Winmostar™ User Manual

Release 11.13.0

X-Ability Co., Ltd.

Jun 25, 2025

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CHAPTER
ONE

INTRODUCTION

Winmostar (TM) provides a graphical user interface that can efficiently manipulate quantum chemical calculations, first principles calculations, and molecular dynamics calculations. From the creation of the initial structure, from the calculation execution to the result analysis, you can carry out the one operation required for the simulation on Winmostar (TM).

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When presenting data created using Winmostar(TM) at a conference or in a paper, for example, please describe Winmostar(TM) itself as follows. Enter the actual version used in the Version field and the year in the Year field.

> Winmostar V11.13.0, X-Ability Co. Ltd., Tokyo, Japan, 2025.

Please refer to the instructions of each software for the citation of solvers and various auxiliary programs called by Winmostar (TM).

1.2 Conventions in this manual

This manual follows the following conventions:

`Ctrl+A`
Indicates keyboard key or key combination operation.

OK
Labels, buttons, etc. Indicates a character string displayed on the GUI.

Tools** → **Preferences** → **Basic** → **License Code
It shows the flow that follows menu, tab, etc. Above example means GUI flow from the menu *Tools* → *Preferences* and click on the tab called *basic* in the opened window and find the label *license code*.

`wmset.ini`, `C\:winmos11\UserPref`
Indicates file name or directory name.

`ls /usr/local/bin`
Command prompt, command to be executed at terminal.

`3.14159`
Indicates input to the text box of the GUI.

Note: Indicates supplementary matter.

Warning: Indicates notes.

1.3 The libraries used

Winmostar uses the following libraries and softwares for some processings.

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```
OpenCubegen
  Cube Generation for Gaussian, Gamess, and MOPAC packages
Author
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  mitsuo.shoji@apchem.nagoya-u.ac.jp
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CHAPTER

TWO

INSTALLATION GUIDE

2.1 Software requirements

Winmostar supports the followings operating systems.

- Windows 11 (64bit)
- Windows 10 (64bit)
- Windows 8 (64bit)
- Windows 7 (64bit)

In the case of Windows Server, please obtain the FREE edition or trial and use it after verifying the operation. macOS and Linux users can use the Windows OS after installing it on a virtual environment such as VirtualBox. It will generally work on 32-bit operating systems, but please evaluate it with a free trial before purchasing.

2.2 Hardware requirements

The minimum spec of Winmostar is as follows.

- CPU and RAM: According to the hardware requirements of Windows 7/8/10/11
- HDD: 20 GB or more free space

It can be used with general office work, PC surfing, etc. A network connection is not required for the software to work, so Winmostar can be used on computers that are not connected to a network. The recommended specs conform to the recommended specs of the solver used together because the Winmostar main unit operates on a relatively low-spec PC. If the recommended specifications of the solver are unknown, prepare a CPU machine with a high floating point arithmetic function (number of cores x frequency). Since HDD and memory can be expanded relatively easily later, standard capacity is acceptable.

2.3 Recommended version of solver

Table 1: Recommended version of solver

MOPAC	6, 7
GAMESS	2020-R2
NWChem	7.0.2
Gaussian	16
Gromacs	5.0.7
LAMMPS	29/Sep/2021 ed.
Quantum ESPRESSO	7.1
OpenMX	3.8

It will generally work with versions other than the ones listed here, but please verify that it works before using it, as it is not guaranteed to work.

2.4 Recommended remote servers

Installation instructions refer to instructions for CentOS, but various Linux OSes such as Ubuntu can be used if they have the following features.

- Communication using SSH and SCP is possible.
- Standard shells such as bash and csh
- Can execute standard UNIX commands
- Various solvers used from Winmostar can be installed and used.

If you want to schedule jobs on the remote server, you need to install the following job scheduler on the remote server. If you do not need job scheduling and can run calculations directly on the node to which you are connected via SSH, you can use the remote server without installing a job scheduler. You can also add the job scheduler of your choice in the Customization in Paid Support.

- **Recommended**
  - Torque, OpenPBS, PBS Professional (PBS)
  - Sun Grid Engine (SGE), Univa Grid Engine (UGE), Altair Grid Engine (AGE)
  - Slurm Workload Manager (SLURM)
  - FUJITSU Software Technical Computing Suite (PJM)
- **Only some functions are supported.**
  - IBM Platform Load Sharing Facility (LSF)

2.5 Installing Winmostar and solvers

If the installation cannot be performed as expected, check *Frequently asked questions · Troubleshooting*.

1. If you have not obtained a license code, you can register and obtain a license at the following link. The differences between the editions can be found in the Features List.
    - FREE edition
    - STUDENT edition
    - PROFESSIONAL edition
    - PROFESSIONAL edition (trial)
2. Download the Winmostar installer for the latest stable version <https://winmostar.com/en/download#latest_stable>`_ .

Note:

- Please check the system requirements with *Hardware requirements*.
- If you have already obtained the installer from a USB flash drive, DVD, or User Portal, you do not need to do this.

3. Double-click the installer to launch it and click “Next. [On the “Select Component” screen, click “Next” with the “64-bit executable file” checked.

Warning:

- If Winmostar is running, close it beforehand.
- The 32-bit version has been deprecated since Winmostar V11.5.0.

4. [Click “Install” to begin installation. If necessary, click Browse to change the destination folder (default is C:\winmos11).

Warning:

- If multibyte characters such as Japanese and double-byte characters and special symbols are included in the installation folder and the name of the higher hierarchy, some modules may cause problems.
- If the text and other items are enlarged or reduced in the display settings, the display may be partially disrupted. For more information here.
- Installation under C:\Program Files is not possible.

Note:

- After the installation is complete, shortcuts will be created in the Start menu and on the desktop.
- If you receive a warning of anti-virus software, please ignore it and continue installation (the same below).
- If the past version of Winmostar has already been installed, it is possible to install it overwritten or change the installation folder to coexist with the past version.
- To upgrade, check *Update* or *Upgrade*.

5. In the case of a new installation, start Winmostar and set the license code in the dialog that appears at the first boot.

   Note:

   - This operation is not necessary if the delivered licensed installer is used.

6. Follow the procedure to build a Cygwin environment for Winmostar.

   Note:

   - NWChem, LAMMPS, Gromacs, MODYLAS, Quantum ESPRESSO, OpenMX, and Towhee are included in CygwinWM. (However, NWChem, LAMMPS, and Quantum ESPRESSO will be included in CygwinWM version 04/05/2023 or later.
   - If you want to run NWChem in parallel, you need to install MPICH according to the NWChem Installation Manual in the next step.

7. For the solver to be used on a Windows PC (local machine) on which Winmostar is installed, follow the instructions in the link below. If you want to perform calculations only on a remote server, you must also install it on the local machine. Some solvers are already installed with CygwinWM and do not need to be installed here.

   - GAMESS Installation Manual for Windows
   - NWChem installation manual for Windows
   - Gaussian installation manual for Windows
   - NAMD installation manual for Windows
   - FDMNES Installation Manual for Windows
   - AkaiKKR installation manual for Windows

If you are using Winmostar V11.4.X or earlier, CygwinWM 07/15/2022 or earlier version, or 32-bit environment (deprecated), please also see below.

- LAMMPS Installation Manual for Windows
- Quantum ESPRESSO for Windows Installation Manual

Note:

- LAMMPS installation is required to use the Polymer Builder. (Winmostar V11.4.X or earlier or CygwinWM 07/15/2022 version or earlier)
- There is no need to install a solver that you do not plan to use.
- If you want to use MOPAC6 with extended maximum number of atoms, you can get it from MOPAC6 (not guaranteed).

8. If necessary, exclude the installation folders of Winmostar, CygwinWM, and solver from the monitoring target in the configuration of the security software you are using.
9. Change the setting to display the extension of each file on Explorer.
   - Not required.

   - If you don't know how to set it up, check *Q. How do I view the extension in Windows Explorer?*.

10. If you want to submit jobs to the remote server and schedule jobs on the remote server, make sure that the *supported job scheduler* is installed on the server. If you do not have Slurm, follow the steps in the link below to install Slurm.

    - Slurm installation method (for Rocky Linux).

Note:

- If job scheduling is not required and calculations can be performed directly on the node to which SSH is connected, there is no need to install a job scheduler on the remote server.
- Various job schedulers other than *Slurm* are also available from Winmostar, so you do not necessarily need to install Slurm. If you are installing a new job scheduler, the procedure for Slurm is relatively simple.

---

11. When submitting a job to a remote server, install the solver used in the destination server according to the following procedure.

- GAMESS installation manual for Linux (only Japanese)
- NWChem installation manual for Linux <https://winmostar.com/en/gmx4wm_en_linux.html>`_
- Gromacs for Linux Installation Manual (only Japanese)
- LAMMPS instllation manual for Linux (only Japanese)
- Quantum ESPRESSO installation manual for Linux (only Japanese)
- OpenMX installation manual for Linux (only Japanese)
- DCDFTBMD installation manual for Linux (only Japanese)

12. Now, you are ready to use Winmostar. Please refer to Tutorials if necessary

2.6 Uninstalling Winmostar

You can uninstall by deleting Winmostar installation folder and shortcut.

2.7 Update

Updates (minor version or revisions) can be performed in the same way as the installation. Example: V11.0.0 to V11.1.0, V10.4.0 to V10.4.5

- If you want to keep the old version, you can take over the settings by copying the files under the UserPref folder of the old version to the following in the UserPref folder of the new version.
- The UserPref folder is located under the Winmostar installation folder.

2.8 Upgrade

Upgrades (major version updates) can be performed in the same way as installations. Example: V8.000→V9.0.0, V10.0.0→V10.0.0

- If you are upgrading from V3, V4, V5 or V6, you can take over the configuration by copying the configuration files atoms1.wmx, winmos_server.ini, wm_nmr.ref, and wm_irscale.ref under the installation folder of the old version to the UserPref folder under V11.
- If you are upgrading from V7, V8 or V9, you can take over the settings by copying wmset.ini, atoms1.wmx, winmos_server.ini, wm_nmr.ref, and wm_irscale.ref under the UserPref folder of the old version to the UserPref folder of V11.
- The UserPref folder is located under the Winmostar installation folder.
- For more information, see V11 Migration Guide, V10 Migration Guide and V9 Migration Guide.

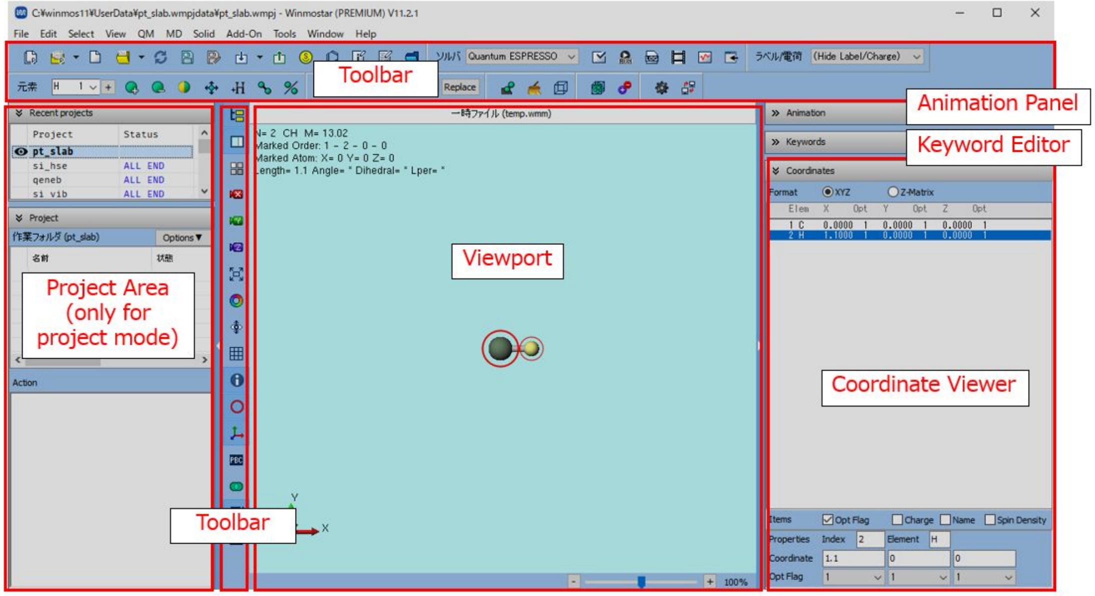
CHAPTER

THREE

MAIN WINDOW

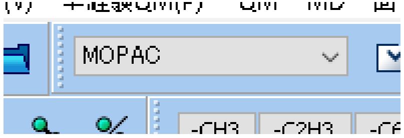
3.1 Role of each part

The window (called **Main Window**) that appears after starting Winmostar has the configuration shown below. In the title of Main Window, the name of the file currently being edited, the license and version of Winmostar in use are displayed.



Toolbar

Here you can also select commonly used functions in the main menu. You can check the role of each button by overlaying the pointer. In addition, only the following functions perform special operations.

- Depending on the solver selected in the *Solver* pull-down menu  (default is MOPAC) in the first row of the upper toolbar, the role of buttons such as *Configure*, *Run* will change.
- Depending on the element selected in the *Select element used in editing operations* pull-down menu, the behavior of *Add Atom* and *Change Element* buttons beside it will change.

Project Display Area

Projects created in the past are displayed in *Recently used projects*. Double-click on an item to open that project. The project display area is only visible in project mode. *Working Folder* displays the working folder for the currently opened project. Clicking on *Options* allows you to select operations for the selected working folder. Double-clicking on an item opens the input file for that working folder. The eyeball icon will appear in the working folder that contains the file displayed in the molecule display area. If that folder is not selected with *working folder*, the eyeball icon will appear red. In *action*, an operation on the working folder selected by *working folder* will appear.

Viewport

The molecular structure currently being edited is displayed. By default, the structure where carbon atom (green) and hydrogen atom (yellow) are bonded is displayed.If the *View → Items → Information* menu is checked, detailed information will be displayed at the top and bottom.Red circle indicates **atom selection marker**.In **group selection** state, atoms are surrounded by blue circles.You can toggle the number displayed on the side of each atom and the type of charge value from the *View → Labels/Charges* menu.The color scheme can be changed from the *Tools → Preferences → View* . If the *:menuselection:* View –> Display items –> Molecular information` menu is checked, detailed information is displayed at the top and bottom. For structures with charge or spin, the total charge (Qtot) and root mean square (Qrms) are displayed at the bottom. For structures with cells, the density and lattice constant are displayed at the bottom. If the dipole moment was calculated directly from the wavefunction obtained in the quantum chemical calculation and read from the log of the quantum chemical calculation, its value is also displayed. For structures with cells, the density and lattice constant are displayed at the bottom. In project mode, the name of the file being displayed is shown at the top of the molecule display area. If the file being displayed is not contained in the working folder selected in the *working folder*, it is displayed in red.

Animation operation area

The animation control buttons are displayed. Click title to show/hide.

Keyword Editor

The settings in the Keyword Settings window for each solver will be displayed. Alias characters such as %WM_XYZ%, %WM_ZMAT%, etc. appear in the molecular structure-dependent parts of the keywords. Click title to show/hide.

Coordinate Viewer

The coordinates of each atom of the molecular structure displayed in Viewport are displayed. The *Display format* at the top allows you to switch the display format. By default *XYZ* is selected.In a state where no group is selected, the line selected in Coordinate Viewer matches the atom with the marker (red circle). You can make a group selection (blue circle) by selecting multiple lines with `Ctrl+left click` or `Shift+left click`. Click on the title to show/hide it.

3.2 Mouse controls

In Viewport, you can operate with the mouse as shown in the table below. Details on how to select molecules/atoms can be found in *Select menu*.

Modifier Key	Left click	Left drag	Right click	Right drag/ Wheel
None	Move marker	Roll camera	Show context menu	Zoom in/out
`Shift`	Select molecule or unselect	Pan camera	Delete atom	
`Ctrl`	Select each atoms or unselect	Select atoms in rectangle area		
`Ctrl+Shift`			Replace with Fragment	

Note that you can also zoom in or out by left-dragging the right end of Viewrport.

3.3 Shortcut keys

In Main Window you can use the shortcut keys in the table below.

Table 1: Basic operations

New	`Ctrl+N`
Open	`Ctrl+O`
Save	`Ctrl+S`
Save As	`Shift+Ctrl+S`
Undo	`Ctrl+Z`
Redo	`Ctrl+Y`
Cut Group	`Ctrl+X`
Copy Group	`Ctrl+C`
Paste Group	`Ctrl+V`
Help	`F1`

Table 2: Modelling

Replace with Fragment	`F6`
Add Atom by Specifying Position	`F4`
Delete atom	`Shift+F4`
Add/Change Bond	`F7`
Delete Bond	`F8`
Move Atom (Translate)	`F5`
Change Element	`Shift+F5`
Add Hydrogens to All Atoms	`Ctrl+H`
Delete Group	`Ctrl+D`
Build Ring	`F9`

Table 3: Modifying structure

Quick Optimization	`Ctrl+G`
Move Group (Direct)	`Ctrl+M`
Rotate Around Axis (2 Marked Atoms)	`Ctrl+R`
Rotate Around Axis (3 Marked Atoms)	`Ctrl+A`
Change Optimization Flags of Group	`Ctrl+I`
Adjust All Bond Length	`Ctrl+J`
Orbit Group Around Marked Atom	`Ctrl+F`
Quick Optimization for Group	`Ctrl+L`

Table 4: Controlling Display

Zoom In	`F3`
Zoom Out	`F2`
Fit to Window	`Ctrl+4`
Align View	`Ctrl+1, 2, 3`
Show Keyword Editor & Coordinate Viewer	`F10`
Export Image	`Ctrl+Alt+I`
Copy Image	`Ctrl+Alt+C`

CHAPTER

FOUR

BASIC OPERATION FLOW

Here, we introduce the basic operation flow of quantum chemical calculation, molecular dynamics calculation, or first principles calculation using Winmostar. Start Winmostar and click on *file* → *new project* in project mode or *file* → *new file* in file mode.

Project Mode
You can manage jobs without being aware of individual files. We recommend using this mode for non-free users.

File Mode
Explicitly operates on individual files, with procedures compatible with V10 and earlier. Use this mode when using the free version or a solver/job scheduler that does not support project mode, or when running calculations using input files for each solver created outside of Winmostar.

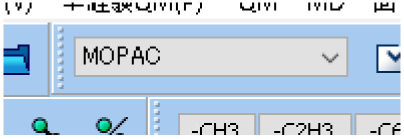
4.1 For project mode

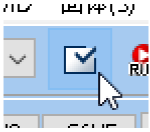
A description of the files that make up the project can be found in *New Project*.

(1) Create initial structure

Click *file* → *New Project* and follow the *Structure Building* procedure to create the system you want to calculate. Click *file* → *New project with current structure* to switch from file mode to project mode, for example, with an existing structure file open. If you want to run calculations on an existing structure file, you can click *file* → *New Project* and then use *file* → *Import File* to load the structure.

(2) Configure simulation conditions

Select the solver you want to use at *Sovlver* pull-down menu 

, and click *Workflow Setup* button . The *# of Jobs* specifies the number of jobs to be executed this time. If *# of Jobs* is 2 or more, jobs are executed sequentially, with the final structure of each job being used as the initial structure of the next job. In the central part of the *workflow settings* window, you specify the calculation conditions for each job. Finally, click *OK*.

(3) Run simulation

- To execute calculations on Windows PC with Winmostar installed (**Local job**)

  In the *Job Settings* window, check *Run Job on this machine* and click *Run*. Enter the number of MPI processes to use (*# of MPI Procs*) or the number of threads per MPI process (*# of Threads/MPI Proc*) (or total threads if no MPI is used) in the *Number of Parallels*

> field . For the parameter and structure scan functions, enter the number of parallels for each calculation. The *Winmostar Job Manager* processes the registered jobs in order. After executing, check the status of each working folder in the *project display area*. If the computation proceeded normally, the state will change from NEW to PEND to RUN to END. If there is an anomaly, the state will be ABORT. *Project Display Area*, hovering the cursor over a working folder will display an error message. Click on the working folder and in the *Actions* click on *Log* to see the log of the calculation. To stop a job, right-click on the job you want to stop in the *working folder* in the *project view area* and click *Stop*.

- When running on a Linux machine connected to the network on Winmostar installed PC (**Remote job**)

  You can also check the instructions at Remote Job Tutorial (Japanese only). In the *Job Settings* window, check the *Run job on remote machine* checkbox. In the *Profile* select the server settings you want to use. If there is no appropriate profile, click *Config* and enter the server information. See *Remote Job Setup Procedures in file mode* for more information. If you need to specify a separate environment variable to use the solver on a remote server, click *New* in the *Template Script*, edit the shell script to use when submitting jobs, and select it in *Template Script*. *options* are arguments for commands (such as qsub) to submit jobs on remote servers. Typically, options are entered that depend on the type of queue you want to use and your machine configuration. You can use *Alias string available for remote job function* in this field to abstractly specify the number of parallels, etc. *Profile* and *Options* can be tested with *Test Connection*. Details of the Test Connection can be found at *Test Connection*. You can also use *Control* to check for free queues, etc.

  > Enter the number of MPI processes to use (*# of MPI Procs*) or the number of threads per MPI process (*# of Threads/MPI Proc*) (or the total number of threads if MPI is not used) in *# of Parallel*. (If you don't use MPI, enter the number of threads per MPI process. (For the parameter and structure scan functions, enter the number of parallels for each calculation.)

  The *job description* can be a description of the working folder that will be created by the execution. This description can be modified later with *Get Info*. Finally, click *Run*. The registered jobs will be executed in order on the remote server. After execution, check the status of each working folder in the *project display area*. If the calculation proceeded normally, the state will change from NEW to SEND to PEND to RUN to END(Rem) to RECV to END(-). If there is an abnormality, the status becomes ABORT. If the job status is not determined successfully, use *Recheck Status*. Error message appears when hovering the cursor over the working folder in the *project display area*. Right-click on the working folder and click *Open Remote stdout* or *Open Remote stderr* to see the standard output and standard error when executed remotely. You can see the log of the calculation by clicking on the working folder and clicking *Log* in *Actions*. If the status is END(-) and you have finished successfully on the remote server, click on the working folder and under *Actions* click *Receive All Remote Output Files* and all output files will be saved to the local Transfer to machine. To stop a job, right-click on the job you want to stop in the *working folder* in the *project view area* and click *Stop*. If you want to check the end of the log or retrieve and visualize some files while the job is running, right-click the target job in the *working folder* of the *project view area* and click *Control Remote Job/Server ` in the :guilabel:`Project View Area*. See *Each function of the Submit Remote Job window* for instructions on how to operate the *Control Remote Job/Server* window that opens.

- If you do not want to run the calculation directly from Winmostar and only want to save the file

  Configure Job window, set up as you would for a local or remote job, then check *Do not run own part after saving file* and click *Save* at the bottom right. Then click *File* → *View in Explorer* to see the set of saved input files, batch files, and shell scripts. If you want to run the job later, use *Run*.

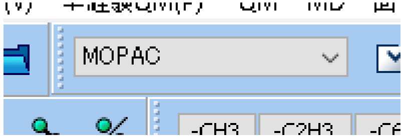
(5) Display and analyze physical quantities

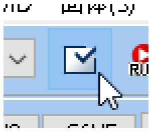
(6) Extend job

(1) Create initial structure

Click *file* → *New File* and follow the *Structure Building* procedure to create the system you want to calculate.

(2) Configure simulation conditions

Select the solver you want to use at *Sovlver* pull-down menu 

, and click *Keyword Setup* button . For some solvers, if you put a pointer over the keyword column, the meaning of that keyword will appear.

(3) Run simulation

- To execute calculations on Windows PC with Winmostar installed (**Local job**)
  - With the configure window open, press the *Run* button.
  - Press the *OK* button to close the configure window. So if you want to modify the keywords directly, enter at *Keyword Editor* or edit the input file from the *Open in Text Editor* using any text editor. Then click the *Run* button on the tool bar 

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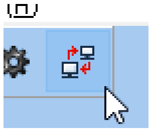
  After clicking *Run*, if the input file is not saved, entering the name of the input file will be saved, then the job will be registered in *Winmostar Job Manager*. *Winmostar Job Manager* will process the registered jobs in order. When you want to abort a job, close the appropriate console window or perform Ctrl-C while the appropriate console window is active.

- When running on a Linux machine connected to the network on Winmostar installed PC (**Remote job**)

  Press the *OK* button to close the configure window. Next, click the *Submit Remote Job* button  on the tool bar to set up connection to the server. See *Remote Job Setup Procedures in file mode* for how to set it up. After that, press the *Send & Submit* button on the *Submit Remote Job* window to save and transfer (send) the input file and register the job at the remote server (submit) at once. Registered jobs are executed in order on the remote server. When the job ends on the remote server Press the *Get All Files* button to transfer the file output from the calculation to the Windows PC where Winmostar is installed. See *Remote Job Operation Procedures in File Mode* for other detailed operations. If you want to abort a job, remember the job ID that appears immediately after you run *Send & Submit*, and in the *Submit Remote Job* window, click *Queue* → *Kill Click `Submitted Job* and enter the job ID.

- If you do not want to run the calculation directly from Winmostar and only want to save the file

For LAMMPS, Gromacs, and Quantum ESPRESSO:

> Go to the *Options* tab in the keyword configuration window, press the *Dump all files for remote* button, enter a file name and save it.

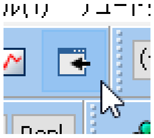
For other solvers:

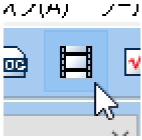
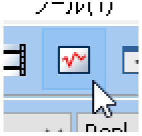
> Close the Keyword Setup window by clicking the *OK* button. Then click *File* → *Save As* to save the file. If you want to save not only the input file but also accompanying files such as shell scripts, use the project mode.

(4) Confirm log

Press the *Open Log File* button  on the toolbar. You are asked which file to open. If the input file of the calculation you want to check log is displayed in the main window, open the file selected by default. The log file is displayed with a text editor, then check whether the job has ended normally or abnormally.

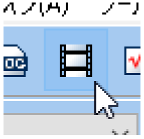
(5) Display and analyze physical quantities

If the job has ended normally, press the *Analysis* button  on the toolbar and select the menu of physical quantities you want to display. You will be asked which file to open, so choose as appropriate. As with log checking, the one associated with the file displayed in the main window is selected by default. When you specify a file, a window for the result display is displayed.

- To visualize the structure optimization process or trajectory, press the *Animation* button on the tool bar .
- To plot changes of energies and temperature during SCF or MD calculation, press the *Energy Plot* button  on the tool bar.
- For analysis of molecular shape, use functions below *Tool menu*.

(6) Extend job

If it is necessary to extend or continue the job, open the configure window again and start the job.

- For MD, check *Continue Simulation* in the configure window.
- For Quantum ESPRESSO, set *Continue* to *Output Direcotory* in the configure window.
- If you want to run simulation after the structure optimization for semi-empirical QM or QM solvers, press the *Animation* button  on the toolbar, display the final structure

on the main window and configure for the next job.

CHAPTER

FIVE

STRUCTURE BUILDING

5.1 Modelling a single molecule

Select one of the following methods.

- Draw and read structure expressions with *file* → *import* → *Structural Formula*.
- Read SMILES format string from *File* → *Import* → *SMILES*.
- Load files in various formats (PDB, mol, mol2, SDF, CIF, xyz, etc.) by *file* → *Import File* or drag and drop into the main window.
- Build 3D molecular structure from directly on the main window.

  Return to the initial structure with *edit* → *Reset Structure* and select the required operation from *Edit menu* as appropriate.

  1. Execute *Replace with Fragment* to the initial structure (carbon and hydrogen atoms) so that the shape approaches a certain degree to the target molecule.
  2. For structures with adjacent aromatic rings, execute *Build Ring*.
  3. Execute *Delete* at the place where you want to delete the unnecessary substructure.
  4. In a place where you want to add a hydrogen atom, execute *To marked atoms (Single), (Double), (Triple)*.
  5. Execute *Element* at the place where you want to change the element of atom.
  6. Execute *Add/Change Bond* where you want to create chemical bonds. Also change the type of binding by the same operation.
  7. Execute *Quick Optimization* to adjust to a reasonable atomic arrangement. (Only when the number of atoms is small)
  8. To explicitly rotate the substructure, execute *Modify Selected Group* → *Rotate Around Axis (2 Marked Atoms)*.
  9. For molecules that can take various conformations, *Tools* → *Conformation Search (Balloon)* and choose a structure with low energy.
- In the case of a polymer, you can model a whole molecule directly, but it is more efficient to use the method of *Creating polymer melt system*.

5.2 Assigning point charges

I will show you how to set up the point charges required for MD calculations on Winmostar. First create a single molecule using the *Modelling a single molecule* method, then assign the charges using the following method. The assigned charges can be displayed and checked by changing *Label/Charge*. Note that there is no need to explicitly set the charge for water molecules, since the water model charge values selected at the time of force field assignment are applied unconditionally. If you want to average or shift the charge of some atoms, use *Average the group's charge* or *Shift Charges of Group*.

- Assign Gasteiger charge.

  Assigning a charge manually by *MD* → *Assign Charges Manually* → *Use AM1-BCC/Gasteiger charges*. For ions, input the charge in *Total charge [e]*. If it is an ion, input the charge in *Total charge [e]*.

- Assign RESP charge automatically.

  :Assigning charges by menuselection:*MD –> manually assign charge –> Use RESP charges* procedure. For ions, enter the charge in *Total charge [e]*.

- Manually assign RESP charges in GAMESS or Gaussian.

  1. In file mode, at *QM* → *GAMESS/Gaussian* → *Keyword Setup* → *Easy Setup*, set the calculation method and basis functions to "HF/6-31G*", select *Method Select :guilabel: `Method* and *ESP/RESP*. For ions, enter the charge in *Charge*.
  2. Close the *Easy Setup* window with the *OK* button and press the *Run* button in the *GAMESS/Gaussian Setup* window to run the calculation
  3. When the GAMESS/Gaussian calculation is finished, get the RESP charge at *QM* → *GAMESS/Gaussian* → *result analysis* → *RESP Charges*.

- Read the charge calculated from the population analysis, e.g. Mulliken or Lowdin charge, for into the main window.
  - In the case of MOPAC, read in the procedure of *MO & Charges (mgf)*.
  - For Quantum ESPRESSO, use *Solid* → *Quantum ESPRESSO* → *Lowdin Charge*.
  - Otherwise, open the log file in the main window.

- Enter a value for the selected atom.
  - *Group select* atoms for which you want to input a charge in the *Viewport*, and then input a charge from *Edit* → *Change Atom Property* → *Charge/Spin Density*.
  - *edit* → *Edit Charge* to enter charge from.

- Edit and assign directly on the text file.
  - Once the molecular structure is saved in *File* → *Save As* in mol2 format, open the mol2 file with any text editor and edit the values in the ninth column of the section starting with `@<TRIPOS>ATOM`. After editing, click on *file* → *Reload* to load the edited structure.

- In the case of polymers, the method of *Creating polymer melt system* is used because it takes time to calculate AM1/BCC and RESP charges of the whole molecule directly.

5.3 Creating an isolated system (gas phase)

1. Create a structure of one molecule (See *Modelling a single molecule*). In the case of quantum chemistry simulation, since the period boundary condition is not used, the subsequent operation is unnecessary.
2. In the case of MD simulation, assign point charges (See *Assigning point charges*).
3. Create a cell by *Edit* → *Create/Build Cell* → *Create/Edit Cell*.

5.4 Creating a small molecule liquid system

1. Create a structure of one molecule (See *Modelling a single molecule*).
2. In the case of MD simulation, assign point charges (See *Assigning point charges*).
3. Save a file by *File* → *Export File* in mol2 or wmm format.
4. Procedures 1 to 3 are performed for all molecular species to be calculated.
5. Select *MD* → *Solvate/Build Cell*.
6. Determine which molecules to put in the system. For the molecules displayed in the main window, press *Add Displayed Molecule*. For water molecules, press *Add Water*. For the other cases, press *Add File*.
7. Enter the number of molecules to be inserted into the system.
8. Perform 6 and 7 for all molecular species you want to calculate.
9. Set the system size at *Simulation Cell* and press *Build* button.

Note:

- If the density is too high, the creation of the system may fail, so start with a low density (about 40 % of the experimental value of the substance of interest or a substance similar to the substance of interest, if known) and adjust the density with *Edit* → *Create/Edit cell* →*Transform Cell* or run the MD calculation and compress gradually to the desired density and pressure with a constant pressure calculation.
- Use *Modify Selected Group* → *Replicate Group*, *Create/Edit Cell* and *Import File* when *CygwinWM* is not installed or it is difficult to arrange with *Solvate/Build Cell*.

5.5 Creating polymer melt system

1. Create a polymer repetition unit to be calculated by the method *Modelling a single molecule*. For example, in the case of polyethylene, create an ethane molecule instead of an ethylene molecule.
2. In the case of MD calculation, the charge is assigned by the method *Assigning point charges* in the state of the repeting unit.
3. In *Molecule Display Area*, left-click two atoms connected with the neighboring repeat unit and register them as monomers by *MD* → *Polymer* → *Register repeat unit*.
4. Depending on the structure of the polymer to be created, perform operations *MD* → *Polymer* → *Homo Polymer builder*, *Block Polymer Builder* and *Random Polymer Builder*.

Tip:

- For example, in the case of a structure like *-[AAABBB]-*, create *AAABBB* using *Block Polymer Builder* first, then open a wpo file generated in the `wpo` folder, register as a new repeat unit at *Register repeat unit* and execute *Homo Polymer builder*.

5. Create a simulation cell by performing the operation *MD* → *Polymer* → *Polymer Cell Builder*.
6. If a small molecule component is dissolved in the polymer, create the dissolved small molecule by the procedure of *Modelling a single molecule* and *Assigning point charges* and save it in mol2 format beforehand. Then, select and insert the mol2 file of small molecule at *MD* → *Insert Molecules*, which was saved after step 5. If the density is not set low in step 5, the insertion of small molecule components may fail.

5.6 Creating gas-liquid interface

1. Create a liquid phase (see *Creating a small molecule liquid system*).
2. In *Edit* → *Transform Cell*, check *Transform only along the selected axis* and *Do not change*, then check *Set incremental length* or *Set total length*, enter a value and press the *OK* button.

Note:

- Select *edit* → *Wrap Around Cell Boundary* before expanding the structure of the liquid phase because there are many atoms with coordinates outside the simulation cell in the structure after MD calculation. For molecular systems, select *relocate molecular units inside the cell*; for inorganic systems, select *relocate atomic units inside the cell*.

5.7 Creating gas-liquid interface

1. Create one of the liquid phases using *Creating a small molecule liquid system*. At this time, a mol2 file should be created in advance for all types of molecules contained in the two phases.
2. Save a file by *File* → *Export File* in mol2 format.
3. Select *MD* → *Solvate/Build Cell*.
4. Decide which and how many molecules to put in the other phase. For water molecules, click *Add Water*. Otherwise, click *Add File* and select the mol2 file.
5. Enter the number of molecules to be inserted into the system.
6. Perform the steps in 4 and 5 for all the molecular species you want to calculate.
7. On the *Simulatoin Cell* tab, check the *Set Lattice Constants* and click the *Same as main window* button. Next, select “triclinic” for the *Box Type*. To the right of the *Set Lattice Constants*, the cell size of the first phase you created is displayed. Click the *Change only one direction*, select Z with the *Select direction*, and enter the specified density with the *Enter density* to automatically set the lattice constants in the z and y directions while keeping the x and y constants fixed.
8. Press the *Build* button.
9. Save a file by *File* → *Export File* in mol2 format.
10. Click *MD* → *Interface Builder*.

11. Click *Browse* button of *Cell 1* in the *Cell* tab, and select the file saved in step 2. Similarly, in *Cell 2*, select the file which was saved in 9.
12. Input the distance between liquid phases in *Direction* tab of *Interval*.
13. Click *Build* button, type the name of the file to save, and then click *Save* button.

5.8 Protein creation (no ligand)

1. Open the pdb file of the protein you want to calculate with Winmostar.
2. Use *Select* → *Select by Molecular Species* to select a group of non-protein components (e.g., binding water, buffers, ligands, etc.), and then use *Edit* → *Modigy Selected Group* → *Delete* to delete the selected group.
3. *Edit* → *Add Hydrogen* → *Using pdb2gmx*. Even if hydrogen appears to be added before the execution, the calculation may fail later if this process is omitted.
4. Click *MD* → *Solvate/Build Cell*. Click *Add Displayed Molecule*, type "1" in *Enter # of molecules* and click the *OK* button. Next, click *Add Water* button, input the number of molecules (about 5000 to 10000) at *Enter # of molecules* and click *OK* button. Then, click the *Build* button.
5. To neutralize the system, place ions with the procedure *MD* → *Generate Ions*. If the message "WARNING: The charges defined on the main window will be discarded. Are you sure you want to continue?" is displayed, click *Yes*.

If the MD calculation is executed after the above procedure, it is desirable to continue the MD calculation after the above procedure because if the file is saved after the above procedure is executed, the residue information may not be saved properly.

5.9 Protein creation (with ligands)

1. Open the pdb file of the protein-ligand complex you want to calculate with Winmostar.
2. Use *Select* → *Select by Molecular Species* to select a group of non-ligand components (proteins, bound water, buffers, etc.), and then use *edit* → *Delete* to delete the selected group.
3. Execute *Edit* → *Add Hydrogens* → *Using OpenBabel*.
4. Save the structure of the ligand in mol2 format with *file* → *Export File*.
5. Open the pdb file of the protein-ligand complex you want to calculate again with Winmostar.
6. Use *Select* → *Select by Molecular Species* to select a group of non-protein components (e.g., binding water, buffers, ligands, etc.), and then use *Edit* → *Modigy Selected Group* → *Delete* to delete the selected group.
7. *Edit* → *Add Hydrogen* → *Using pdb2gmx*. Even if hydrogen appears to be added before the execution, the calculation may fail later if this process is omitted.
8. Click *Solvate/Build Cell*. Click *Add Displayed Molecule*, type "1" in *Enter # of molecules* and click the *OK* button. Next, click *Add Water* button, input an appropriate number of molecules at *Enter # of molecules* and click *OK* button. Then, click *Add mol2 File* button, open the mol2 file saved in step 4, type "1" in *Enter # of molecules*, and click *OK* button. Do you want to arrange these molecules in a random manner? If asked, click *No*. Then, click the *Build* button.

9. To neutralize the system, place ions with the procedure *MD* → *Generate Ions*. If the message "WARNING: The charges defined on the main window will be discarded. Are you sure you want to continue?" is displayed, click *Yes*.

If the MD calculation is executed after the above procedure, it is desirable to continue the MD calculation after the above procedure because if the file is saved after the above procedure is executed, the residue information may not be saved properly.

5.10 Preparation of inorganic crystals

If you already have the crystal data you want to calculate, such as a CIF file, open the file with Winmostar. If such a file does not exist, perform the following operations.

1. Click on *solid* → *Crystal Builder*.
2. Select the following item at the top right of *Crystal Builder* window.
    - Select the classification of a crystal from *Crystal System* of *Lattice*.
    - Select a space group of a crystal from *Space Group* of *Lattice*. The choices of *Space Group* are changed by *Crystal System*.
    - In *Lattice Constants*, input the lattice constants of the crystal to be computed.
3. *Crystal Builder* Input an atom of an asymmetric element in the list at the bottom right of the window.
    - Double-click on the *Atom* field and enter the type of element.
    - Double-click the fields of *X* , *Y* , *Z* to fill in the coordinates.
    - Add an atom by *Add* button.
    - Removes a selected atom by clicking *Remove* button.
4. Click the *OK* button to apply the structure specified by the crystal builder to the main window.
5. If you want to distort the crystal, use the *edit* → *create/edit cell* → *Transform Cell* function.
6. If you want to change the unit lattice of the crystal without changing the crystal structure, perform the following operations. If you want to convert between primitive and conventional cells, use the *solid* → *Convert Lattice (Primitive-Conventional)* function. To convert a hexagonal cell to a rectangular cell, use the *solid* → *Convert lattice to equivalent rectangular cells* function. If you want to convert a unit cell with a rotation matrix, use the *solid* → *Transform Unit Cell* function.
7. If the symmetry of the created structure or the structure of the loaded file is broken from the original one, the *solid* → *Refine Lattice* function may improve the symmetry.

5.11 Preparation of inorganic crystals (with point defects or elemental substitutions)

1. Open a CIF file of the crystal with no defects or create a crystal structure with the method *Preparation of inorganic crystals*.
2. Click on *Solid* → *Generate Supercell*. Increase the value of *a* , *b* , *c* and specify the size of the supercell (first, about 2 in each direction). Finally, click the *OK* button.
3. In the main window, left-click on the atom you want to create a point defect, or the atom you want to replace the element with, and a red marker will appear.

4. To create a point defect, click *Edit* → *Delete atom*.
5. To replace an element, select the element from *Edit* → *Select Element for Editing Ops* and then click on *Edit* → *Change Atom Property* → *Element*.

5.12 Creation of inorganic slabs (surfaces)

1. Open a CIF file of the crystal in bulk, or create a crystal structure with *Preparation of inorganic crystals*.
2. Click on *solid* → *Build Cluster Model*.
3. Enter the items above *Generate Slab* button, *Miller indices (h k l)* etc., then click the *Generate Slab* button.
4. Click the *Generate Slab* button after enteringthe following items below *Generate Slab* button. If the atomic configuration of both the front and back of the slab structure you want to create is not among the choices of *Surface configurations*, ensure that the atomic arrangement on at least one side is the desired structure, then click *OK* and delete an unwanted atomic layer with *Delete* function in the main window. To make the atomic layer thicker in advance, increase the value of *Minimum slab size* above *Generate Slab* button .
5. If you want to change the cell orientation without changing the structure, perform the following operations. If you want to convert a hexagonal cell to a rectangular cell (for example, if you want to create a solid-solid interface but the shape of one ab-plane is different from that of the other), use the *solid* → *Convert lattice to equivalent rectangular cells* function . To convert a unit cell with a rotation matrix, use the *solid* → *Transform Unit Cell* function.
6. If the symmetry of the created structure is broken from the original one, the *solid* → *Refine Lattice* function may improve the symmetry.

5.13 Creation of molecular adsorption surfaces

1. Create a molecule to be adsorbed by the method *Modelling a single molecule*.
2. Save a file by *File* → *Export File* in wmm or mol2 format.
3. Create a surface with the method *Creation of inorganic slabs (surfaces)*.
4. If necessary, click on *solid* → *Generate Supercell*. Increase the value of *a* , *b* and specify the size of the supercell. Finally, click the *OK* button.
5. Click (mark) the atom directly below the position on the slab surface where you want the molecule to be adsorbed, then click *Edit* → *Add Atom* → *Adding dummy atoms to the center of gravity of a group*.Set the Axis to z, set the Distance appropriately, and click OK.
6. Click *MD* → *Replace Molecules* Species=(unknown) and click OK. Then open the file exported in step 2.
7. If you want to rotate adsorbed molecules, use *Edit* → *Modify Selected Group* → *Rotate by Aligning Marked Atoms* or *Rotate (Numerical)*. If you want to translate the adsorbed molecules, use *Edit* → *Modify Selected Group* → *Move (Numerical)*. For example, if you want to adjust the distance between the surface first layer and a specific atom in an adsorbed molecule, first click the atom in the surface first layer, then click the specific atom in the adsorbed molecule, then Ctrl+click the adsorbed molecule to select the group. Then click *Edit* → *Edit Group* → *Move (Numerical)*, change *Definition* to Relative coordinate between marked atoms and change the value of *Z*.

5.14 Creation of solid interfaces (grain boundaries)

1. Create one solid using the method *Creation of inorganic slabs (surfaces)*.
2. Save the file as a cif from *file* → *Export File*.
3. Create the other solid using the *Creation of inorganic slabs (surfaces)* method. Now, if the shape of the ab plane is different from the shape of the ab plane of the structure created in 1, use the *solid* → *Transform Unit Cell* function to re-create the cell.
4. Save the file as a cif from *file* → *Export File*.
5. Click *MD* → *Interface Builder*.
6. Click *Browse* button of *Cell 1* in the *Cell* tab, and select the file saved in step 3. Similarly, in *Cell 2*, select a file which was saved in step 5.
7. Enter the distance between solids in *Interval* on *Direction* tab. Then check *Specify interval on selected axis between outermost atoms* of *Interval*
8. If you move to the *Repeat* tab, the top two (a-axis and b-axis) of the three *Suggest* buttons can be pressed. Click the *Suggest* button, select a row whose value of *Ratio* is close to 1 and the system size is not too large, and click the *Set* button.
9. Click *Build* button, type the name of the file to save, and then click *Save* button.
10. Select one of the solids as a group by Ctrl+Left dragging. See *Select menu* for details.
11. Click *edit* → *group editing* → *Move (Numerical)* to move the group in the X and Y direction. If you enable *view* → *Show Multi-View*, it is easier to see the position.

5.15 Creating Molecular Crystals

At present, Winmostar does not have the ability to generate stable structures of physicochemically valid molecular crystals from the structure of a single molecule, so it is necessary to use a structure file of a molecular crystal obtained from a database or other source as a starting point. In such a structure file, the coordinates of molecules across the boundaries of the simulation cell are far apart, and the process will fail if such a structure file is directly used to perform force field assignment for molecular dynamics calculations such as Gromacs and LAMMPS. In this section, we introduce a processing method to prevent the force field assignment from failing as follows. Note that the following processing is not necessary when only first-principles calculations such as Quantum ESPRESSO and OpenMX are performed.

1. Draw and read structure expressions with *file* → *import* → *Structural Formula*.
2. *Edit* → *Wrap Around Cell Boundary* and check *Wrap for each atom* and click *OK*.

CHAPTER

SIX

DETAILS OF EACH MENU WINDOW

6.1 File menu

6.1.1 New Project

Create a new project. The file structure of the created project is as follows. Renaming of each file/folder is not supported. Since renaming of projects is not supported, it is recommended to leave a note in the Description of *File* → *Project* → *Get Info* about the role of the project, etc. Similarly for working folders, you can leave notes in the Description of *File* → *Project* → *Selected Working Folder* → *Get Info*. When moving project files, move the entire wmpjdata folder.

- `.wmpjdata` folder: a folder containing all the files in the project. Drag and drop this folder into Winmostar to open the project.
- `.wmpj` file: A file containing information about the project. Drag and drop this file into Winmostar to open the project.
- `temp.wmm` : This file contains information on the molecular structure being edited.
- `index.ndx`: the file where information on groups registered with *select* → *register group* is stored.
- `.wmps*` file: the workflow configuration file used for this project.
- `work*` folder: working folder
- `Exec*` folder: contains the files that control the jobs in each working folder.

6.1.2 New project with current structure

Create a new project using the structure currently displayed in the molecule display area.

6.1.3 Open Project

Open an existing project.

6.1.4 Open Recent Project

Open a recently opened project file.

Clear History

Empty the history of recently opened project files.

6.1.5 Project

Get Info

View information about the open project. Some information can be edited here.

Open Temporary File

Open a temporary file of the opened project.

Show in Explorer

Open the wmpjdata folder of the opened project.

Parameter/structure scan result display

You must purchase an add-on to use this feature. After a parameter scan or structural scan calculation, the results of each calculation can be tabulated.

Check All
Check all working folders in Working Folders.

Uncheck All
Uncheck all working folders in Working Folders.

Check Selected
Check the selected working folders in Working Folders; you can use Shift or Ctrl to select multiple working folders in Working Folders.

Working Folders
Check the working folder that contains the calculation results you want to visualize.

X Axis
Selects the value of the X axis for visualization.

X Axis
Selects the value of the Y axis for visualization.

Options

Export csv
Outputs a csv file listing the physical properties for each working folder. When outputting a csv file from a graph, you can only select one physical property, but this function allows you to output multiple physical properties.

Export Animation
Create a wmm file with the values selected in End Structure and Property. For example, if you want to create a Volume-Total Energy graph, create an animation with this feature and then use the Custom Plot feature to select Volume for the X axis.

Interpolate Structure at Specified Volume
When a structure with a different volume is scanned, it interpolates the structure at the specified volume.

Draw
Create a graph with the conditions you set.

Stop multiple jobs

Stops selected running jobs in a project at once.

Selected Working Folder

Each function in this menu operates on the working folder selected with *working folder* in the project display area on the left of the main window. The same menu is displayed by right-clicking on the *working folder* in the project display area.

Open Coordinate (Initial)

Displays the initial structure in the selected working folder. In most cases, this will be the input file for the job. For the second and subsequent working folders in a series of generated working folders, the same initial structure as the first working folder will be displayed until the job is executed. After the job is executed, the original initial structure of the working folder is displayed.

Run

Runs the job in the selected working folder. Select *Do not run jobs after saving files* in the *Job Settings* window and use this function if you want to start the job later.

Stop

Stops (kills) jobs in the selected working folder.

Show Workflow Setup

Displays workflow settings for the selected work folder.

Show Keyword Setup

Displays keyword settings for the selected work folder. This corresponds to the contents of Details in the workflow settings.

Show Job Setting

Displays job settings for the selected working folder.

Control Remote Job/Server

Performs remote server operations for jobs in the selected working folder. Available only for remote jobs.

Show Command for Job Submission

Displays the command when a job in the selected working folder is submitted (SUBMIT) on a remote server. Available only for remote jobs.

Show Result of Job Submission

Displays the result of submitting (SUBMIT) a job in the selected working folder on a remote server. Available only for remote jobs.

Receive All Remote Output Files

Transfers all output files related to the job in the selected working folder from the remote server to the local machine. If the job has ended normally, the zip file generated automatically at the end of the job is acquired. For jobs that have not finished successfully, the zip file is created and retrieved at the timing of this operation. Available only for remote jobs.

Open Remote stdout

Opens the standard output on the remote server for the job in the selected working folder. Available only for remote jobs.

Open Remote stderr

Opens the standard error on the remote server regarding the job in the selected working folder. Available only for remote jobs.

Delete Remote Working Folder

Deletes the data in the selected working folder on the remote server. This operation cannot be reverted. It is available only for remote jobs.

Get Info

You can change the Description of the selected working folder; the Description will be the string set in the *job description* in the *job settings* window.

Recheck Status

Re-checks the status of the selected working folder. If for some reason the status is not determined correctly for a remote job (for example, ABORT is displayed even though the job has ended normally), this function will re-determine the status.

Delete

Deletes the selected working folder. This operation cannot be reverted.

Show in Explorer

The selected working folder is displayed in Explorer.

6.1.6 New File

Create a new file.

Hint: The shortcut is `Ctrl+N` .

6.1.7 Open File

Read the molecular structure from file into the main window. It corresponds to the format of various software. Use *Import File* if you want to load the structure without switching the current mode file.

Hint: The shortcut is `Ctrl+O` .

6.1.8 Open Recent File

Open a recently opened file.

Clear History

Empty the history of recently opened files.

6.1.9 Reload

Re-load the file opened in the main window.

6.1.10 Save

Overwrites the currently open file or project. For details, see *Save As* .

Hint: The shortcut is `Ctrl+S` .

6.1.11 Save As

Save the molecular structure displayed in the main window as a different name. After saving, the saved file will be reopened. If you simply want to output the structure in the specified format without reopening it, use *Export File*. It is recommended that you enter the file name and the folder name including all files (all upper layers) with one-byte alphanumeric characters only.

- If multi-byte characters such as double-byte alphanumeric characters or Japanese characters or spaces are included, some processing may cause problems.
- Underscores can be used.

If multiple types of charges are set at the same time (e.g., Mulliken and Lowdin charges) and saved in a file format that contains information on a single type of charge (e.g., mol2), the charge with the highest priority type is output. User charges have the highest priority, followed by NBO, Mulliken, and Lowdin charges, with ESP charges having the lowest priority. If multiple types of charges are set at the same time and you want to output the charge with the lowest priority among them, use *Edit Charge* to remove the information of the charge with the highest priority. When saving an input file of various solvers, a file is created based on the contents of *Keyword Editor* and *Coordinate Viewer*. If the keyword of the solver you want to save is not displayed in Keyword Editor, Configuration window will open automatically. For MOPAC, GAMESS, Gaussian, NWChem, the coordinates are output in the format selected in *File* → *Coordinate Format*.

Hint: The shortcut is `Shift+Ctrl+S`

6.1.12 Close

Closes the currently open project or file and returns to the startup screen.

6.1.13 Import File

Loads an existing molecular structure file. You can either discard the current structure and load it, or append it to the current structure and load it. *Open File* opens the file in file mode when it is read in, but this function overwrites the structure of the molecular display area with the structure of the imported file without switching modes or files.

6.1.14 Import Recent File

Import recently used files.

6.1.15 Import

It reads a specific type of molecular structure.

SMILES

Molecular structure is generated from SMILES format string and read into the main window. When *Import SMILES* window opens, enter the SMILES format string in the text box and press *Import* button. Internally, conformational search by Bolloon or OpenBabel is also executed at the same time. A working folder named `*_smiles_tmp` will be created as an intermediate file.

Structural Formula

Create a molecule by entering a structural formula. Internally, JSME draws the structural formula, and Balloon or OpenBabel generates the 3D structure by generating SMILES from JSME.

Sample File

Load the files in the Samples folder.

6.1.16 Export File

Outputs the current molecular structure in an arbitrary file format. The detailed behavior of file output follows *Save As*.

6.1.17 Export

Outputs the contents displayed in the main window in the selected format.

SMILES

Outputs the molecular structure displayed in the main window as a string in SMILES format. Not available when multiple molecules are displayed in the main window. Use OpenBabel on Cygwin. “Do you want to generate SMILES after completing the hydrogen atoms?” dialog, if “yes”, OpenBabel is executed via mol2 format with the -b option, if “no”, OpenBabel is executed via xyz format.

Warning: To use this function, *CygwinWM setup* is required.

Structural Formula

The image of the structural formula of the molecular structure displayed in the main window is output in SVG format. It can not be used when multiple molecules are displayed in the main window. I use OpenBabel on Cygwin.

Warning: To use this function, *CygwinWM setup* is required.

Image

Outputs the contents displayed in the main window in BMP or JPG format.

CHARMM crd File

Outputs the molecular structure displayed in the main window in CHARMM crd format.

LAMMPS data File (for metal)

The molecular structure displayed in the main window is output in LAMMPS data format (readable with the read_data command), with the format units=metal. The data file is generated assuming that the force field is set in the various potential files.

SDF File

Outputs the molecular structure displayed in the main window in SDF format.

6.1.18 Get Info

Displays detailed information about the molecular structure displayed in the main window.

6.1.19 Open in Text Editor

Open the file displayed in the title of the main window with the text editor selected in the configuration window.

Note: After editing with the text editor, selecting *Reload* , you can reflect the change on the main window.

6.1.20 Show in Explorer

Open the directory one level higher than the file displayed in the title of the main window.

6.1.21 Exit

Quit Winmostar.

6.2 Edit menu

It is a menu related to modeling function of atomic/molecular structure. See *Select menu* for how to select atoms to be edited. Automatically generated bonds are generated when the interatomic distance is less than (sum of covalently bonded radii) × (coefficient). The coefficient defaults to `` 1.15``, and this value can be changed with *Tools* → *Preferences* . Functions with mouse operations such as *Add atom by*, *Rotate group on axis (selection 2 atoms, mouse control)* can be canceled by unchecking the `Esc` key or the menu of the same function.

6.2.1 Undo

Revert various editing operations. It is possible up to 50 times.

6.2.2 Redo

Redo the undone operation. It is possible up to 50 times.

6.2.3 Undo text

Restore the edited contents in *keyword display area*.

6.2.4 Reset Structure

New Project or *New File* will return to the initial structure when clicked.

6.2.5 Select Element for Editing Ops

Select element to be applied in *Add atom by* or *Element* .

6.2.6 Add atom by

Specifying Position

Add atoms to the position you click in *Viewport*. The types of atoms to be added are selected by *Select element for editing ops* pull-down menu 

of *Toolbar*.

Hint: You can also operate with `F4` or from *Toolbar*.

Specifying Position and Connectivity

Add atom by specifying joint relation and coordinate in Z-Matrix format at the same time. The types of atoms to be added are selected by *Select element for editing ops* pull-down menu 

of *Toolbar*. First click on the place where the atom is placed, then click on three connecting atoms (Na, Nb,Nc) in Z-Matrix notation in order.

Adding dummy atoms to the center of gravity of a group

Adds a dummy atom at the specified distance away from the atom with the marker (red bold circle). You can select the direction (axis) to add.

Dummy atoms added along selected 2 atoms

Add a dummy atom on a straight line passing through two atoms with markers (red round, red circle).

Adding dummy atoms to the center of gravity of a group

Group Add dummy atoms to the position of the center of gravity of the selected structure.

6.2.7 Delete atom

Delete the atom marked with *marker*.

Hint: You can also operate it with `Shift + F4` or *Toolbar*.

6.2.8 Change attributes of atoms

Element

The element of the selected atom is changed to the element selected by the *Select element for editing ops* pull-down menu 

in the *Toolbar*. If a group is selected, all atoms selected in the group are targeted.

Hint: You can also operate with *Chg* button of `Shift + F5` or *Toolbar*.

Note: *Lp 0* is a Lone pair, *Cb 104* is a Capped bond used to cut out a molecular structure in MOPAC, *++ 105* to *-108* is a MOPAC sparkle, *Tv 109* is a MOPAC translation vector , *Xx 110* through *Z 112* means the dummy atom of each solver.

Optimization Flags

Changes the optimization flag for the selected atoms. The optimization flag is a flag that specifies whether each degree of freedom should be fixed (flag is '0') or variable (flag is '1') in the structural optimization calculation. By default, all degrees of freedom are variable (1). If a group is selected, all atoms selected in the group are targeted. If *General* is selected in *Solver*, the selected flag for X, Y, and Z is set as it is. If a specific solver is selected in *Solver*, the corresponding flag will be set for each.

Warning: In the case of OpenMX, if `0` is displayed on the *Coordinate Viewer*, `1` is displayed when saving the file, and conversely `1` is displayed, the output is `0`. In other words, the operation follows the `` Variable`` and `` Fixed`` notation of this function.

Charge/Spin Density

Changes the value of the charge (User charge) or spin density of the selected atoms. If a group is selected, all group-selected atoms will be affected. If *Overwrite* is checked, all values of the selected atoms will be overwritten with the input values. If *Scale* is checked, all values of the selected atoms will be scaled equally.

Note: If you want to display User Charge or Spin Density on the main window, select *User Charge* or *Spin Density* of *View* → *Labels/Charges*.

Connectivity

Click on the three connecting atoms (Na, Nb, Nc) in the Z-Matrix of the atom with the marker in order to set again.

Occupancy

Changes the occupancy of the site where the marked atom is located or the site where the group-selected atom is located. The total value of *Occupancy* must be 1. Sites with an occupancy set other than 1 will be treated by Winmostar as if there are multiple atoms in the site. The same is the behavior when a CIF file with Occupancy set is read.

Atom Name

Changes the atomic name of the site where the highlighted atom is placed or group selected atoms, affecting read/write in PDB, mol2, and gro formats.

Residue Name

Changes the residue name of the site where the marked atom is placed or the group-selected atom, affecting read/write in PDB, mol2, and gro formats.

Residue Number

Changes the residue number of the site where the marked atom is placed or group selected atoms, affecting read/write in PDB, mol2, and gro formats.

6.2.9 Move atom

Translate

Drag and move *marker* atom on *Viewport*.

Hint: You can also operate it with `F5`.

Translate (with hydrogen)

Drag and move the atoms with *marker* and the hydrogen bonded to them on the *Viewport*.

Hint: You can also use `Ctrl+F5` or `Alt` + drag.

Translate While Keeping Z-Matrix

Drag and move the atom with *marker* and the atom connected with Z-Matrix on the *Viewport* at the same time. Suitable for movement by functional group.

Change Dihedral

Drag and move the atom with *marker* on the *Viewport*. Only the dihedral angle of Z-Matrix changes.

Change fractional coordinates

:ref:Specifies the fractional coordinate of the atom with the *marker*.

6.2.10 Add/Change Bond

A bond is created between two atoms with markers (red round, red circle). If it has already been created, the type of join is changed. As types of bonds, single, double, triple, aromatic ring (1.5-fold), red are defined as 5. Please use red coupling for presentation and other purposes.

Hint: you can also operate with `F7` or *Toolbar*.

6.2.11 Delete Bond

Delete the bond between 2 atoms with markers (red round, red circle).

Hint: You can also operate with `F8` or *Delete bond* button of *Edit button area*.

6.2.12 Add Hydrogens

Make up for missing hydrogen atoms. If you import a file whose bond distance is extremely different from the original equilibrium length (such as ChemDraw or PubChem mol format), you may not be able to add hydrogen normally. In that case, please use *Edit → Automatically Adjust Atoms/Bonds* –> *Adjust All Bond Lengths*.

To all atoms

Automatically adds hydrogen to all atoms. If atoms are group selected, hydrogens are added only to the atoms.

Hint: You can also operate with `Ctrl + H`.

To marked atoms (Auto)

Add hydrogens to the markered atom. If atoms are group selected, hydrogens are added to the atoms.

Hint: You can also operate with *+ H* button of *Toolbar*.

To marked atoms (Single), (Double), (Triple)

Add one to three hydrogens with markers to the atoms. If atoms are group selected, hydrogens are added to the atoms.

Using pdb2gmx

Use the Gromacs **`gmx pdb2gmx`** command to automatically add hydrogen to proteins read from pdb or gro files. If the original pdb or gro file contains atoms that do not have amino residue information, the process will fail. An intermediate file is created in a working folder called `* _protonate_tmp`.

Note: If the structure displayed in the main window contains molecules other than proteins such as ligands and solvents, delete them with *Select* → *Select by Molecular Species* and *Edit* → *Modify Selected Group* → *Delete* in advance.

Warning: To use this function, *CygwinWM setup* is required.

Using OpenBabel

We will automatically add hydrogen using OpenBabel. It is mainly used for ligand molecules cut out from pdb file. An intermediate file is created in the working folder named `* _protonate_tmp`.

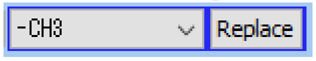
Note: If the structure displayed in the main window contains molecules other than proteins such as ligands and solvents, delete them with *Select* → *Select by Molecular Species* and *Edit* → *Modify Selected Group* → *Delete* in advance.

Warning: To use this function, *CygwinWM setup* is required.

6.2.13 Delete All Hydrogens

Delete all hydrogen atoms.

6.2.14 Replace with Fragment

Replaces Marked atoms (thick red circles) with the parts (substituents) selected with the *Fragment to be replaced with* pull-down menu  on the *Toolbar*. In the pull down menu, - *CHCH* - and - *CH* - are parts for making a polycyclic structure, which are generated to point in the direction of the atom with the second marker (thin red circle). If a group has been selected, each group-selected atom will be replaced. Fragment registration and deletion is done via *Save Fragment* and *Delete Fragment*.

Hint: You can also operate with `F6`, *Replace* button, or by right-clicking an atom.

6.2.15 Select Fragment

Select the fragment to be replaced with *Replace with Fragment* . The order of fragments can be changed in `fragment_list.txt` in the user configuration folder (`UserPref`).

Save Fragment

Register the molecular structure displayed in the main window as a fragment. Atoms with markers (bold red circles) will be set as connections during the substitution.

Delete Fragment

Deletes the registration of a fragment selected by *fragment* in the *Toolbar*.

6.2.16 Build Ring

When selecting the same function with markers (thick red circle, fine red circle) attached to 2 atoms at both ends of the connected 4 atoms, it generates aromatic rings containing the 4 atoms in the skeleton.

Hint: You can also operate it with `F9`.

Hint: For example, if you move a marker to H on both ends of the HCCH portion of a benzene molecule and call this function, a naphthalene molecule will be created.

6.2.17 Modify Selected Group

Do the operation on the atom for which *group selection (blue circle)* was performed.

Rotate group on axis (selection 2 atoms, mouse control)

Rotate the group-selected structure around a vector between two atoms with two markers (red thick circle, red thin circle) as axes by mouse operation.

Hint: You can also operate with `Ctrl + R`.

Rotate group on axis (select 2 atoms, specify values)

Rotate the group-selected structure around a vector between two atoms with two markers (red thick circle, red thin circle), specifying a numerical value.

Rotate Around Axis(3 Marked Atoms)

Rotate the group selected structure around the normal vector of the plane defined by three atoms with a marker (These can be confirmed by top left *Marked Order* on *Viewport*).

Hint: You can also operate with `Ctrl + A`.

Rotate Group Around Marked Atom

Rotate group-selected structure around the atom with *marker (thick red circle)*.

Hint: You can also operate with `Ctrl + F`.

Rotate (Numerical)

The structure group selected is rotated around the atom or geometric center marked with *marker (red circle)* by slider operation or numerical input. Specify the Euler angles.

Hint: You can also operate with `Ctrl + F`.

Rotate by Aligning Marked Atoms

Rotates the group-selected structure so that it is oriented with respect to a specific axis or plane.

Align principle axis to target direction
Rotate the inertia spindle so that its major axis points in the specified direction.

Align 2 marked atoms to target direction
Rotate so that the two atoms marked face the specified axis. The two atoms marked must be included in the group-selected structure.

Align 3 marked atoms to target plane
Rotate so that the marked 3-atom is included in the specified plane. The marked 3 atoms must be included in the group-selected structure.

Move (Direct)

Move group-selected structure in *Viewport*.

Hint: You can also operate with `Ctrl + M`.

Move (Numerical)

Translate selected group structure by slider operation or numerical input.

- If Definition = Relative coordinate from original position: specify coordinates relative to the position before the move.
- If Definition = Relative coordinate between marked atoms: Specifies the relative coordinate between two marked atoms. Before activating this function, you must first click (mark) an atom that is not included in the group of atoms to be moved, then click (mark) an atom whose position relative to the atom you want to specify and that is included in the group of atoms to be moved, and then select the group of atoms to be moved. The group of atoms to be moved must be selected.
- If Definition = Absolute coordinate for center of mass: specifies the absolute coordinates for the center of mass of the group.
- For Definition = Absolute coordinate for center of geometry: Specify the absolute coordinate for the geometric center of the group; Direction specifies the direction of movement; for Two marked atoms, the vector between the last two clicked atoms is used as the direction.

Quick Optimization

We will optimize structure using molecular force field for group selected structure.

Hint: You can also operate with `Ctrl + L`.

Creates bonds between adjacent atoms in a group

Automatically generates bonds between neighboring atoms in the group-selected structure. Adjacency is determined by Voronoi splitting.

Hint: You can also operate with `Ctrl + L`.

Delete bonds in a group

Deletes bonds in the group-selected structure. Bonds between atoms that are not group-selected and atoms that are group-selected are not deleted.

Cut

Cut the group-selected structure to the clipboard.

Hint: You can also operate with `Ctrl + X`.

Copy

Copy the group-selected structure to the clipboard.

Hint: You can also operate with `Ctrl + C`.

Paste

Paste the group-selected structure from the clipboard. After pasting, drag to determine the position.

Hint: You can also operate with `Ctrl + V`.

Replicate Group

Duplicate and arrange the group-selected structures at regular intervals. Specify the arrangement interval and number of copies in each direction in the subwindow.

Delete

Delete the group-selected structure or any other structure. When a part of the structure in the molecule is deleted, hydrogen atoms are automatically supplemented to the disconnected part.

Hint: You can also operate with `Ctrl + D`.

Change Optimization Flags of Group

groupSet the optimization flags for all components of the XYZ coordinates of the selected structure to `0` (fix) or `1` (free). See *Optimization Flags* for more information on the optimization flags. For more fine-grained control, choose *edit* → *change attribute* → *Optimization Flags*.

Hint: You can also operate with `Ctrl + I`.

Fix/Unfix Groups (Z-Matrix)

Sets the optimization flags of all components of Z-Matrix for the group selected structure to `0` (fix) or `1` (free). See *Optimization Flags* for more information on the optimization flags. For more fine-grained control, choose *edit* → *change attribute* → *Optimization Flags*.

Shift Charges of Group

The total point charge of the group-selected structure is uniformly shifted to the specified value. This function is useful when you want to reduce the total system charge to 0, such as when performing MD calculations.

Average the group's charge

Corrects the sum of the point charges that a group-selected structure has to their average value. This is useful if you want to average the charges of equivalent atoms (e.g. the three hydrogen atoms of a methyl group) after running *Use RESP charges* or *RESP Charges*.

6.2.18 Automatically Adjust Atoms/Bonds

Quick Optimization

We will perform structure optimization using molecular force field. The algorithm used can be changed with *Tools → Preferences menu*. If the method is "Winmostar", the algorithm used in Winmostar before V10 is used. The number of applicable atoms is limited, but the process is faster. If the method is "OpenBabel", the OpenBabel installed in CygwinWM is used. Although the process is slower, there is no limit to the number of atoms that can be applied, and parameters such as the type of force field can be finely tuned.

Hint: You can also operate with `Ctrl + G`.

Regenerate All Bonds

Determine the presence and type of bonds from interatomic distances and reassign the bonds.

Adjust All Bond Lengths

Adjust the coupling length to a reasonable value to some extent.

Hint: Please use this function with *Quick Optimization*, if necessary.

Delete all bonds

Delete all bonds.

Regenerate Z-Matrix

Automatically regenerate Z-Matrix. Connection atom is also set automatically.

Convert Aromatic Rings to Single and Double Bonds

Change the aromatic ring bond to a combination of a single bond and a double bond.

Change unknown elements to hydrogen.

Change the atoms recognized as Lp or dummy atoms to hydrogen.

Hint: This is useful, for example, for converting deuterium to hydrogen in a CIF file.

Assign different residue numbers to each molecule.

Assign a different residue number to each molecule. A group of atoms connected by bonds is recognized as a molecule.

Assign different residue numbers to each molecule.

Assign a different residue number to each molecule. A group of atoms connected by bonds is recognized as a molecule.

Remove all optimization flags

Set the optimization flags for all atoms to their default (variable) values.

Overwrite Bonds from File

Overwrites the bond information for the current structure with the bond information for the structure written in the specified file. If the bond order changes from the order before force field assignment after force field assignment in MD calculations (LAMMPS, Gromacs, etc.), save a file in mol2, wmm, etc. format before force field assignment and load the file with this function after force field assignment, and the bond order will be restored to the one before force field assignment. If you save the file in mol2, wmm, etc. format before force field assignment, and then load the file with this function after force field assignment, you can restore the bond information before force field assignment. This function is useful in cases where a force field has been assigned once and an MD calculation has been performed, but the bond order has changed since the initial force field assignment and the force field cannot be assigned again. The bond order after force field assignment is determined by Winmostar's criterion based on the bond equilibrium length of the assigned force field, so the aforementioned phenomenon occurs for some types of force fields.

Distribute Charge of Selected Atom in Residue

It distributes the charge of the selected atom to the other atoms in the residue to which it belongs. With this function, the total charge within the same residue does not change before and after the deletion of a selective atom.

Merge Overlapping Atoms

For all atoms in the system, look for atoms with overlapping coordinates and elements, and for those that overlap, consolidate them into one. A threshold value can be set to determine whether or not the coordinates overlap.

6.2.19 Renumber/Sort

Exchange Between 2 Marked Atoms

Exchange the numbers of the two atoms with the marker. It is mainly used when editing Z-Matrix.

Sort by Atomic Number

Sorts the atoms so that they are ordered by atomic number.

Sort by H atoms and Others

Arrange the atom numbers so that they are in the order of atoms other than hydrogen, hydrogen atoms.

Sort by Molecular Species

We will rearrange the order of the atoms so that molecules of the same kind are continuous.

Renumber Across Each Molecule

Number the molecules sequentially from the end within the molecule. This is useful, for example, when selecting both ends of a polymer.

6.2.20 Adjust Axes

Set to Camera Coordinate

Redefine the molecule by redefining the current direction of the camera's line of sight as Z axis, the camera upward direction as Y axis, and the camera right direction as X axis.

Set Using 3 Marked Atoms

The normal direction of the plane passing through the three atoms with the marker is taken as the Z axis, and the vector passing through the two atoms with the marker is taken as the X axis.

Set to Principal Axes

Rotate the entire system so that the principal axis of inertia matches the X, Y, Z axes. The long axis is the X axis.

Set Origin to Marked Atom

Set atoms with markers as origin.

Set Origin to Lower Bound Edge of Cell

Rewrite the coordinate system so that the cell's origin coordinates are (0, 0, 0).

Swap Axes

Swap the axes and recreate the coordinate system.

6.2.21 Invert Coordinates/Chirality

Invert along X/Y/Z/a/b/c Axis

Inverts the specified axis and recreates the coordinate system.

Generate Enantiomer

Generate an enantiomer of the molecular structure displayed in the main window adjacent to the current structure.

6.2.22 Create/Edit Cell

Create/Edit Cell

Create the simulation cell

- *Set Margin* is checked, it creates cell borders at a specified distance from the minimum and maximum values for each direction of the molecular structure shown in the main window. If *Use Cubic Cell* is checked, a cubic cell will be created.
- :guilabel:If *Set Dimension* is checked, a cell with the specified size cube will be created.

Transform Cell

1. *How to transform cell* specifies how to transform the cell.
    - Check the *Transform only along the selected axis* if you want to deform the cell only along the selected axis. Check *Set incremental length* for length, *Set total length* for size after deformation, or *Set normal strain* for vertical strain. or *Set density* to specify the deformed density.
    - Check *Transform similarly* to deform the cells similarly. Select *Set target density* to specify the density of the transformed cells, or *Set target volume* to specify the volume of the transformed cells.
    - Check *Transform by shear strain* if you want to apply a shear strain. Specify the direction to be deformed and the strain to be applied.
    - Check *Transform by angle* if you want to change the angle of a cell. Specify the type and value of the angle to be transformed.
2. *Atomic positions* specifies how to move atoms.
    - Check *Do not change* if you want to keep the position of the atoms and only change the cells.
    - If you want to change the position of the atoms fixed as the cell is deformed, check the *Move with keeping fractional coordinates* checkbox. For molecular systems, check *Keep intramolecular coordinates*, then intramolecular coordinates are kept fixed.

Edit Cell Manually

The *Create/Edit Cell* window opens, where you can create or edit simulation cells such as MD calculations and plane wave DFT calculations. If the cell does not exist, clicking the *Create* button creates a cell at a distance of` Distance` from the minimum and maximum values in each direction of the molecular structure displayed in the main window. Click the *Expand* button to expand the cell size in the specified direction. On the right side of the *Create/Edit Cell* window, you can edit the cell size value directly. Click *Lattice Vecors*, *Lattice Constants*, *LAMMPS Tilt Factors* to change the cell size notation.

Note:

- You can also display the lattice parameters in the *Viewport* by checking *Preferences* → *View* → *Items to be drawn* → *Lattice constant*.
- Even if you change the cell size with this function, the coordinates of the atoms do not change, so if you want to change atomic coordinates similarly to the cell size, use *Transform Cell*.
- If you want to return atoms outside the simulation cell to the simulation cell before editing, use the *Wrap Around Cell Boundary* function.

6.2.23 Delete Cell

Delete Cell.

6.2.24 Wrap Around Cell Boundary

We return the coordinates of the atoms outside the simulation cell into the cell taking into account the period boundary. Mainly in molecular systems *Wrap for each molecules*, mainly in inorganic systems *Wrap for each atoms*.

Note:

- If *Display-> Wrap Around Cell Boundary* → *Do not wrap* is selected, it will be easier to check the change of coordinates.
- In tne *Display* → *Wrap Around Cell Boundary* function, only the display changes and the coordinates do not change, but in this function the coordinates actually change.

6.2.25 Edit Charge

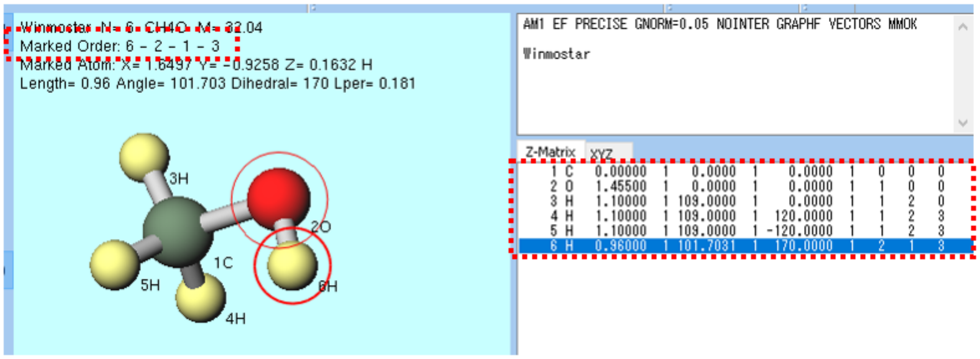
Edit the value of the charge. Specify the type of charge and set it to user charge. You can also delete specified charges. It can be adjusted so that the total charge is at a specific value.

6.3 Select menu

It is a menu related to the function of selecting atoms or molecules.

Hint: How to select atoms

There are two ways to select an atom: **The method using a red circle marker** and **the method using a blue circle group selection**. **The method using the red circle marker** is mainly used for operation on one atom.The marker moves to the atom that was left-clicked in Viewport.In the example of the methanol molecule in the figure below, the oxygen (red) and hydrogen (yellow) of the OH (hydroxy) group are left clicked. The red thick circle is drawn to the atom to which the marker is finally attached, and the red thin circle is drawn to the atom attached the marker one before.The marker also moves by left clicking at *Coordinate Viewer* in the right red frame of the figure below.Last four atoms marked are internally stored and displayed as shown in the upper left red frame of the figure below.The number of each atom can be confirmed in *Viewport* by selecting *View → Labels/Charges → Show Number & Element* or *Coordinate Viewer*.



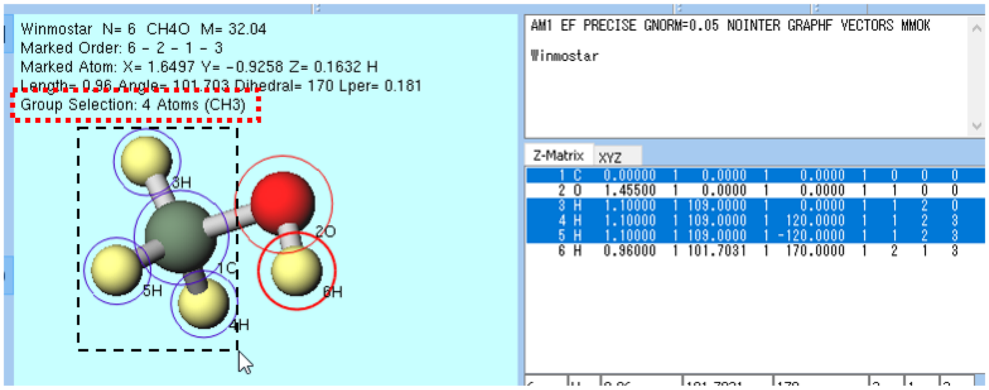
```
Winmostar  N= 6  CH4O  M= 32.04
Marked Order: 6 - 2 - 1 - 3
Marked Atom: X= 1.6497 Y= -0.9258 Z= 0.1632 H
Length= 0.96 Angle= 101.703 Dihedral= 170 Lper= 0.181
```

```
AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar
```

```
  1 C   0.00000  1    0.0000  1     0.0000  1   0   0   0
  2 O   1.45500  1    0.0000  1     0.0000  1   1   0   0
  3 H   1.10000  1  109.0000  1     0.0000  1   1   2   0
  4 H   1.10000  1  109.0000  1   120.0000  1   1   2   3
  5 H   1.10000  1  109.0000  1  -120.0000  1   1   2   3
  6 H   0.96000  1  101.7031  1   170.0000  1   2   1   3
```

The method using group selection of the blue circle is mainly used for operations on multiple atoms.You can select a group by `Ctrl+left drag` , `Ctrl+left click` or `Shift+left click` in *Viewport*.You can also select a group by using the function of *Select* menu.In the example of the methanol molecule in the figure below, after `Ctrl+left drag` around the CH3 (methyl) group, it can be confirmed that the CH3 group atoms are surrounded by blue circles.You can also select a group by `Ctrl+left click` in *Coordinate Viewer*.On the upper left of *Viewport*, the number of atoms and composition of the group selected are displayed



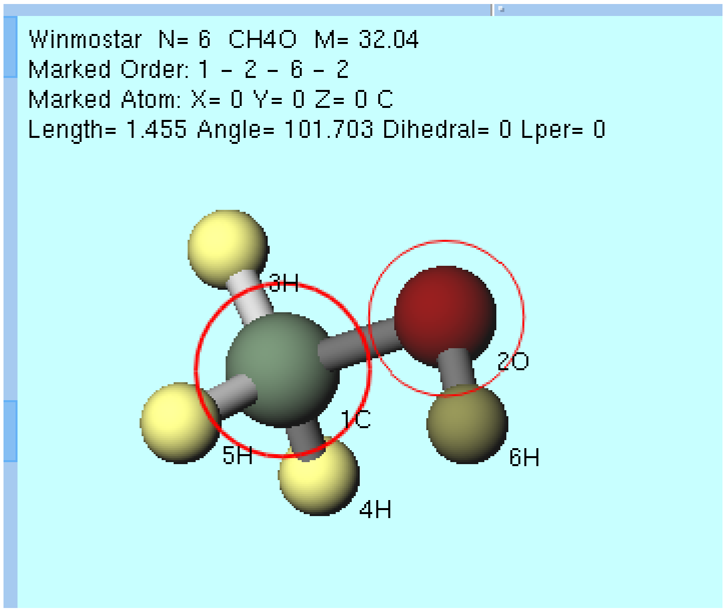
```
Winmostar  N= 6  CH4O  M= 32.04
Marked Order: 6 - 2 - 1 - 3
Marked Atom: X= 1.6497 Y= -0.9258 Z= 0.1632 H
Length= 0.96 Angle= 101.703 Dihedral= 170 Lper= 0.181
Group Selection: 4 Atoms (CH3)
```

```
AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar
```

```
  1 C   0.00000  1    0.0000  1     0.0000  1   0   0   0
  2 O   1.45500  1    0.0000  1     0.0000  1   1   0   0
  3 H   1.10000  1  109.0000  1     0.0000  1   1   2   0
  4 H   1.10000  1  109.0000  1   120.0000  1   1   2   3
  5 H   1.10000  1  109.0000  1  -120.0000  1   1   2   3
  6 H   0.96000  1  101.7031  1   170.0000  1   2   1   3
```

Select Partial Structure Split by 2 Marked Atoms is executed automatically when you execute an operation on multiple atoms such as *Edit → Modify Selected Group* in a state where no group is selected. Specifically, the substructures that are divided by two atoms with a red thick circle and a red thin marker attached are selected as a group. In the example of a methanol molecule shown below, after oxygen (red) and carbon (green) are moved in the order of `left click` and the marker is moved, *Edit → Modify Selected Group → Rotate group on axis (selection 2 atoms, mouse control)* is selected, the group with the last marker on the CH3 group is automatically selected (highlighted on the screen).



Winmostar N= 6 CH4O M= 32.04
Marked Order: 1 - 2 - 6 - 2
Marked Atom: X= 0 Y= 0 Z= 0 C
Length= 1.455 Angle= 101.703 Dihedral= 0 Lper= 0

6.3.1 Select All

Select all atoms as a group.

6.3.2 Select None

Cancel the group selection.

6.3.3 Invert Selection

Select a group that has not been selected as a group, and cancel the group selection of the group that was selected until then.

6.3.4 Select by Molecular Species

It opens with *Use List* tab of *Select by* window checked *Molecular Species*.Click on each line in the list in the window and the corresponding molecular species are selected.

Note: When calculating from protein pdb files, this function can be used to extract proteins, ligands, bound water, buffers, etc.

6.3.5 Select by Molecules

It opens with *Use List* tab of *Select by* window checked *Molecules*.Click on each line in the list in the window and the corresponding molecule is selected.

6.3.6 Select by Elements

It opens with *Use List* tab of *Select by* window checked *Elements*.Click on each line in the list in the window and the corresponding element is selected.

6.3.7 Enter Selection Language

It opens with *Use Selection Language* tab of *Select by* window.If you click on *Apply* button after describing in the text box, the corresponding atoms are selected.The following syntax is supported in the selection language.

Table 1: Basic syntax

`element C H`	Select all carbon and hydrogen atoms.
`index 1-3 6 8`	Select 1, 2, 3, 6 and 9th atoms.
`compid 1`	Select the molecular species whose CompID is 1. The correspondence between CompID and molecular species can be confirmed in the list under *Apply* button.
`moleid 1-3`	Select 1, 2 and 3rd molecules. You can see the numbers of molecules in the list under *Apply* button.
`site 1`	Select the first atom (site) in each molecule. You can see the numbers of sites for each molecule in the list under *Apply* button.
`charge 0.5`	Select the atoms whose atom name is CA. A tolerance of ± 0.1% is provided.
`resname GLY`	Select the atoms whose residue name is GLY.
`name CA`	Select the atoms whose atom name is CA.
`x< 10`	Select the coordinates where the x-coordinate is less than 10 Angstrom. (No space between x and <.) Similarly, y and z can be used. You can also use `x>` , `x=>` and `x<=`.
`bondto H`	Select the atom to be bonded to the H atom.

The residue name and atom name can be used when PDB or gro format file is opened.

Table 2: Composite syntax using logical operators

`(compid 1) and (site 1)`	It is a molecular species whose CompID is 1 and the first site in the molecule is selected.
`(current) and (element H)`	Select only hydrogen atom among atoms currently selected in the group.
`(resname GLY) and (not (element H))`	Select the atom whose residue name is GLY and other than hydrogen.

In addition to `and`, `not` you can use `or` and `xor`. When using these logical operators, use the parentheses `()` as in the example above. Also, if you enter `%2==0` where you enter an integer, it will assign a sequence of numbers where the remainder divided by two is zero. For example, typing `site %3==1` will select atoms with sites 1, 4, 7, 10… will be selected.

6.3.8 Select Partial Structure Split by 2 Marked Atoms

Substructures that are separated between two atoms with the first and second markers are selected. Details are described in *Select menu* with pictures.

6.3.9 Group selection of atoms bound to the current group

Selects an additional group of atoms bound to the current selection group.

6.3.10 Group selection of atoms adjacent to the current group

Select a group of atoms adjacent to the current selection group. Here, adjacent atoms are defined as those atoms that have the same Voronoi boundary when Voronoi splitting is applied to all atoms.

6.3.11 Group selection of molecules adjacent to the current group

Select a group of molecules adjacent to the current selection group. Here, adjacent atoms are defined as atoms that have the same Voronoi boundary when Voronoi splitting is applied to all atoms.

6.3.12 Select Atoms Around Marked Atom

Select a group of atoms that exist within a specified distance from the marked atom.

6.3.13 Select Molecules Around Marked Atom

Selects a group of molecules whose center of gravity is within a specified distance from the marked atom.

6.3.14 Select Residue with Marked Atom

Select Residue with Marked Atom. Residues with the same residue number and consecutive atom IDs are determined to be the same residue.

6.3.15 Select Groups by Enlarging Each Molecular Species

Enable group selection of atoms by zooming in on the molecule in 3D for each molecular species. In the Create Group window, use Target to switch molecular species and Ctrl+click on the left side of the window to select atoms (sites). Click the Add button to register the selected sites, and click OK to create a group for each molecule's registered sites.

6.3.16 Register Selected Group

Name and register the selected group so that it can be called from *Select Registered Group*.

6.3.17 Select Registered Group

Call the group registered with *Register Selected Group*. When LAMMPS is executed, the groups listed here are output in the ndx file. If you want to take over the registered group even after restarting Winmostar, export to the ndx file using *Export Groups to Index File (ndx)* and then read it using *Import Groups from Index File (ndx)*.

6.3.18 Import Groups from Index File (ndx)

Reads the group output to the ndx file and makes it accessible from *Select Registered Group*.

6.3.19 Export Groups to Index File (ndx)

Outputs the groups registered in *Select Registered Group* to the ndx file.

6.3.20 Add Selected Group to Index File (ndx)

Add the group selected group to the specified ndx file.

6.3.21 Concatenate and Transpose Groups

This function combines multiple groups with equal number of atoms in them and transposes the order. For example, if group A contains 1, 2, 3, and group B contains 4, 5, and 6, and this function is applied to groups A and B, three groups will be created: 1 4, 2 5, and 3 6.

6.4 View Menu

6.4.1 Show Project Area

Show/Hide the project display area in the main window.

6.4.2 Show Keywords & Coordinates Areas

Switch show or do not show Keyword Editor and Coordinate Viewer on the main window.

6.4.3 Show Multi-View

Make Viewport three views.

6.4.4 Coordinate Format

Specifies the display format in the coordinate display area. To switch the output format of coordinates in the solver's input file, select the output format in the various solver keyword setting windows.

Hint: *Coordinates display area* You can also toggle the checkbox at the top.

6.4.5 Reset View

Return the camera to the default position.

6.4.6 Align View

Change the direction of the line of sight of the camera.

6.4.7 Zoom In/Out

Expand or reduce the field of view.

6.4.8 Always View Center

If checked here, even if the displayed molecular structure changes, the center of gravity at that point will always be the gaze point of the camera. If it is not entered, gaze point will not change unless explicit gaze change.

6.4.9 View Marked Atom

Specify atom attached with marker (thick red circle) as gaze point.

6.4.10 Pan

Drag left on the main window to move the line of sight in parallel.

6.4.11 Rotate

Around Center

Drag left in the main window to rotate the camera around the point of interest.

Around X, Y, Z-Axis

Drag left in the main window to rotate the camera around each axis.

Around Line of Sight

Drag left in the main window to rotate the display.

Rotate the display (Numerical)

Enter the rotation angle of the display.

6.4.12 View Preset

Save and load display settings at once.

6.4.13 Perspective

If checked here, perspective is applied to Viewport.

6.4.14 Enable Depth Cueing

If this is checked, fog is applied to Viewport. This makes it easy to distinguish between atoms in front and back. Fog strength can be set with *Tools → Preferences menu*.

6.4.15 Enable Specular Lighting

If this is checked, the atoms will be glossed over in the molecular display area.

6.4.16 Items

Check the items to be displayed in Viewport.

6.4.17 Label/Charge

In Viewport, a label (annotation) and a sphere showing the magnitude of the charge are displayed beside each atom.

(Hide Label/Charge)	Hides the label and charge display. (initial state)
Number&Element	Displays the serial numbers of the atoms and the element names.
Number	Displays the serial numbers of the atoms.
Element	Displays the the element names.
Mulliken Charge	Displays the Mulliken charge read when various log files are opened.
ESP Charge	Displays ESP or RESP charge read when various log files are opened.
Lowdin Charge	Displays Lowdin charge read when various log files are opened.
NBO Charge	Displays Lowdin charge read when various log files are opened.
Show User Charge	*Edit* → *Chnge Atom Property* → *Charge/Spin Density* and *MD* → *Assign Charges* and other functions to display the charge assigned by the user.
Show Spin Density	Spin density read when various log files are opened Display the spin density assigned by *Edit* → *Change Atom Property* → *Charge/Spin Density*.
Show Difference Density	Show Difference Density

6.4.18 Dipole/Transition Moment

Show Dipole/Transition Moment

Displays the dipole moment or transition moment read when various log files are opened.

Select Transition Moment

Select the transition moment to be displayed.

Change Scaling Factor

Specify the magnitude when displaying dipole/transition moment.

6.4.19 Molecular Representation

Select the expression method (model) of the molecule.

6.4.20 Wrap Around Cell BOundary

The display method when the atomic coordinates are smaller than the top and bottom of the cell while the cell is being created is shown below. The coordinate value itself does not change with this function. *Edit* → *Wrap Around Cell Boundary*, you can set the value of the coordinates to the position of the atom displayed in this function.

6.4.21 Transparency

Set transparency/opaqueness and adjust transparency for selected groups or all atoms.

6.4.22 Winmostar Viewer

Display the structure displayed in Viewport using *Winmostar Viewer*.

6.4.23 External viewer

Displays the structure displayed in Viewport with various external programs.

Jmol

Start Jmol.

Mercury

Start Mercury. If the file being read is CIF, use that file.

ChemscapeChime

Start MDL Chime.

Ray Tracing (POV - Ray)

It outputs a file in POV - Ray format and renders it using POV - Ray.

OpenSCAD

Output the OpenSCAD format file and start OpenSCAD. You can create data for 3D printers.

6.4.24 Copy Image

Copy the image of Viewport to the clipboard.

6.5 *QM* → *MOPAC* menu

It is a menu related to MOPAC. MOPAC6 and MOPAC7 are bundled with Winmostar. If you wish to use other MOPACs, please obtain the MOPAC itself separately and set the path in the Preferences window.

6.5.1 Workflow Setting

Sets up and executes the MOPAC calculation flow in project mode. Local jobs in project mode will use the binary specified in *MOPAC(1)* in *Tools* → *Preferences* → *Program Path*.

Preset
Loads and saves a preset of settings.

# of Jobs
Specifies the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File* → *Project* → *Scan Results* to tabulate the calculation results.

Import
Import the settings output by Export. Click the arrow to the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Run a calculation or generate a file with your settings. See *For project mode* for details.

Details
Set up detailed calculation conditions. The *Configure* will be launched.

Task
Specifies the type of calculation.

	Configuration details
Energy	Method=1SCF
Optimize	Method=EF
IR	Method=FORCE
Optimize(TS)	Method=TS
IRC(Forward)	Method=IRC=1 LARGE=50
IRC(Reverse)	Method=IRC=-1 LARGE=50
Scan	Method=EF Add the specified Scan content to the last line of input.

Method
Specify the calculation method (Hamiltonian).

UHF
Specify whether the calculation should be done in a closed or open shell system.

Charge
Specify charge.

Multiplicity
Specifies spin multiplicity.

6.5.2 Configure

Set calculation condition of MOPAC. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. Behavior when clicking *Run* is see *(1) Run MOP6W70, (2) Run MOP7W70, (3) Run MOPACX*. return to the default state with *Reset* button. . Save the current state as the default state with *Save as Default* button. Restore the default state to the factory condition with *Save as Default* → *Clear Default Settings*.

Easy Setup
The simple setting window is displayed.

Hamiltonian
Specify the Hamiltonian to use. The Hamiltonian supported by each version of MOPAC is as follows.

Hamiltonian	Version of MOPAC being implemented
AM1	MOPAC 6, MOPAC 7, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012, MOPAC2016
PM3	MOPAC 6, MOPAC 7, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012, MOPAC2016
RM1	MOPAC 2007, MOPAC2016
AM1 EXTERNAL=RM1.rm1	MOPAC 7.1, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012
PM6	MOPAC 2007, MOPAC 2009, MOPAC 2012, MOPAC2016
PM7	MOPAC 2012, MOPAC2016
MINDO/3	MOPAC 6, MOPAC 7, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006
MNDO	MOPAC 6, MOPAC 7, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012, MOPAC2016
MNDO-d	MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012, MOPAC2016

Method
Specify the calculation method.

EF
Perform structure optimization calculation by EF (Eigen Vector Following) method.

TS
Find the transition state.

FORCE
Perform vibration analysis.

1SCF
Perform SCF calculation only once. (Structure optimization is not performed.)

IRC
Perform unique reaction coordinate calculation. Energy is not preserved.

IRC=1
Specify the inverse direction of the 1st reference vibration and calculate the unique reaction coordinate.

IRC=-1
Specify the positive direction of the first reference vibration and perform the unique reaction coordinate calculation.

Charge
Specify the value of the charge.

Multiplicity
Specify multiplicity.

OPEN
Specify the number of electrons and the number of orbits in open shell calculation.

MM

MMOK
Molecular dynamics correction is added to CONH bond.

NOMM
Molecular mechanics correction is not added to CONH bond.

GNORM
Specify the threshold value of the energy gradient norm.

LARGE
Information is output for each specified cycle.

GRAPH
Create a file to graphically display molecular orbitals. (GPAGH/GRAPHF)

EXTERNAL
Read parameter file on disk.

STEP
Specify the step width in reaction coordinate calculation.

POINT
Specify the number of calculation points in reaction coordinate calculation.

STEP1/2
Specify the step size in the grid calculation.

POINT1/2
Specify the number of calculation points in the grid calculation.

AUX
Create an AUX file for use with another program.

BONDS
It outputs the final bond order matrix.

ENPART
Specify the energy split that resolves the energy into 1 center and 2 center terms.

ESP
Calculate electrostatic potential.

EXCITED
Optimize the singlet first excited state.

GEO-OK
Ignore the check if the atom is close to abnormal.

NOINTER
Interatomic distance is not output.

OLDFPC
We use the same reference physical quantity value as the old version MOPAC.

POLAR
Calculate the polarizability.

PRECISE
Set the convergence judgment condition to 100 times stricter.

SYMMETRY
Define the structure using symmetry and equivalent conditions.

UHF
Perform unrestricted Hartree-Fock calculation.

VECTORS
The final eigenvector (wave function) is output.

XYZ
Calculation is performed using the XYZ coordinate system.

Others
Fill in other keywords.

Coordinate format
Specifies the format of the atomic coordinates (XYZ or Z-matrix).

Reset
Reset settings.

Import
Loading configuration file.

Export
Output configuration file.

6.5.3 Import Keywords

Only keywords (calculation conditions) are read from the existing MOPAC input file.

6.5.4 (1) Run MOP6W70, (2) Run MOP7W70, (3) Run MOPACX

If MOPAC input file is opened in the main window, execute MOPAC using that file. If it is not open, save the input file of MOPAC and execute MOPAC. When saving the input file, the output format of coordinates changes according to the choice of *Coordinate Format* (*Z-Matrix* or *XYZ*) and *Coordinate Viewer* of *Z-Matrix* / *XYZ* tab. It is assumed that different versions of MOPAC are set for *(1) MOP6W70 execution* , *(2) MOP7W70 execution*, and *(3) MOPACX execution*, and that both are used in different situations. The *(1). The difference between :guilabel:`(1) Execute MOP6W70*, *(2) Execute MOP7W70*, and *(3) Execute MOPACX* is the program path of MOPAC to be launched. The program path used for each menu can be changed in *Tools* → *Preferences* → *Program Paths*. The default *MOP6W70* is MOPAC6 and *MOP7W70* is MOPAC7, both of which are built in Winmostar. The *(3) Execute MOPACX* is intended for use with programs such as MOPAC2012, which you can obtain and specify separately. Following file will be generated with execution. For example, the file/folder name when the input file is `water.dat` is shown together.

type	Description
out file `water.out`	It summarizes the outline of the calculation result.
arc file `water.arc`	It is a file summarizing the details of the calculation result.
mgf file `water.mgf`	This file is output by specifying the keyword GRAPH and contains information used to draw molecular orbitals.
Working Folder `water_mop_temp\`	Working folder.

6.5.5 Open Log File (out)

Open out file in a text editor.

6.5.6 Open Log File (arc)

Open arc file with a text editor.

6.5.7 Animation

Optimization (arc)

Select the arc file and display the animation of the molecular structure. For the animation display operation method, see *Animation operation area*.

IRC, STEP (out)

Select out file and display animation of IRC calculation. For the animation display operation method, see *Animation operation area*.

6.5.8 Analyses

MO & Charges (mgf)

Select the mgf file and display the molecular orbital. `GRAPHF` must be set on *keyword*. Refer to *Energy Level Diagram window*, *Surface Setup / Cubgen window* for how to operate the subwindow. Show charges when you select *View → Label/Charges → Show Mulliken Charge*.

IR (out)

Select the out file and display the IR spectrum. Vibration calculation must be set with *keyword*. Refer to *IR Spectrum Window* for how to operate the subwindow.

6.5.9 Use Job Manager

When checked, use *Winmostar Job Manager* when executing MOPAC. Otherwise, Winmostar will be in a wait state until calculation by MOPAC is completed, and the output result of MOPAC will be automatically loaded into the main window. It can also be set from *Tools → Preferences menu*.

6.6 *QM → CNDO/S* menu

It is a menu related to the CNDO/S program. The CNDO/S program is bundled with Winmostar. The CNDO/S program is a slight modification of the P083 program registered in the former Japan Chemistry Program Exchange Organization (JCPE, the present Japan Computer Chemistry Society) to correspond to Winmostar. The manual of P083 is *here <https://winmostar.com/jp/manual_third_party/cndos_man.pdf>*. The CNDO/S program (: file: *cndosw.exe*) has been compiled with gfortran.

6.6.1 Workflow Setting

Set up and run the CNDO/S calculation flow in project mode.

Preset
Recalls and saves a preset of settings.

# of Jobs
Specifies the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File → Project → Scan Results* to tabulate the calculation results.

Import
Import the settings output by Export. Click the arrow at the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Runs a calculation or generates a file with your settings. See *For project mode* for details.

Details
Set up detailed calculation conditions. The *Configure* will be launched.

Task
Specify calculation details. (UV-Vis only)

Method
Specify calculation method.

Charge
Specify the charge.

Multiplicity
Specifies spin multiplicity.

6.6.2 Configure

Set calculation conditions of CNDO/S. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. Behavior when clicking *Run* is see *Run*.

Method
Specify the calculation method. (CNDO or INDO)

Multiplicity
Specify multiplicity.

Basis set
Specify the basis function. (SP or SPD)

BONDS
Specifies to output the bond order

NOINTER
If checked, interatomic distance will not be output.

SHORT
It outputs a simplified log.

OUTMO
It outputs a file for MOLMOL 2.

Repulsion integral

Specify the expression of repulsion integral.

- Parisian
- Ohno
- Nishimoto - Iga
- Theoretical

Nuclear repulsion energy

Specify the expression of inter-nuclear repulsion energy.

- Za * Zb / 1

- Za * Zb * Gamma ab

PKAPPA
p Specify the value of kappa for electrons.

DKAPPA
d Specify the value of kappa for electrons.

Charge
Specify the charge.

# of CI
Specify the number of states to include in the CI calculation of the excited state. (Max 500)

# of excited states
Specify the number of excitation states to output the bond order.

6.6.3 Import Keywords

Only keywords (calculation conditions) are read from the existing CNDO/S input file.

6.6.4 Run

If the input file of CNDO/S is open in the main window, execute CNDO/S with that file. If it is not open, save the CNDO/S input file and execute CNDO/S. Following file will be generated with execution. For example, the file/folder name when the input file is: file: *water.cnd* is also shown.

type	Description
lst file `water.lst`	Calculation log file.
Working Folder `water.cnd_temp\`	Working folder.

6.6.5 Open Log File (lst)

Open the lst file with a text editor.

6.6.6 Analyses

UV-Vis

Select lst file and display UV-Vis spectrum and molecular orbital. Refer to *UV-Vis Spectrum window*, *Energy Level Diagram window*, *Surface Setup / Cubgen window* for how to operate the subwindow.

6.7 *QM* → *GAMESS* menu

It is a menu related to GAMESS. In order to use GAMESS you need to install GAMESS separately. The way to install GAMESS is described in *Installing Winmostar and solvers*.

6.7.1 Workflow Setup

Sets up and executes the GAMESS calculation flow in project mode. Local jobs in project mode will use the binary specified in *GAMESS(1)* in *Tools* → *Preferences* → *Program Path*.

Preset
Import and saves a preset of settings.

# of Jobs
Specify the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File* → *Project* → *Scan Results Viewer* to tabulate the calculation results.

Import
Import the settings output by Export. Click the arrow to the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Run a calculation or generate a file with your settings. See *For project mode* for details.

Details
Set up detailed calculation conditions. The *Configure* will be launched.

Task
Specifies the type of calculation. Keywords without a group name beginning with $ are from $CONTRL.

	Setting details
Energy	RUNTYP=ENERGY
Optimize	RUNTYP=OPTIMIZE
IR	RUNTYP=HESSIAN
Raman	RUNTYP=RAMAN
TDDFT	RUNTYP=ENERGY TDDFT=EXCITE $TDDFT NSTATE=10
Optimize(TS)	RUNTYP=SADPOINT $STATPT HESS=CALC
Optimize(TDDFT)	RUNTYP=OPTIMIZE TDDFT=EXCITE $TDDFT NSTATE=10
IRC(Forward)	RUNTYP=IRC $STATPT HESS=READ $IRC FORWRD=.TRUE. NPOINT=20 MXOPT=40 SADDLE=.TRUE.
IRC(Reverse)	RUNTYP=IRC $STATPT HESS=READ $IRC FORWRD=.FALSE. NPOINT=20 MXOPT=40 SADDLE=.TRUE.
Optimize+IR	RUNTYP=OPTIMIZE $STATPT HSSEND=.TRUE.
Optimize(TS)+IR	RUNTYP=SADPOINT $STATPT HESS=READ HSSEND=.TRUE.

Method

Specifies the calculation method (Hamiltonian). Keywords without a group name beginning with $ are from $CONTRL.

	Setting details
Various DFTs	DFTTYP=Various DFTs (For DFT-D3) $DFT IDCVER=3
MP2	MPLEVL=2 $SYSTEM MEMDDI=500
CCSD	CCTYP=CCSD

Basis set

Specifies a basis function.

Charge

Specify charge.

Multiplicity

Specify spin multiplicity.

Solvent

Specify PCM solvent type.

6.7.2 Configure

Set calculation conditions of GAMESS. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. See the *(1) Run GAMESS, (2) Run GAMESS* for the behavior when clicking *Run*. Return to the default state with *Reset* button. Save the current state as the default state with *Save as Default* button. Restore the default state to the factory condition with *Save as Default → Clear Default Settings*.

Easy Setup

Shows the simple setting window.

NCPUS

Specify the parallel number.

NODES (FireFly)

Specify the directory of the node used for calculation.

Basic Tab

$CONTRL

ICHARG

Specify charge.

A LOT
Specify spin multiplicity.

SCFTYP
Specify SCF calculation method.

RUNTYP
Select the calculation purpose.

COORD
Specifies the format of the molecular structure coordinates. It is linked to the $DATA coordinate format.

MAXIT
Specify the upper limit of the SCF calculation iteration number.

NZVAR
Specifies the number of internal coordinates. %NZVAR% is assigned 5000 if ZMAT contains DLC=.T. AUTO=.T., 3N-6 if RUNTYP=OPTIMIZE with IFREEZ and 1 numerator and 5 or more atoms, and 0 otherwise.

EXETYP
To specify whether or not to actually perform the calculation, specify CHECK to check the input.

NOSYM
Specify whether to use symmetry in calculation.

NPRINT
Specify the detail level of the output.

LOCAL
Specify the method of localization of the trajectory. (Default 0 = not)

PP
Specify Pseudopotential (Effective Core Potential, ECP).

DFTTYP
Specify the basis function system of the density functional theory method.

TDDFT
Specify whether energy calculation of excited state is performed using time-dependent DFT method

CITYP
Specify whether to perform placement interaction (CI) calculations.

CCTYP
Specify whether or not to perform combined cluster (CC) calculations.

ISPHER
Specifies whether the basis functions should be treated as Cartesian or spherical harmonic functions. (Default -1 = Cartesian)

MPLEVL
Specify whether to perform Moller-Plesset perturbation (MP) calculations.

Others
Fill in other keywords.

$BASIS

Basis Set
Specifies the base function system, reflected in GBASIS, NGAUSS, NDFUNC, NFFUNC, DIFFSP, and DIFFS.

GBASIS
Specify the base set of the base function system.

NGAUSS
Specify the number of Gaussian functions

EXTFIL
Read the basis function from an external file.

NDFUNC
Specify the number of added d-polarization functions

NFFUNC
Specify the number of added f-polarization functions

NPFUNC
Specify the number of added p-polarization function

DIFFSP
Specify whether to add sp-diffuse function

DIFFS
Specify whether to add s-diffuse function

Others
Fill in other keywords.

Advanced tab

$SYSTEM

timl
Specify calculation time limit (default 525600 minutes)

MWORDS
Specify memory usage (default 1 MW)

MEMDDI
Specify maximum summed memory usage for DDI. (Default 1MW)

Others
Fill in other keywords.

$SCF

DIRSCF
Specify whether to use direct SCF calculation method.

DAMP
We use Davidson damping to create Fock matrix.

CONV
Specify the threshold of density change at SCF convergence judgment. (Default 1.0D - 05)

Others
Fill in other keywords.

$GUESS

GUESS
Specify how to calculate the initial wave function.

Others
Fill in other keywords.

$STATPT

NSTEP
Specify the upper limit of the number of steps of structure optimization. (Default 20)

OPTTOL
Specify the threshold of the energy gradient. (Default 0.0001 Hartree/Bohr)

METHOD
Specify algorithm for structure optimization.

HESS
Specify how to obtain the Hessian matrix.

HSSEND
Specifies whether or not a Hessian matrix is desired at the end of the calculation.

Others
Fill in other keywords.

$FORCE

TEMP
Specifies the temperature (Kelvin) in thermodynamic data calculations. (default 298.15)

Others
Fill in other keywords.

Z-Matrix tab

Set "DLC=.T. AUTO=.T." if RUNTYP=OPTIMIZE, (# atoms)>5 & (# mols)=1
If checked, set %ZMATDLC%. Set %ZMATDLC% to "DLC=.T. AUTO=.T." if RUNTYP=OPTIMIZE without IFREEZ and with 1 numerator and 5 or more atoms.

DFT tab

$DFT

LC
Specify whether to perform long distance correction. (Only for BLYP, BOP and BVWN)

MU
Specify the value of long-distance correction parameter. (Default 0.33)

DC
Specifies whether Grimme's empirical dispersion force correction should be applied.

IDCVER
Specifies the version of Grimme's empirical dispersion force correction.

Others
Fill in other keywords.

$TDDFT

NSTATE
Specify the number of desired states (excluding the base state).

NRAD
Specify the number of grid points in the radial direction for deriving the derivative of density functional. (Default 48)

NLEB
Specify the number of lattice points in the angular direction. (Default 110)

Others
Fill in other keywords.

MP2 tab

$MP2

CODE
Specify the directory of the node used for calculation.

Others
Fill in other keywords.

Solvent tab

$PCM

SOLVNT
Specify the solvent.

SMD
Specify whether to use SMD (Solvent Model Density).

IEF
Specifies the type of PCM model.

ICAV
Specifies whether Cavitation energy should be calculated.

TABS
Specify temperature (Kelvin). (default 298.0)

Others
Fill in other keywords.

$PCMCAV

RADII
Specifies the type of cavity radius.

Others
Fill in other keywords.

IRC Tab

$IRC

FORWRD
Specifies forward or reverse direction.

PACE
Specify IRC calculation method.

NPOINT
Specify the number of IRC points.

MXOPT
Specify the maximum number of steps for structural optimization at each IRC point.

STRIDE
Specifies the distance between IRC points.

SADDLE
Specifies whether the structure of $DATA is a saddle point.

OPTTOL
Specifies the threshold value of the energy derivative to determine if a minimum point has been reached.

Comment tab
Fill in your comments.

Preview tab
A preview of the configuration keywords will be displayed.

Import $HESS
Import $HESS from the punch file.

Import $VEC
Import $VEC from the punch file.

Reset
Reset settings.

Import
Read the basis function from an external file.

Export
Output configuration file.

6.7.3 Import Keywords

Only keywords (calculation conditions) are read from the existing GAMESS input file.

6.7.4 (1) Run GAMESS, (2) Run GAMESS

If the input file of GAMESS is opened in the main window, execute GAMESS using that file. If it is not open, save the input file of GAMESS and execute GAMESS. When saving the input file, the atomic coordinate format of $DATA changes according to the setting of COORD in $CONTRL; for ZMTMPC, the format is MOPAC's Z-matrix format, otherwise it is Cartesian format. *(1) GAMESS run* , *(2) GAMESS run* are intended to be used with different versions of GAMESS, depending on the situation. The difference between *(1) Execute GAMESS* , *(2) Execute GAMESS* is the program path of GAMESS to be invoked. The program path used for each menu can be changed in *Tools* → *Preferences* → *Program Paths*. To use the external basis function file (: command: *$ BASIS EXTFIL = .T.*), Put `basis.lib` in the same directory as GAMESS's EXE file. For WinGAMESS, specify **`setenv EXTBAS ../ basis.lib`** in :file:` runscript.csh`. Following file will be generated with execution. As an example, the file/folder name when the input file is `water.inp` is also shown.

type	Description
out file `water.out`	Calculation log file.
bat file `water.inp.bat`	This is a batch file for running GAMESS.
pun file `water.pun`	It is a punch file for detailed result analysis.

The job is run through *Winmostar Job Manager*.

6.7.5 Open Log File (out/log)

Open the out file with a text editor.

6.7.6 Show log excerpts

Excerpts of key information from the out file.

6.7.7 Animation(Optimization)

Create and display animation such as structure optimization, scanning, IRC calculation, etc. from the out file information. For the animation display operation method, see *Animation operation area*.

6.7.8 Analyses

Molecular Orbitals, Charge

Retrieve and display molecular orbital and charge information from out file information Information on the charge read can be displayed in Viewport by selecting *View* → *Labels/Charges* → *Show Mulliken Charge* and so on. See *Energy Level Diagram window* , *Surface Setup / Cubgen window* for subwindow operation.

UV-Vis Spectra

Displays UV-Vis spectra from information in out files. See *UV-Vis Spectrum window* for subwindow operation.

NMR Spectra

Display NMR spectra from information in out file. See *NMR Window* for subwindow operation.

IR/Raman

Display vibration spectra (IR or Raman spectra) from the information in the out file. After loading the IR spectrum from the out file of `RUNTYP = HESSIAN`, if you subsequently read the out Raman spectrum of :command: *RUNTYP = RAMAN* in this menu, both spectra are displayed simultaneously in the subwindow can. Refer to *IR Spectrum Window* for how to operate the subwindow.

RESP Charges

Calculate point charge based on RESP method from punch file. The punch file to be loaded must be output from a calculation performed with the *RESP/ESP* setting selected in the *Preference* → *Easy Setup*. The spin multiplicity is treated with the assumption of 1. After being asked "Do you assign the same charge to an atom that is structurally equivalent to a molecule?", when you click *Yes*, it internally uses acpype, and when you click *No*, it internally uses AmberTools directly to calculate the RESP charge. Basically, it is recommended to click *Yes*, but in such cases, click *No*. It is expected that the results of both calculations will not change significantly. If you want to average the charges of structurally equivalent atoms (e.g. the three hydrogen atoms of a methyl group) after choosing *No*, use *Average the group's charge*. Note that Firefly is not supported by this feature.

Warning: To use this function, *CygwinWM setup* is required.

6.7.9 Edit PDB file

Editing of atom deletion etc. is done while leaving residue information etc. of PDB data etc.

6.8 *QM* → *Gaussian* menu

It is a menu about Gaussian. In order to use Gaussian you need to install Gaussian separately.

6.8.1 Workflow Settings

Sets up and executes the Gaussian computation flow in project mode. Local jobs in project mode will use the binary specified in *Gaussian* in *Tools → Preferences → Program Path*.

Preset
Recalls and saves a preset of settings.

# of Jobs
Specifies the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., when you open an SDF file). After the scan calculation is finished, use *File → Project → Scan Results* to tabulate the calculation results.

Import
Load the settings output by Export. Click the arrow to the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Run a calculation or generate a file with your settings. See *For project mode* for details.

Details
Set up detailed calculation conditions. The *Configure* will be launched.

Task
Specifies the type of calculation. Note that CHelpG charges are read as ESP charges when the log file is read.

	Configuration details
Energy	
Optimize	opt
IR	freq=noraman
IR+Raman	freq=raman
TDDFT	td=(nstates=10)
NMR	nmr
Optimize(TS)	opt=(ts,noeigentest,calcfc)
Optimize(TDDFT)	opt td
IRC(Forward)	irc=(forward,maxpoint=20,stepsize=5,calcfc) No pop designation
IRC(Reverse)	irc=(reverse, maxpoint=20, stepsize=5, calcfc) No pop designation
Optimize+IR	opt freq=noraman
Optimize+IR+Raman	opt freq=raman
Optimize(TS)+IR	opt=(ts,noeigentest,calcfc) freq=noraman
RESP	Pop=mk

Method
Specify the calculation method (Hamiltonian).

	Configuration details
HF	HF
Various DFTs	functional name (For DFT-D3) Empirical Dispersion=gd3
MP2	MP2

Basis set
Specify the set of basis functions.

Charge
Specify the value of the charge.

Multiplicity
Specify Spin multiplicity.

Solvent
Specify solvent type and solvent calculation method.

6.8.2 Configure

Set calculation conditions of Gaussian. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. Behavior when clicking *Run* is see *Run*. Return to the default state with *Reset* button. Save the current state as the default state with *Save as Default* button. Restore the default state to the factory condition with *Save as Default* → *Clear Default Settings*.

Easy Setup
Show the simple setting window.

%nprocshared
Specify the parallel number(Number of CPU cores used).

Link0

%Chk=file
Specify the checkpoint file.

%Mem=n
Specify the amount of dynamic memory in 8 bytes words. It is also possible to specify units of KB, MB, GB, KW, MB, GW. (Default: 800 MB)

Comment
Write a comment.

#

Specify the beginning of the route section.

#N

Output is done at the standard level. (Default)

#P

Perform detailed output. The execution time at the start and end of each link, and the information on convergence of SCF are output.

#T

Specify a concise output that only outputs important information and results.

Charge

Specify the value of the charge.

Multiplicity

Specify Spin multiplicity.

Additional Chg./Multi.

Specify additional charge and spin multiplicity.

Hamiltonian

Specify the Hamiltonian to use.

Ltd.

Perform Hartree-Fock calculation. Unless explicitly specified, RHF is used for singlet and UHF is used for higher multiplicity.

rhf

Restricted Hartree-Fock calculation is performed.

uhf

Unrestricted Hartree-Fock calculation is performed.

am1

We will perform semi-empirical calculations using AM1 Hamiltonian.

pm3

We perform semi-empirical calculation using PM3 Hamiltonian.

pm3mm

We perform semi-empirical calculations using PM3 Hamiltonian with molecular dynamics correction on HCON binding.

b3lyp

Compute the density functional method combining the Becke 3 functional with the LYP nonlocal correlation functional.

ub3lyp

Unrestricted version of b3lyp.

mp2

Following Hartree-Fock calculation, Moller-Plesset correlation energy correction up to the second order is performed.

ump2

It is an Unrestricted version of mp2.

mp4

Following Hartree-Fock calculation, Moller-Plesset correlation energy correction up to the fourth order is performed.

ump4
It is an Unrestricted version of mp4.

cis
Calculate the excited state using one-electron excitation CI.

cisd
Calculate the excited state using two electron excitation CI. (Synonymous with CI)

indo
We will perform semi empirical calculations using INDO Hamiltonian.

ondo
We will do semi-empirical calculations using CNDO Hamiltonian.

gvb
Perform general valence bond (GVB) calculation.

Basis
Specify the set of basis functions.

Pop
Control of molecular orbital output, electron density analysis, atomic charge distribution and so on.

none
It does not output molecular orbits and does not analyze electron density.

minimal
It outputs atomic charge and orbital energy.

regular
We output 5 occupied orbits and 5 virtual trajectories. Also output density matrix and Mulliken electron density analysis.

full
All occupied orbits and virtual trajectories are output. Also output density matrix and Mulliken electron density analysis.

mk
Output charge fitted to electrostatic potential in Merz-Singh-Kollman scheme.

chelp
Outputs charge fitted to electrostatic potential with CHelp scheme.

chelpg
Outputs charge fitted to electrostatic potential with CHelpG scheme.

(full,chelp)
Outputs charges fitted to the electrostatic potential in the CHelp scheme, all occupied orbitals and virtual orbitals. It also outputs the density matrix and Mulliken electron density analysis.

(fullchelpg)
Outputs charges fitted to the electrostatic potential in the CHelpG scheme, all occupied orbitals and virtual orbitals. It also outputs the density matrix and Mulliken electron density analysis.

(full,npa)
Outputs NBO (Natural Bond Orbital) charges by Natural Population Analysis, all occupied orbits and virtual orbits. It also outputs the density matrix and Mulliken electron density analysis.

OPT/IRC
Controls structural optimization or IRC calculations.

opt
Perform structure optimization.

opt=z-matrix
Structure optimization is performed with internal coordinates.

opt=modredundant
Add, delete, or modify the definition of redundant internal coordinates (including search and bound information). An input section is required after the structure specification.

opt=(ts,noeigentest,calcfc)
Optimize for transition state. We do not test curvature. Calculate the force constant for the first time.

opt=tight
Tighten the threshold for determining convergence of force and coordinate changes.

irc=(forward, maxpoint=20, stepsize=5, calcfc)
Tracks a forward reaction path. Specify the number of points on the path and the step size. Calculates force constants for the first time.

irc=(reverse, maxpoint=20, stepsize=5, calcfc)
Tracks the reaction path in the reverse direction. Specify the number of points on the path and the step size. Calculates force constants for the first time.

OptMaxCyc
Sets the maximum number of structural optimization steps.

Scrf
run the calculation with solvent effects.

SCF
Controls SCF calculations.

scf=tight
Convergence decision for normal SCF calculation. (Default)

scf=qc
Use second-order convergence method.

scf=xqc
If the first-order convergence method does not converge, switch to the second-order convergence method halfway through.

scf=vshift[=N]
Shifts orbit energy by N*0.001 Hartree, default value of N is 100.

Freq
Controls the calculation of force constants and frequencies.

freq
Calculate force constants and frequencies.

freq=raman
We calculate the Raman intensity in addition to the IR intensity.

freq=vcd
Calculate oscillating circular dichroism (VCD) intensity in addition to normal frequency analysis

freq=noraman
Only IR intensity is calculated and Raman intensity is not obtained.

freq=nraman

Calculate the polarizability derivative by numerically differentiating the analytical dipole derivative for the electric field.

freq=nnraman

Calculate the polarizability derivative by numerically differentiating the analytical polarizability on nuclear coordinates.

NMR

Controls NMR calculations.

nmr

Perform NMR calculations.

nmr=giao

Perform NMR calculations using the GIAO method. (Default)

nmr=csgt

NMR calculations using the CSGT method.

nmr=igaim

Perform NMR calculations using atomic center coordinates as gauge origin.

TD

td

Calculate excited state energies using the time-dependent Hartree-Fock or DFT method. (default singlet).

td=(nstates=n)

For the n states, we obtain the energy of the excited state using the time dependent calculation method. (Default 3)

td=50-50

Half of the states are calculated as singlet and the other half as triplet. Valid only for closed-shell systems.

td=triplets

Calculate the triplet state. Valid only for closed-shell systems.

EmpiricalDispersion

Enable empirical dispersion power.

pfd

Add Petersson-Frisch dispersion power.

gd2

Add D2 version of Grimme dispersion force.

gd3

Add D3 version of Grimme dispersion force.

gd3bj

Add D3 version of Grimme dispersion force with Becke-Johnson damping.

Config ONIOM

Set up ONIOM calculation. You must have assigned each atom to a layer with beforehand.

Hamiltonian

Set the Hamiltonian for each layer.

Basis

Sets the basis function for each layer.

gfinput
Outputs the basis function system in the same format as the input format.

gfprint
It outputs the basis function system in tabular form.

nosymm
Do not reorient the coordinates, run the calculation with the input orientation.

guess=read
Read initial wave function from checkpoint file

geom=check
Fetch the molecule specification section from the checkpoint file.

fchk
Create the Test.FChk file.

counterpoise
Perform a counterpoise calculation. The fragment number set for each atom is assigned the residue number on Winmostar. Note that the *Assign different residue numbers to each molecule.* function can be used to assign different residue numbers to each molecule at once.

Subsection
Fill in other keywords.

Coordinate format
Specifies the format of the atomic coordinates (Cartesian or Z-matrix).

Reset
Reset settings

Import
Output configuration file.

Export
Output the Cube file.

6.8.3 Import Keywords

Only keywords (calculation conditions) are read from the existing Gaussian input file.

6.8.4 Run

If Gaussian's input file is opened in the main window, use Gaussian to execute it. If it is not open, save the Gaussian input file and run Gaussian. Gaussian's program path can be changed with:: menuselection: *Tools –> Preferences –> Program Path*. Following file will be generated with execution. For example, the file/folder name when the input file is: file: *water.gjf* is shown together.

type	Description
log file `water.log`	Calculation log file.
bat file `water.gjf.bat`	It is a batch file for running Gaussian.
Working folder `water_gau_tmp\`	Working folder.

The job is run through *Winmostar Job Manager*.

6.8.5 Open Log File (log/out)

Open the log file with a text editor.

6.8.6 Animation

Optimization

Creates and displays animation of structural optimization calculation from information of log file. For the animation display operation method, see *Animation operation area*.

IRC/modred

Creates and displays animation of IRC calculation from information of log file. For the animation display operation method, see *Animation operation area*.

6.8.7 Analyses

Molecular orbitals, Charge

Retrieve and display molecular orbital and charge information from log file information Information on the charge read can be displayed in Viewport by selecting *View* → *Labels/Charges* → *Show Mulliken Charge* and so on. See *Energy Level Diagram window* , *Surface Setup / Cubgen window* for subwindow operation.

UV-Vis Spectra

Displays UV-Vis spectra from log file information. Refer to *IR Spectrum Window* for how to operate the subwindow.

See UV-Vis Spectrum window for subwindow operation.

Display NMR spectra from log file information. See *NMR Window* for subwindow operation.

IR/Raman

Displays vibration spectra (IR or Raman spectra) from information in the log file. Refer to *IR Spectrum Window* for how to operate the subwindow.

RESP Charges

Calculate the point charge based on the RESP method from the esp file. The esp file to be read must have been output from a calculation performed by selecting *RESP/ESP* in *Configure* → *Easy Setup*. Spin multiplicity is assumed to be 1. Internally, RESP charge is calculated using Antechamber. To use this function, you need to use G09.C.01 or later version; if you use the version before G09.C.01, you need to change the IOP.

Warning: To use this function, *CygwinWM setup* is required.

Assigning ONIOM layers

Show Layer Flags
Displays the flags for the layers assigned to each atom.

Unset Layers for All Atoms
Delete flags for all atom layers.

Select Atoms in High/Middle/Low Layer
Group selection of atoms set to High/Middle/Low Layer, used to confirm atoms set to High/Middle/Low Layer.

Set Selected Group to High/Middle/Low Layer
Set the atom of the selected group to High/Middle/Low Layer.

Select All
Group selection of all atoms.

Select None
Deselect group selection.

6.8.8 FormChk

Launch Formchk in the G16W, G09W, and G03W utilities to create and display formatted .fch files from .chk files.

6.8.9 Import Fchk (Cubegen) File

Run Cubegen from the G16G, G09W, or G03W utility and create a Cube file by reading the .fch file. If Cubegen is not available, use Winmostar's built-in OpenCubegen. For how to operate the subwindow, please refer to *Surface Setup / Cubgen window* and the following.

Property

- **MO**
  Molecular orbital
- **Density**
  Electron density
- **ESP**
  ESP
- **Spin**
  Spin density (alpha - beta)
- **Alpha**
  alpha spin density
- **Beta**
  beta spin density
- **Current Density**
  Current Density
- **Shielding Density**
  Shielding Density

Type
Specify the option of the Density keyword. (HF, MP 2, CI, QCI)

Cube
Output the Cube file.

OpenCubegen supports fchk files up to approximately 2 GB. The upper size limit depends on the molecule size and basis functions. We plan to remove the fchk file size limitation in the future.

6.8.10 Import Cube File

Read and display the Cube format file. For GAMESS pun file, convert it to Cube file. For how to operate the subwindow, please refer to *Surface Setup / Cubgen window* and the following.

cube Manipulation
Perform operations on cube files specified in *File 1* and *File 2*.

- **map**
  Map the data in the lower column to the data in the upper column. (Example mapping ESP to Density)
- **subtract**
  We will cover the difference between the data of the two cube files.

sub 2
We will cover the difference between the squares of the data of two cube files.

add
We will cover the sum of two cube files.

Cube
The calculation result of the cube file targeted by Map is output and displayed.

Cubegen
Start Cubegen, read the fch file and create a Cube file. For details, see *Import Fchk (Cubegen) File*.

6.9 *QM* → *NWChem* menu

It is a menu related to NWChem.

6.9.1 How to set up NWChem

To install NWChem, install CygwinWM after the 2023/04/05 version, which contains `nwchem.exe` in `/opt_win/NWChem*/bin/` of CygwinWM. To run MPI parallel calculations, install MPICH according to the NWChem for Windows Installation Manual. The configuration for using NWChem from Winmostar is done at *Tools → Preferences menu*. If you have newly installed Winmostar V11.5.0 or later and are using CygwinWM 2023/04/05 version or later, no configuration is required. First, under *Program Path → NWChem*, select `nwchem.exe` for the NWChwm you want to use. Next, under *Calculation → mpiexec (NWChem)*, select *MPICH* or *Select* and select `mpiexec.exe` for the MPI you are using. If you want to use NWChem stored in CygwinWM, select *MPICH*. Finally, in *Calculation → Options for mpiexec (NWChem)*, enter the argument for **`mpiexec.exe`**, which does not need to be changed if you use NWChem in CygwinWM. How to install NWChem on a remote machine is described in *Installing Winmostar and solvers*.

6.9.2 Workflow Setting

Sets up and executes the Gaussian computation flow in project mode. Local jobs in project mode use the binary specified in *NWChem* of *tools → preferences → program path*.

Preset
Load and save a preset of settings..

# of Jobs
Specify the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It is possible to run multiple calculations in which only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each line of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File → Project → Parameter/Structure Scan Results* to tabulate the calculation results.

Import
Loads the settings output by Export. Click the arrow to the right of the button to recall settings previously used in the same project or on Winmostar.

Export
Output configuration file.

OK
Runs a calculation or generates a file with your settings. See *For project mode* for details.

Details
Set up detailed calculation conditions. The *Configure* will be launched.

Task
Specifies the type of calculation.

	Configuration details
Energy	task energy
Optimize	task optimize
IR	task frequencies
IR+Raman	task raman property response 1 8.8559E-2
TDDFT	task tddft energy notriplet nroots 10 Noautosym True
NMR	task energy task property property shielding
Optimize(TS)	task saddle
Optimize(TDDFT)	task tddft optimize notriplet civecs nroots 10 grad root 1 Noautosym True
Optimize+IR	task optimize task frequencies
Optimize(TS)+IR	task saddle task frequencies
NEB	task neb No Mulliken No Dipole

Method

Specify the calculation method (Hamiltonian).

	Configuration details
HF	task scf
Various DFT	XC Functional name (for DFT-D3) Disp vdw 3

Basis set

Specifies the basis function.

Charge

Specify the charge.

Multiplicity

Specify the DFT spin multiplicity.

Solvent

Specify the solvent type.

6.9.3 Configure

Set calculation conditions of NWChem. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. Behavior when clicking *Run* is see *Run*. Return to the default state with *Reset* button to.

Easy Setup

Show the simple setting window.

Use MPI

When checked, MPI is used. Enter the parallel number next to the checkbox.

Basic Tab

Start-up mode

Use “start” to start a new calculation, or “restart” to continue from a calculation that has already been performed.

Title

Specify the title.

Memory

Specify the memory usage.

Basis

Specify the basis function system. Choose cartesian/spherical. Specify exception for some atoms with Exception.

Task
Specify the calculation method (theory) and calculation purpose (operation).

Charge
Specify the charge.

DFT

- **Multiplicity**
  Specify the DFT spin multiplicity.
- **XC**
  Specifies the exchange-correlation functional of the DFT..
- **cam**
  Specifies a long-distance correction.
- **Disp**
  Specify empirical dispersion force correction.

SCF

- **Multiplicity**
  Specify the SCF multiplicity.
- **Wave Function**
  Specify the calculation theory of SCF.

Property

- **Mulliken**
  Mulliken Select whether to output electric charge.
- **Shielding**
  Select whether to perform NMR calculation.
- **Dipole**
  Select whether to output dipole moment.

Advanced tab

Set tolguess
Specify the precision of initial guess.

ECP
Specify the potential of ECP.

Driver (Optimize)

- **MaxIter**
  Specify the maximum number of iterations for optimization.
- **Convergence**
  Specify the precision of structural optimization.
- **Others**
  Describe other input elements.

Geometry

- **noautoz**
  Set not to convert internal coordinates.
- **noautosym**
  Set to not use symmetry.

Symmetry
Specify the symmetry.

Others
Describe other input elements.

SCF/DFT

MaxIter
Specify the maximum number of cycles for SCF/DFT energy calculation.

Direct
Specify Direct calculation (2-electron integrals are calculated each time).

Others
Describe other input elements.

Solvent tab

COSMO

Solvent
Specify the solvent type.

Dielec
Specifies the dielectric constant of the solvent.

Ificos
Specifies how the solvent area is divided.

do_cosmo_smd
Configures the use of the SMD method.

do_gasphase
Sets whether the gas phase is calculated before the solvent calculation.

Others
Describe other input elements.

TDDFT tab

NOSINGLET
Sets whether or not to calculate the excited singlet.

NOTRIPLET
Sets whether or not to calculate the excited triplet.

CIVECS
Specifies saving of CI vectors to a file.

Nroots
Specifies the number of excited states to be calculated.

Target
Specifies the solution number of the target's excited state.

TargetSym
Specifies the symmetry of the target's excited state.

Grad Root
Specifies the solution number of the target excited state for the TDDFT derivative calculation.

Others
Describe other input elements.

NEB/String tab

It becomes effective when neb or string is specified as Operation of Task.

NBeads

Specify the number of beads.

KBeads

Specify the spring constant of NEB.

MaxIter

Specify the maximum number of iterations for optimization.

StepSize

Specify the optimization step size.

NHist

Specify the number of histories to use in the quasi-Newton method.

Freeze1

Set whether to fix the first bead with ZTS.

FreezeN

Set whether to fix the last bead with ZTS.

Convergence

Choose the convergence condition from loose/default/tight.

XYZ_Path

Specifies the initial path file. Used for restarting calculations, etc.

Print_Shift

Output paths for each step you specify.

EndGeom

Specify the coordinates of the last bead. You can specify a file by loading it with the Load button. Load format that can be read with Winmostar in XYZ format. You can also edit with the Edit button.

Others tab

Other Settings

Describe other input elements.

Coordinate format

Specifies the format of the atomic coordinates (Cartesian or Z-matrix).

Reset

Reset settings.

Import

Loading configuration file.

Export

Output configuration file.

6.9.4 Import Keywords

Only the keyword (calculation condition) is read from the existing NWChem input file.

6.9.5 Run

If NWChem's input file is open in the main window, use NWChem to execute the file. If it is not open, save the input file of NWChem and run NWChem. The program path of NWChem can be changed with *Tools → Preferences → program path*. Following file will be generated with execution. For example, the file/folder name when the input file is: file: *water.nw* is shown together.

type	Description
out file `water.out`	Calculation log file.
movecs file `water.movecs`	It is a file that summarizes detailed information of calculation.
bat file `water.bat`	It is a batch file for running NWChem.
Working folder `water.nw_temp\`	Working folder.

The job is run through *Winmostar Job Manager*.

6.9.6 Open Log File (out)

Open the out file in a text editor.

6.9.7 Animation

Optimization

Create and display animation such as structure optimization from the out file information. For the animation display operation method, see *Animation operation area*.

NEB/String

Create and display NEB, String calculation animation from xyz file information. For the animation display operation method, see *Animation operation area*.

6.9.8 Analyses

Molecular Orbitals, Charge

Retrieve and display molecular orbital and charge information from out file information Information on the charge read can be displayed in Viewport by selecting *View* → *Labels/Charges* → *Show Mulliken Charge* and so on. See *Energy Level Diagram window* , *Surface Setup / Cubgen window* for subwindow operation.

UV-Vis Spectra

Displays UV-Vis spectra from information in out files. Refer to *IR Spectrum Window* for how to operate the subwindow.

NMR Spectra

Display NMR spectra from information in out file. See *NMR Window* for subwindow operation.

IR/Raman

Display vibration spectra (IR or Raman spectra) from the information in the out file. Refer to *IR Spectrum Window* for how to operate the subwindow.

6.10 MD menu

It is a menu on the molecular dynamics method. Also, with almost every feature *CygwinWM* is required.

6.10.1 Solvate/Build Cell

This function is mainly used for the following two purposes.

1. Arrange solvent molecules around the molecules displayed in the main window
2. Create liquid phase by arranging low molecules

There are three kinds of molecules that can be arranged as follows.

- Molecule displayed in the main window
- Molecules preserved in mol 2 format
- water molecule

A working folder with `_builder_tmp` added to the end of the current file name is created, and processing using Packmol is performed in that folder. Details are described in `packmol.bat` and `packmol.log` under the working folder. `output.pdb` under the working folder is the file containing the final generated molecular structure.

Add Displayed Molecule
Add molecules displayed in the main window. After pressing the button, enter the number of molecules to be added. If only one is placed, other molecules are aligned with the coordinates fixed for the molecules displayed in the main window.

Add File
Add molecules from a previously saved molecular structure file to the system. After pressing the button, specify the location of the file and enter the number of molecules to add. If the number of molecules to be added is 1, specify whether the molecules are to be placed randomly or fixed to the coordinates written in the file. When placing a ligand molecule cut from a PDB file, the placement is usually fixed. When performing MD calculations using point charges (RESP charges, etc.) obtained from QM calculations, etc., the file specified here must contain information on the point charges. The point charge information can be maintained in mol2, wmm, or other formats.

Add SMILES
Specify the type of molecules you want to arrange in SMILES format.

Add Water
Add water molecules to the system. After pressing the button, enter the number of molecules to be added. The water molecule model is selected from *Water Model* in *Options* tab.

Delete
Deletes the selected item in the above list.

Simulation Cell

Set Density
Specify the density of the simulation cell to be created. If it is too large, you may not be able to insert the molecule sufficiently, so in case of liquid phase it is usually set to about 0.5~0.8 g/cm ^{3}.

Set Margin from Solute
When choosing *Solvate* for *Method*, specify the distance between the molecule displayed on the main window and the simulation cell.

Set Lattice Constants
Specify the size of the simulation cell directly. When you press : guilabel:*Same as main window* button, the same value as the cell set in the main window is entered.

Same as main window
Sets the lattice constant of the cells displayed in the molecular display area.

Change only one direction
Used to move one lattice constant to the specified density while keeping two lattice constants fixed. It can be used by selecting triclinic in *Box Type*. This is especially useful when creating interface structures.

Box Type
Specify the shape of the simulation cell.

Option

Water Model
Specify the water model added by *Add Water*. The coordinate data of the specified water model will be quoted from the library of the topology file installed in Gromacs on Cygwin.

Packmol Parameters

Tolerance

Specify tolerance parameter of Packmol.Specifies the minimum distance between atoms.

Tolerance(Fixed)

Specifies the minimum distance between atoms and the tolerance parameter in Packmol for molecules with Fixed Position. This is useful when you do not want to place solvent in a slab or protein.

Margin

Specify the width of the area where no atoms are placed near the edge of the cell when using Packmol.

Random seed

Specify the seed of random number when using Packmol.

Do not rotate

Align molecules without changing their orientation. It is intended for the creation of nematic liquid crystal phases, etc.

Automatically change random seed every time

The seed of random number when using Packmol is automatically changed every time.

Use PBC if Margin=0 and Packmol supports it

When using CygwinWM 2025/7/1 version or later, if Margin is 0, the molecules are placed considering the periodic boundary condition. If not checked, there will be no molecules that straddle cell boundaries. This feature is not available for Packmol in CygwinWM prior to the 2025/7/1 version.

SMILES converter

Specify the program to use when turning SMILES entered in Add SMILES into a 3D structure.

Shift origin to cell center

Sets the origin to the center of the cell.

Reset

Resets the settings in this window.

Build (Multi)

Create simulation cells according to the settings in this window. Multiple patterns are generated with different random seeds. The random seed used is the value of *Random seed* in the first structure, the value of *Random seed* plus one in the second structure, and the value of *Random seed* plus two in the third structure. The third structure uses the value of *Random seed* plus two (as below). This is useful to increase the number of samplings by performing multiple MD calculations with different initial coordinates using the structure scan.

Build

Create a simulation cell according to the contents set in this window.

6.10.2 Insert Molecules

You can add multiple molecules stored in mol 2 format to the structure displayed in the main window. If no simulation cell has been created, create it with *Create/Edit Cell* or *Solvate/Build Cell* beforehand. If you want to add only one additional molecule without changing the coordinates, please select *Import File*. Basic operation is the same as *Solvate/Build Cell*.

6.10.3 Assign Charges Automatically

Automatically assign charges to multiple molecules. A working folder with `_charge_tmp` at the end of the current filename is created and processed. See *Use AM1-BCC/Gasteiger charges* , *Use RESP charges* , *Use OPLS-AA charges* for more details.

Set … for all components
If checked, charges will be calculated for all molecular species displayed in the main window using the method specified in the pull-down menu. If unchecked, select a Method for each atomic species.

Except for components that are already charge
If checked, even if *Set … for all components* is checked, no new charge will be assigned to molecules that have already been assigned.

Except for protein, monoatomic ion and water
When checked, no charge is assigned to proteins, monatomic ions, and water molecules in this function. In the MD calculation of proteins, it is necessary to check the box because it takes time to calculate the charge by methods such as AM1-BCC and the charge is automatically assigned from the residue name when assigning the force field.

Method
Select the method to assign the charge.

Charge
Set the charge for that molecular species. The charge is specified as 0 for neutral molecules and +1, -1 for ions.

6.10.4 Assign Charges Manually

Use AM1-BCC/Gasteiger charges

Calling this function while only one molecule is displayed in the main window allocates point charge to each atom by AM1 - BCC or Gasteiger method. Internally I use the Acpype program on Cygwin. It is used when creating a file in mol 2 format to be inserted by charge allocation of solute molecules or *Solvate/Build Cell* or *Insert Molecules*. When allocating charge to non-neutral polyatomic ions, it is necessary to use RESP charge or this function. For polyatomic ions, enter the charge into *Total charge [e]*. A working folder with the `_acpype_tmp` appended at the end of the current file name is created and processed in that. Details are listed on `temp.sh`, `temp.log` under working folder. The value of the charge written in the working folder below `input.acpypeinput_GMX.itp` will be the result.

Use RESP charges

Calculate RESP charge using GAMESS. See *RESP Charges* for details. The GAMESS keywords (including basis functions and calculation methods) and the number of parallels are set in the *Tools → Preferences menu Keywords for automatic RESP charge calculation (GAMESS)* and :guilabel:` Number of parallels for automatic RESP charge calculation with GAMESS` on the *Calculation* tab of the *Calculation*.

Use OPLS-AA charges

Use mktop to calculate OPLS-AA charges

6.10.5 Polymer

See *MD → Polymer Menu*.

6.10.6 Interface Builder

See *MD → Interface Builder menu*.

6.10.7 Replace Molecules

Replaces all molecules of the specified molecular species with other molecules. Please save the newly placed molecule (one molecule) in wmm or mol2 format before calling this function.

6.10.8 Generate Ions

Replace water molecules with monoatomic ions. It is necessary to arrange water molecules in the system in advance. To place water, use *Solvate/Build Cell*. It is mainly used to neutralize the charge in the system in protein systems. Internally run **`gmx genion`** on Cygwin.

Neutral
In the case of *True*, we arrange the ions so that the charge of the whole system becomes neutral, and *Number of Cations* and *Number of Anions* are ignored. In the case of *False*, the number of ions described in *Number of Cations* and *Number of Anions* are respectively allocated.

Concentration
Specify the concentration of ion to be substituted.

Cations/Anions
Specify the type of cations and anions from the pulldown.

Number of Cations/Number of Anions
Specify the number of cations and anions. This setting is valid when *Neutral* is *False*.

Execute
Run **`gmx genion`** on Cygwin. A working folder with the file name `_genion_tmp` at the end of the current file name is created and processed in that. Details are described in `temp.sh`, `temp.log` under the work folder. On the way, automatic creation of a temporary topology file (`temp.top`) may fail if the molecules in the system are inappropriate. Details of the topology file creation are output in `temp_top_tmp` in the working folder.

6.10.9 LAMMPS

See *MD → LAMMPS menu*.

6.10.10 Gromacs

See *MD → Gromacs menu*.

6.10.11 MODYLAS

MODYLAS Configure, calculation execution, animation display, energy display. Basically it behaves similarly to *MD → Gromacs menu*.

6.11 *MD → Polymer* Menu

The procedure for preparing the polymer system is as follows.

1. Model the repeat unit and execute *Register repeat unit*.
2. Register the polymer using the monomer registered in 1 *Homo Polymer builder*, *Block Polymer Builder*, *Random Polymer Builder*.
3. In the *Polymer Cell Builder*, construct the cell using the polymer registered in 2.

If you want to create a low molecular-polymer mixed system, create a polymer system by the above procedure and then add low molecules with *Insert Molecules*.

6.11.1 Register repeat unit

register the repeat unit to use at *Homo Polymer builder*, *Block Polymer Builder*, *Random Polymer Builder*.The file is saved with the extension `wmo` in the save destination of the monomer file set by *Settings*. The `wmo` file is a mol2 file with Winmostar's own comment added.

1) Create the structure of the repeat unit you want to register in the main window.
2) Left click on Head and Tail 2 atoms, red circle's *marker*, and call this function.

[Head], [Tail]

The number of the selected Head atom and Tail atom is displayed.

[OK]

Enter a registration name for the repeating unit, register the repeating unit and close the window. A monomer file will be created.

[Cancel]

Discard the settings and close the Register Monomer window.

6.11.2 Homo Polymer builder

Create a homo polymer for use with *Polymer Cell Builder* from the repeat units registered with *Register repeat unit* and register. It is stored in the save destination of the polymer file set with *Settings* with `wpo` extension. The `wpo` file is a mol2 file with Winmostar's own comment added. The charge of the whole polymer is the product of the charge of the monomer (repeat unit) used and the degree of polymerization. Charges for atoms deleted by polymerization are equally allocated to the atoms of the whole polymer.

[Degree of Polymerization]
Specify the degree of polymerization.

[Repeat Unit]
Display selected repeat units.

[Display]
Display selected repeat units.

[Delete]
Delete the selected monomer file.

[Tacticity]

[Isotactic]
Make an isotactic polymer.

[Syndiotactic]
Make a syndiotactic polymer.

[Atactic]
Make atactic polymer.

[Racemo Ratio]
When selecting an atactic polymer, specify the racemism rate (0 <x <1.0).

[Head/Tail Configulation]

[Head to Tail]
Combine the head atom of the repeat unit and the tail atom by overlapping.

[Head to Head]
Combine the Head and Head atoms of the repeat unit. Also, combine the Tail and Tail atoms of the monomer.

[Build]
Register the polymer. A polymer file is created.

[Close]
Close the window.

6.11.3 Block Polymer Builder

Create a block polymer for use with *Polymer Cell Builder* from the monomers registered with *Register repeat unit* and register it. It is stored in the save destination of the polymer file set with *Settings* with `wpo` extension. The `wpo` file is a mol2 file with Winmostar's own comment added. The way to assign electric charge is the same as *Homo Polymer builder*.

[First Repeat Unit]
Select the first repeat unit from list.

[Last Repeat Unit]
Select the last repeat unit from the list.

[Middle Repeat Unit]
Select an intermediate repeat units from the repeat unit list. In [Number], enter the number of repeating.

[>>Add>>]
Registers the selected repeat unit in the list.

[<<Delete<<]
Delete selected items from list.

[Display]
Display selected repeat units.

[Delete]
Delete selected repeating units.

[Build]
Creates a polymer based on the contents of the list. A polymer file will be created.

[Close]
Close the window.

6.11.4 Random Polymer Builder

Create a random polymer for use with *Polymer Cell Builder* from the monomers registered with *Register repeat unit* and register it. It is stored in the save destination of the polymer file set with *Settings* with `wpo` extension. The `wpo` file is a mol2 file with Winmostar's own comment added. The way to assign electric charge is the same as *Homo Polymer builder*.

[Degree of Polymerization]
Specify the degree of polymerization. Enter the number including the beginning and the end.

[First Repeat Unit]
Select the first repeat unit from the list. If you want to assign the first repetition unit randomly, leave blank.

[Last Repeat Unit]
Select a tail repeat unit from the list. If you want to assign the tail repeat unit randomly, leave it blank.

[Middle Repeat Unit]
Select an intermediate repeat unit from the list.

[>>Add>>]
The set repeat unit name and occurrence rate (0 < x < 1.0) will be reflected in Middle Repeat Unit.

[<<Delete<<]
Delete selected items from list.

[Display]
Display selected repeat units.

[Delete]
Register the set repeting unit name and occurrence rate (0 < x < 1.0) in the list.

[Sum of Ration]
The total value of the ratios listed in the Internal repeat unit List is displayed.

[Definition of Ratio]

[Probability of Each Monomer]
Generate intermediate repeat unit according to appearance rate [Add]. The ratio of the final intermediate repeat unit does not necessarily correspond to the appearance rate.

[Proportion in Total Monomers]
The ratio of finally obtained intermediate repeat unit is proportional to the appearance rate [Add].

[Number of Patterns]
Specifies the number of patterns of polymers.

[Use Specific Random Seed]
If you want to use a specific random number type, check the box and specify the value. If not specified, you will get a pattern with a different structure.

[Build]
Create polymers based on the contents of the listings. Polymer files will be created under the polymer name folder for the number of patterns.

[Close]
Close the window.

6.11.5 Polymer Cell Builder

Build a simulation cell using the polymer registered in *Homo Polymer builder*, *Block Polymer Builder*, and *Random Polymer Builder*. When using *Solvate/Build Cell*, it is difficult to create each molecule rigidly in the simulation cell, so it is difficult to create polymers with high density. However, when using this function, while executing energy minimization calculation using LAMMPS It can be created at a relatively high density for placement. The internal process is as follows

1. Place each polymer in a straight line.
2. Only the main chain of each polymer is extracted for structural optimization.
3. Structure optimization is performed by adding side chain atoms that can be added to the extent that each atom is not in contact with each other.
4. Repeat 3 until all atoms have been added.

[Polymer Available]

[Display]
Show the selected polymer.

[Delete]
Delete the specified polymer file.

[>>Add>>]
The selected polymer is reflected in the Polymers Used list.

[<<Delete<<]
Remove the selected polymer from the Polymers Used list.

[Simulation Cell] tab

[Set Density]
Specify the density.

[Set Dimensions]
Specify a cube cell.

[Cubic Cell]
Specifies the length of a rectangular cell in each direction.

[Periodic Boundary Condition]

[X],[Y],[Z]

Toggle in the direction that imposes periodic boundary condition.

[Options] tab

[MPI]

LAMMPS used for optimization at creation runs in MPI parallel.

[Processes]

Specify number of MPI ranks.

[Non-bonded inter-atomic distance tolerance]

Specifies the minimum allowable distance between unbonded atoms. If it cannot be created with the specified tolerance, it will gradually reduce the tolerance, so it may not always be within the tolerance. Changes of the tolerance are output to the log.

[Randomly select random polymers to be used]

For Random Polymer, randomly select the polymer to be used. If it is not checked, use them in order.

[Use Specific Random Seed]

If you want to use a specific random number seed, check the box and specify the value. If not specified, you will get a different structure each time.

[Do not twist each polymers]

Place each polymer in a straight line.

[Build]

Create a simulation cell.

[Close]

Close the window.

6.11.6 Map Repeat Unit

We allocate registered repeat units to DPD particles and acquire the molecular structure of all atoms MD.

6.11.7 Settings

Specify the folder to register the monomer and polymer.

[Monomer(*.wmo) Folder]

Specify the folder to save the monomer file.

[Polymer(*.wpo)Folder]

Specify the folder to save the polymer file.

[OK]

Save the settings and close the window.

[Cancel]

Discard the settings and close the window.

6.12 *MD → Interface Builder* menu

Join the two simulation cell files (mol2 or cif format) prepared in advance to create an interface model. *Tools → Preferences menu* allows you to switch between the new and old features. The features of the new spec are as follows

Cell Tab

Specify the two phases (Cell1 and Cell2) across the interface.

Use displayed cell

Specify the model displayed in the main window as a phase.

Load from file

Loads models from structural files in various formats and specifies them as phases.

Direction Tab

Axis perpendicular to interface

Specifies the axis in the vertical direction of the interface.

Order

Specify the order of Cell1 and Cell2 joined.

Interval

Specify the interval between Cell1 and Cell2.

Specify interval between cell boundaries

The entered value is the distance between cell boundaries.

Place atoms on cell boundaries on both sides

If checked, the atoms placed just above the cell boundary are copied and placed on both sides of the interface vertical. If *Axis perpendicular to interface* is c-axis, atoms with a fractional coordinate of 0 or 1 on the c-axis (or z-axis in the case of a rectangular cell) are copied to position 1 or 0 respectively.

Specify interval on selected axis between outermost atoms

The specified value is the *Axis perpendicular to interface* is the distance between the outermost atoms on the selected axis.

Adjusting cell size parallel to interface

Specifying how to adjust the horizontal cell size of the interface

Scaling cells to average size

Doing Affine deformation so that the horizontal cell size of the created interface model is the average of the cell sizes of Cell 1 and Cell 2.

Scale to size of…

Doing Affine deformation of the atomic positions to match the selected cell size to the other cell size.

Extend size of smaller cell while keeping atomic positions

The atomic positions are not changed, but the smaller cell size is changed to the larger cell size.

Repeat Tab

Number of cells

Specify the number of supercells in Cell 1 and Cell 2 when creating the interface model. Clicking the *Suggest* button and the ratio of the cell size is shown for the numbers of Cell1 and Cell2. It is recommended to choose a combination for which *Ratio* close to 1.

Operation for atoms outside each cell
Specify how to handle atoms that are located outside the cell.

Wrap for each molecule
Molecules are moved inside the cell taking into account the periodic boundary.

Wrap for each atom
Atoms are moved inside the cell taking into account the periodic boundary.

Do nothing
Do nothing

Build button
The interface model is created based on the settings.

The features of the previous version are as follows

Cell Files
Specify the information of the two cells (Cell 1 and 2) to be joined. After setting each item, click the [Next] button.

Cell 1 and Cell 2

[Browse]
Specify the file (mol 2 or cif format) to be joined. It is also possible to specify files by dragging and dropping them.

[Lattice Constants]

[a],[b],[c],[Alpha],[Beta],[Gamma]
The cell constant is displayed.

Direction
Specify the direction to join the cells and the spacing between the cells. After setting each item, click the [Next] button.

Direction

[a-axis]
Combine two cells along the a-axis direction.

[b-axis]
Combine two cells along the b-axis direction.

[C-axis]
Combine two cells along the c-axis direction.

Order

[Normal]
Place Cell 2 on Cell 1.

[Reverse]
Overlay Cell 1 on Cell 2.

[Interval]
Specify the interval between cells. It is not the distance between the two sides but the length along the axis.

[Scaling cells to average size]
If there is a difference in cell size, it stretches to the average size.

[Padding small cell to the size of large cell]

If there is a difference in the size of the cell, put a vacuum in the smaller cell and align it with the larger cell.

Repeat

Specify the number of repeats for each cell. Finally click the [Build] button.

Number of Cell 1 and Cell 2

[a-axis]

Specify the number of reports in cell 1 or cell 2 in the a-axis direction.

[b-axis]

Specify the number of repeats in cell 1 or cell 2 in the b axis direction.

[C-axis]

Specify the number of repeats in cell 1 or cell 2 in the c-axis direction.

[Suggest]

We will present a combination of repeat numbers so that Cell 1 and Cell 2 are closer in size. The combination with Ratio close to 1 reduces the distortion of both cells. Click on the column and press the Set button, or double-click it to take effect.

Lattice Constrants

[a],[b],[c],[Alpha],[Beta],[Gamma]

The lattice constant of the cell after bonding is displayed.

[Build]

Save the joined cells. Processing time may be prolonged if the size of the system is large.

6.13 *MD → LAMMPS* menu

It is a menu related to LAMMPS.

6.13.1 How to set up LAMMPS

To install LAMMPS, install CygwinWM version 2023/04/05 or later, which contains `/opt_win/LAMMPS*/bin/` in `lmp_serial.exe` and `lmp _mpi.exe` and so on. The configuration for using LAMMPS from Winmostar is done at *Tools → Preferences menu*. If you have newly installed Winmostar V11.5.0 or later and are using CygwinWM 2023/04/05 version or later, no configuration is required. First, select the LAMMPS `lmp_serial.exe`, `lmp_mpi.exe` or `lmp.exe` to use with *program path → LAMMPS*. (When you select `lmp_serial.exe` to run MPI, the `lmp_mpi.exe` in the same folder is automatically used.) Next, under *Calculation → mpiexec (LAMMPS)*, select *MPICH* or *Select* and choose the MPI `mpiexec.exe` you want to use. If you want to use LAMMPS stored in CygwinWM, select `/opt_win/MSMPI/Bin/mpiexec.exe` under CygwinWM. Finally, at *Calculation → Options for mpiexec (LAMMPS)*, enter the arguments for **`mpiexec.exe`**. If you use LAMMPS in CygwinWM, enter **`-np %WM_NUM_PROC%`**. If you want to add a potential file, click *Tools → Preferences menu → Calculation → MD → LAMMPS potential folder → Open potential directory* and in the opened folder Add potential files to the opened folder. How to install LAMMPS on a remote machine is described in *Installing Winmostar and solvers*.

6.13.2 Assign Force Field

Set the force field. The choices vary depending on the type of solver. After assigning a forcefield, use *Get Info* to check the assigned forcefield. In the case of LAMMPS, if a gro file containing velocities is open in the main window at the time this function is used, a data file containing velocities is generated. Similarly, in the case of Gromacs, if a data file with velocities is open, a gro file with velocities is generated; this is useful when you want to take over Gromacs and LAMMPS calculation data with velocities. Once you assign a force field and run the MD calculation, the bond order is automatically determined from the equilibrium length of the force field parameters. Depending on the type of force field, the bond order determined at that time may be different from the bond order before the force field assignment. Some force fields are affected by the bond order. Use *Overwrite Bonds from File* if you want to return to the bond order before force field assignment.

Automatically assign parameters

Assign new force field parameters. Structures connected to each other by bonds in the molecule display area will be recognized as a single molecule.

(General)

Specifies the force field for molecules other than proteins and water molecules. Internally, **`acpype`** is used for GAFF, GAFF2, OPLS/AA-L+GAFF, an in-house program for Dreiding, a proprietary extension of OpenBabel for UFF, and mktop for OPLS-AA. The configuration for Dreiding is described in `polymer/dreiding.lib.txt`. Check *Universal Force Field* for details on UFF.

Exception

For specific molecules, assign the user specified LJ parameters without using the force field selected in (General). In the left column of the subwindow, check the molecule you want to specify the LJ parameter and enter the LJ parameter in the right column.

Note: For example, when you want to allocate LJ parameters to solid phase atoms in a solid-liquid interface system.

(Protein)

Specify the force field of the protein. Here, the atom to which the name of the amino acid residue is assigned in the PDB or gro format is recognized as a protein. Internally, **`gmx pdb2gmx`** is used.

Warning: This function can not be used when reading the molecular structure from a file not including residue name.

(Water)

Specify the force field of the water molecule. You must specify the selected water model with *Solvate/Build Cell*. Internally we get the parameters from the library of Gromacs topology installed in Cygwin.

Add [position_restraints] for protein

If a protein exists, write information (`[position_restraints]` section) to constrain the position in the topology file with *-POSRES* on the *Advanced* tab. Ignored when protein is absent.

Add [position_restraints] for selected atoms

For the molecule specified by the user, write information (`[position_restraints]` section) to constrain the position in the topology file with *-POSRES* on the *Advanced* tab. For example, when fixing solid phase in solid-liquid interface system.

Add [distance/angle/dihedral_restraints] for selected atoms

For the molecule specified by the user, write information to constrain distance, angle, dihedral angle to topology file by *-POSRES* on the *Advanced* tab.

Dump Now
Based on the current settings, generate a topology file.

Note:

- If you want to customize the forcefield information by editing it with a text editor, first save the file containing the forcefield information using *Dump Now* and edit the top for Gromacs or the data file for LAMMPS with a text editor.
- Next, for Gromacs, import the gro file at *File* → *Import File* (select *Discard and import*), then at *Assign Force Field* select :guilabel:` Select *Use parameters written in topology file* and click the *OK* button. You will then be asked for the location of the top file, so open the top file you just saved and edited.
- For LAMMPS, import the data file at *File* → *Import File* (select *Discard and import*), then at *Assign Force Field*, select *Use the parameters written in file opened on :guilabel: `main window* and click on the *Next* > button. If the force field information is not written in the data file, you will get a *Choose the type of force field*, choose the type of generic force field you want to use and click the *OK* button.
- Charges are taken from the structure displayed in the main window. If more than one type of charge is set in the main window (for example, if the GAMESS log file is opened and Mulliken charge and Lowdin charge are set), the following order of priority is used: (high priority) User charge > NBO charge > Lowdin charge > ESP charge > Mulliken charge (low priority). When the file is opened and the Mulliken charge and Lowdin charge are set (for example, when the file is opened and the Mulliken charge and Lowdin charge are set), the order of priority is User charge > NBO charge > Lowdin charge > ESP charge > Mulliken charge (low priority).

Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)
(for LAMMPS) Select if you want to use the potential for inorganic materials, ReaxFF or DPD. After pressing the *Next* > button, specify the type of force field you actually want to use. pair_style and Potential file must be set in [Tools]-[Preferences]-[Calculations] to allow the user to enter them freely.

Use parameters written in topology file
(For Gromacs) Select this option if you want to run MD calculations using a top file that already exists. The corresponding gro file must be opened or imported in the main window. If you edit the structure after opening or importing it, the correspondence with the top file will be broken and the calculation will not be possible. If you want to use this function after editing the structure after opening or importing it to the extent that it does not affect the force field information (for example, editing only the coordinates without changing the bonds), export the structure in gro format after editing it and open or import that file before using this function.

Use parameters written in file opened on main window
(For LAMMPS) Select this option if you want to run the MD calculation using a data file that already exists. The main window must have the data file you want to use open or imported. If you edit the structure after opening or importing the file, the correspondence with the top file will be broken and the calculation will not be possible. After pressing the *Next* > button, specify the type of force field to use.

6.13.3 Workflow Setup

Set up and run the LAMMPS calculation flow in project mode. 12-Step Compression in Preset is the polymer equilibration procedure described in [Hofmann2000] , [Larsen2011] . Also, 21-Step Compression-Decompression is the polymer equilibration procedure described in [Larsen2011].

Preset
Import and saves a preset of settings.

# of Jobs
Specify the number of jobs.

Enable parameter/structure scan

This feature requires the purchase of an add-on. It is possible to run multiple calculations in which only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For the structure scan, select %WM_STRUCT% for the *Target Variable* with the animation appearing in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File* → *Project* → *Scan Results* to tabulate the calculation results.

Import

Import the settings output by Export. Click the arrow at the right of the button to recall settings used in the past on the same project or Winmostar.

Export

Output settings to file.

OK

Run a calculation or generate a file with your settings. See *For project mode* for details.

Details

Set detailed calculation conditions. The *Configure* will be launched.

Ensemble

Specifies the type of ensemble.

	Setting details
Minimize	Ensemble=minimize
NVT	Ensemble=nvt
NPT	Ensemble=npt
NPT(aniso)	Ensemble=npt Pressure control=aniso
NPT(z)	Ensemble=npt Pressure control=z
NVE	Ensemble=nve
NPH	Ensemble=nph
NPH(z)	Ensemble=nph Pressure control=z
NPT+Rescale Cell	Ensemble=npt Rescale cell size=True
NVE+Rescale Vel	Ensemble=NVE Rescale velocities=True
NVT(DPD)	Ensemble=nve
NVT(SLLOD)	Ensemble=nvt Reset COM=Disable Enable SLLOD=True

Temperature
Specify the temperature.

Pressure
Specify the target pressure.

Simulation time
Specify simulation time.

# of snapshots
Specify number of dump and xtc outputs.

Initial velocity
If Random, the first speed is generated randomly; if From parent, the last speed of the previous job is inherited.

Free boundary condition
Calculate with free boundaries instead of periodic boundary conditions.

	Setting details
True	Boundary=fff Neighbor search=nsq Reset COM motion=angular
False	Boundary=ppp Neighbor search=bin Reset COM motion=linear

Precision
Set calculation precision.

	Setting details
Low	Cutoff(vdW)=10 Cutoff(Coulomb)=10 Log interval=10 Time step(fs)=2 Tchain=3 Pchain=3 Shake tolerance=1e-5 PPPM order=4 K-space accuracy=1-e5
Medium	Cutoff(vdW)=12 Cutoff(Coulomb)=12 Log interval=20 Time step(fs)=1 Tchain=3 Pchain=3 Shake tolerance=1e-6 PPPM order=4 K-space accuracy=1e-6
High	Cutoff(vdW)=15 Cutoff(Coulomb)=15 Log interval=40 Time step(fs)=0.5 Tchain=1 Pchain=1 Shake tolerance=1e-9 PPPM order=6 K-space accuracy=1e-9

6.13.4 Configure

Set calculation condition of LAMMPS. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. Behavior when clicking *Run* is see *Run*. *Assign Charges Automatically* will be launched automatically if there is a molecule to which no charge is assigned. If no force field is assigned, *Assign Force Field* will be launched automatically. Return to the default state with *Reset* button. Save the setting except Force Field with *Save* button. Load the setting saved by *Save* with the *Load* button.

Continue Simulation

Execute a continuous job. For details, see *Run*.

Preset

Specify the preset of the calculation condition. Each preset changes the following keywords.

	Minimize (fast)	NVT (fast)	NPT (fast)	NVE (fast)
Pair style	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long
Time step		2.0	2.0	2.0
# of time steps	5000	5000	5000	5000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	p p p	p p p	p p p	p p p
Reset COM motion	linear	linear	linear	linear
Tchain		3	3	
Pchain			3	
Shake tolerance		1e-5	1e-5	1e-5
Dump interval (dump)	100	100	100	100
Dump interval (xtc)	100	100	100	100
Log interval	10	10	10	10
Cutoff (vdW)	10.	10.	10.	10.
Cutoff (Coulomb)	10.	10.	10.	10.
PPPM order	4	4	4	4
K-space accuracy	1e-5	1e-5	1e-5	1e-5

	Minimize (medium)	NVT (medium)	NPT (medium)	NVE (medium)
Pair style	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long
Time step		1.0	1.0	1.0
# of time steps	10000	10000	10000	10000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	p p p	p p p	p p p	p p p
Reset COM motion	linear	linear	linear	linear
Tchain		3	3	
Pchain			3	
Shake tolerance		1e-6	1e-6	1e-6
Dump interval (dump)	200	200	200	200
Dump interval (xtc)	200	200	200	200
Log interval	20	20	20	20
Cutoff (vdW)	12.	12.	12.	12.
Cutoff (Coulomb)	12.	12.	12.	12.
PPPM order	4	4	4	4
K-space accuracy	1e-6	1e-6	1e-6	1e-6

	Minimize	NVT	NPT	NVE
Pair style	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long	lj/cut/coul/long
Time step		0.5	0.5	0.5
# of time steps	20000	20000	20000	20000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	p p p	p p p	p p p	p p p
Reset COM motion	linear	linear	linear	linear
Tchain		1	1	
Pchain			1	
Shake tolerance		1e-9	1e-9	1e-9
Dump interval (dump)	400	400	400	400
Dump interval (xtc)	400	400	400	400
Log interval	40	40	40	40
Cutoff (vdW)	15.	15.	15.	15.
Cutoff (Coulomb)	15.	15.	15.	15.
PPPM order				
K-space accuracy				

	Minimize (vapor,fast)	NVT (vapor,fast)	NPT (vapor,fast)	NVE (vapor,fast)
Pair style	lj/cut/coul/cut	lj/cut/coul/cut	lj/cut/coul/cut	lj/cut/coul/cut
Time step		2.0	2.0	2.0
# of time steps	5000	5000	5000	5000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	f f f	f f f	f f f	f f f
Reset COM motion	angular	angular	angular	angular
Tchain		3	3	
Pchain			3	
Shake tolerance		1e-5	1e-5	1e-5
Dump interval (dump)	100	100	100	100
Dump interval (xtc)	100	100	100	100
Log interval	10	10	10	10
Cutoff (vdW)	10.	10.	10.	10.
Cutoff (Coulomb)	10.	10.	10.	10.
PPPM order				
K-space accuracy				

	Minimize (vapor)	NVT (vapor)	NPT (vapor)	NVE (vapor)
Pair style	lj/cut/coul/cut	lj/cut/coul/cut	lj/cut/coul/cut	lj/cut/coul/cut
Time step		0.5	0.5	0.5
# of time steps	20000	20000	20000	20000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	f f f	f f f	f f f	f f f
Reset COM motion	angular	angular	angular	angular
Tchain		1	1	
Pchain			1	
Shake tolerance		1e-9	1e-9	1e-9
Dump interval (dump)	400	400	400	400
Dump interval (xtc)	400	400	400	400
Log interval	40	40	40	40
Cutoff (vdW)	15.	15.	15.	15.
Cutoff (Coulomb)	15.	15.	15.	15.
PPPM order	6	6	6	6
K-space accuracy	1e-9	1e-9	1e-9	1e-9

	Minimize (ReaxFF)	NVT (ReaxFF)	NPT (ReaxFF)	NVE (ReaxFF)
Pair style	reax/c	reax/c	reax/c	reax/c
Time step		0.5	0.5	0.5
# of time steps	20000	20000	20000	20000
Ensemble	minimize	nvt	npt	nve
Generate initial velocity		True	False	False
Temperature		300	300	
Pressure			1.0	
Boundary Condition	p p p	p p p	p p p	p p p
Reset COM motion	linear	linear	linear	linear
Tchain		1	1	
Pchain			1	
Shake tolerance		1e-9	1e-9	1e-9
Dump interval (dump)	400	400	400	400
Dump interval (xtc)	400	400	400	400
Log interval	40	40	40	40
Cutoff (vdW)	15.	15.	15.	15.
Cutoff (Coulomb)	15.	15.	15.	15.
PPPM order				
K-space accuracy				

MPI

Specify MPI parallel number.

Basic

Units

Specify the unit system.

real

It is mainly specified by molecular system (A, fs, Kcal/mol).

metal

It is mainly specified by crystal system (A, ps, eV).

lj

It is mainly specified by DPD calculation (dimensionless unit).

Atom Style

Specify the type of system to calculate. *Units* changes accordingly.

Pair Style

Select the method of interaction calculation. lj/cut/coul/long and boundary is ppf, the command kspace_modify slab 3 is automatically added and the calculation is performed using the PPPM method considering the 2-D periodic boundary condition.

Force Field/Potential File

If *Units* is real, specify the type of force field. Affects the special_bonds, bond_style, angle_style, dihedral_style, and improper_style keywords. Select the potential file when *Units* is other than "real". List the files in the `Potential` folder directly under the folder where you installed the LAMMPS main unit. The choices will change according to *Pair Style*.

Time Step

Specify the step size of time integration. Units are selected according to the selected *Unit*.

# of Time Steps

Specify the maximum number of time integration steps.

Ensemble

Specify the type of time integration. `nvt` (canonical ensemble with constant temperature), `npt` (temperature, constant pressure ensemble), `nve` (micro and canonical ensemble with constant volume and energy), `minimize` (CG Energy minimization by law).

Generate Velocity

If you check, the initial speed will be given.

Random Seed

Specify the seed of the pseudorandom number at the time of initial velocity occurrence.

Temperature

Specify the target temperature. At the time of annealing calculation, specify the temperature of the start condition.

Tdamp

Specify the time constant parameter for temperature control.

Use berendsen thermostat

Use fix temp/berendsen instead of fix nvt or npt to control temperature.

Use velocity rescaling

Use fix temp/rescaling instead of fix nvt or npt for temperature control.

Pressure Control

Specify how cells are moved during pressure control.

Pressure

Specify the target pressure.

Pdamp

Specify the time constant parameter of pressure control.

Use berendsen barostat

Use fix press/berendsen instead of fix nph or npt to control pressure.

Advanced

Boundary X Y Z
Specify the periodic boundary condition. `p` (periodic), `f` (non-periodic and fixed), `s` (non-periodic and shrink-wrapped), `m` (non-periodic and shrink-wrapped with a minimum value). If pair_style is lj/cut/coul/long and boundary is ppf, the command kspace_modify slab 3 is automatically added and the calculation is performed using the PPPM method considering the 2-D periodic boundary condition.

Energy Tolerance
minimize Specifies the truncation error on energy during calculation.

Force Tolerance
minimize Specifies the truncation error on force during calculation.

Reset COM Motion
In the case of xy, only the center-of-gravity motion is frozen in the x and y directions, but not in the z direction.

Reset Interval
Specify *Reset COM Motion* frequency in time step

Tchain
Specify the number of stages of Nose-Hoover chain.

Pchain
Specify the number of stages of pressure control.

Velocity rescaling interval
Specify how often to apply speed scaling.

Velocity rescaling window
Specify the window (allowable range from set temperature) when applying speed scaling.

Velocity rescaling fraction
Specifies the fraction at which to apply speed scaling; if 1.0, it will match the set temperature immediately after application.

Control temperature of specific group only
This function controls only the temperature of a specific group. To do this, register a group to be controlled with *Select Registered Group* and press *Select Group* button to select the group.

Constrain hydrogen atoms
We restrict hydrogen atoms by SHAKE method.

SHAKE tolerance
Specify the truncation error of the SHAKE method.

Automatically disable Shake if CH4-like molecule exists
Automatically disables the SHAKE method when methane like molecules are included.

Set "box tilt large"
Specify the allowable degree of deformation of the simulation cell.

Enable dynamic load balancing
Enable dynamic load balancing.

Output

Dump Interval (dump)
Specify the frequency of outputting coordinates in dump format as the number of time steps.

Dump Interval (xtc)
Specify the frequency of outputting coordinates in xtc format as the number of time steps.

Dump Interval (xyz)

Specify the frequency of outputting coordinates in xyz format by time step number.

Dump Interval (restart)

Specify how often to output the restart file, in number of time steps.

Log Interval

Specify the frequency of writing energy variables to the log file by time step number.

Print log in high precision

Increases the number of digits of the energy variable to be written to the log file.

Sort dump file by id

Makes the order of particles in the dump file sorted by id (consecutive number).

Flush log

Flush each time when the log is output.

Include velocities in dump custom

When outputting in dump format, also output the velocity.

Extra variables for log

Add any variables to thermo_style.

Dump interval (dipole)

Specify the frequency of outputting time series data of dipole moments for the entire system in terms of the number of time steps.

Calculate Fluctuation Properties

Calculates and outputs on-the-fly specific heat and isothermal compression ratio from fluctuations of thermodynamic quantities.

Calculate Thermal Conductivity

Calculate and output the thermal conductivity on-the-fly from the autocorrelation function of the atomic flow velocity and the Green-Kubo equation. This method uses the fix ave/correlate command, so the length of the autocorrelation function is fixed.

Calc interval

Specifies how often the autocorrelation function is calculated.

ACF length

Specifies the length of the autocorrelation function. The maximum time for an autocorrelation function is (Calc Interval)×(ACF Length)×(Time Step).

Calculate viscosity

Calculates and outputs viscosity on-the-fly from the autocorrelation function of the pressure tensor and the Green-Kubo equation. This method uses the fix ave/correlate command, so the length of the autocorrelation function is fixed.

Calc interval

Specifies how often the autocorrelation function is calculated.

ACF length

Specifies the length of the autocorrelation function. The maximum time for an autocorrelation function is (Calc Interval)×(ACF Length)×(Time Step).

Calculate heat flux relaxation

Output autocorrelation functions for atomic heat flow. This method uses the fix ave/correlate/long command (multiple-tau correlator), so you can automatically get long-time autocorrelation functions depending on the simulation time. Thermal conductivity can be calculated separately from post-processing.

Calc interval
Specifies how often the autocorrelation function is calculated.

Dump Interval
Specifies the output frequency of the autocorrelation function.

Calculate stress relaxation
Output autocorrelation function for the pressure tensor. This method uses the fix ave/correlate/long command (multiple-tau correlator) so you can automatically get long autocorrelation functions depending on simulation time. Viscosity can be calculated separately from post-processing.

Calc interval
Specifies how often the autocorrelation function is calculated.

Dump Interval
Specifies the output frequency of the autocorrelation function.

Calculate dipole relaxation
Outputs the autocorrelation function of the dipole moments for the entire system. This method uses the fix ave/correlate/long command (multiple-tau correlator) so you can automatically get long-time autocorrelation functions depending on simulation time.

Calc interval
Specifies how often the autocorrelation function is calculated.

Dump Interval
Specifies the output frequency of the autocorrelation function.

Interaction

Modify cutoff radii not to exceed L/2
If checked, Cutoff(vdw) and Cutoff(Coulomb) are automatically adjusted so that they do not exceed half the lattice constant.

Neighbor Search
Specify algorithm for near particle search.

Neighbor Skin
Specify the extra radius of the search radius when searching for nearby particles.

Cutoff(vdw)
vdw (LJ) Specifies the cutoff radius of the potential.

Enable Long Range Correction
Specify the presence or absence of the vdw potential cut-off correction term.

Cutoff(Coulomb)
Coulomb (electrostatic) Specify the cutoff radius of the potential.

Disable Ewald(PPPM) if no charge exists
Automatically disables the Ewald (PPPM) method when the system has no charge.

Automatically set Nmesh
The number of meshes of the PPPM method used when *Pair Style* = `lj/cut/coul/long` is automatically set from K-space accuracy.

Nmesh for kx, ky, kz
Specify the mesh number of PPPM method.

PPPM Order
Specify Spline interpolation order of PPPM method.

K-space accuracy
Specify the allowable relative error of PPPM method.

Non-equiliibrium (1)

Enable Elongation
Enable decompression calculation. *Ensemble* can be specified when it is not `minimize`.

Affine Transformation
Specify whether to modify the atom position according to the simulation cell and to affine (similarity) deformation during elongation calculation.

Eng. Strain Rate
Specify the extension speed at extension calculation with industrial strain. *Max Eng. Strain* shows the predicted value of the strain at the final step.

Preserve Volume
During elongation calculation, deform the cell size in the direction perpendicular to the elongation direction so that the volume of the simulation cell is kept constant.

Enable Pulling
Enable Pull calculation to move a specified atom group at a constant speed. *Ensemble* can be specified when it is not `minimize`.

Pulled Atoms
Press *Select Group* button and select the group in the state where the atoms you want to pull are registered by *Select Registered Group* in advance.

Pull Velocity
Specify the pull speed for Pull calculation.

Enable Simulated Annealing
Enable annealing calculations (calculation to change the temperature at a constant speed). *Ensemble* can be specified when `nvt`, `npt`. The value of *Temperature* is the temperature at the beginning, and the value of *Final Temperature* is the temperature of the final state.

Final Temperature
Specify the temperature of the final state at the time of annealing calculation.

Annealing Rate
The heating or cooling rate at the time of annealing calculation is displayed.

Enable pressurization
Enable annealing calculations (calculation to change the temperature at a constant speed). *Ensemble* can be specified when `nvt`, `npt`. The value of *Temperature* is the temperature at the beginning, and the value of *Final Temperature* is the temperature of the final state.

Final Pressure
Specify the temperature of the final state at the time of annealing calculation.

Enable electric field
Gives an external electric field. If you select *Sine wave*, the electric field is given sine wave. When *Constant* is selected, the electric field is given in static.

Amp & Freq
Gives the intensity (Amp) and frequency (Freq) of each direction. If *Sine wave* in *Enable electric field* is selected, the following formula is used to give the electric field, where A is the intensity and f is the frequency. If you choose *Constant*, only the intensity is used.

$$A\sin(2\pi ft)$$

Non-equiliibrium (2)

Enable adding force
Target atoms applies a force in the z-direction to the atoms specified in *Target atoms*. The force applied is the value of *Target Pzz* and the area of the XY plane of the simulation cell. In solid-liquid interfacial systems, this is useful when you want to apply a force to a solid (slab) and adjust the pressure throughout the system. The position of the center of gravity in the z-direction of the atom applying the force is output to thermo_style in the variable v_GrpAddForceCOMz and can be monitored using *Energy Plot*.

Target atoms
Press the *Select Group* button with the atoms you want to force registered beforehand with *Select Registered Group* and select that group.

Target Pzz
Enable adding force

Enable direct density control
Force the simulation cell to be linearly deformed so that the density is at the value of *Density at final step* at the final step. The deformation is analogous. This is useful when the pressure control is not stable but you want to compress the system to some extent.

Density at final step
:guilabel:Specifies the density of the final step in the *Enable direct density control* feature.

Enable SLLOD method
Enable SLLOD method calculation.

Shear strain rate
Specifies the shear rate for SLLOD method calculations.

Restraint

Enable Restraint
Calculation is performed by constraining the distance between specified two atoms. *Ensemble* can be specified when it is not `minimize`.

Restrained Atoms
When you click the *Set* button, the two atoms with the markers become the target of the constraint.

Bond Length
Specify the constraint distance between two atoms at the time of constraint calculation.

Initial Strength
Specify the spring coefficient of the constraint potential in the starting state at the time of constraint calculation.

Final Strength
Specify the spring coefficient of the constraint potential in the final state at the time of constraint calculation.

Enable Position Restraint
Calculate with the absolute coordinates of the specified atom fixed. The temperature of the unfixed atom is output to the log as TempFree.

Restrained Atoms
Press *Select Group* button to select the group with the atoms to be constrained registered with *Select Registered Group* in advance, .

Use spring potential
If *Restrained Atoms* is checked, the atoms will be restrained by the spring potential from their initial position. If *Reset positions of restrained atoms after run* is checked, the atoms will be

returned to their initial positions after the calculation is finished, so they will not move away from their initial positions even if you repeat the continue simulation. If the *Restrained positions of atoms after run* checkbox is checked, the position will be returned to the initial position after the calculation.

Spring constant

Specify the spring coefficient when using the spring potential.

Reset positions of restrained atoms after run

When using the spring potential, the position of the constrained atoms is reset to the initial position after the calculation is complete.

Automatic

Rescale velocities to..

Use it when you want to bring the system temperature closer to the target temperature in the NVE ensemble. Calculate the scaling factor from the average temperature under calculation and the temperature entered here and scale the velocity of each particle in the final structure.

Rescale cell size to..

It is used when calculating with the NVE or NVT ensemble in the state close to the set pressure after calculating with the NPT ensemble. Scale the final structure to the average cell size under calculation.

Additional Commands

Add any command just before the read_data line, after the various fix commands, just before the run (or minimize) line, and just after the run (or minimize) line.

Manual entry

The contents of the generated LAMMPS input script (in file) will be displayed. You can also edit directly at this location. Any additional information you add here will be discarded when you edit other keywords. If you want to avoid this, fill in the Additional Commands field.

Options

Restore Working Folder

Click this button to return the working folder to the state before execution, such as when the continued job terminates abnormally.

Dump all files for remote

Output files necessary for job execution under Linux environment. The same file as the file generated by *Remote job* function is output.

Generate gro & ndx files every time

If it is not checked, gro and ndx files will not be generated for continuous jobs.

Extra File

Click Add to copy the selected files to the working folder; click Clear to clear the added files.

Reset

Reset settings.

Import

Loading configuration file.

Export

Output configuration file.

6.13.5 Run

Execute LAMMPS. The execution method differs depending on the situation.

- **(Default)** ***Continue Simulation*** **is unchecked and** ***Automatically assign parameters*** **or** ***Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)*** **in** ***Assign Force Field*** **is selected**
  Create a new data file (file containing coordinates and topology) and start the job.
- ***Continue Simulation*** **is unchecked and** ***Use parameters written in file opened on main window”*** **in** ***Assign Force Field*** **is selected**
  Start the job using the data file opened in the main window.
- **When** ***Continue Simulation*** **is checked**
  Start the job using the `lmp_tmp_final.data` located in the working folder associated with the data file opened in the main window.

Following file will be generated with execution. As an example, the file/folder name when the input file is `water.data` is also shown.

type	Description
out file `water.log`	This is the log file of LAMMPS.
bat file `water.bat`	LAMMPS and its pre/post processing
Working Folder `water_lmp_tmp\`	Working folder.

The following files are generated in the working folder. Only the main files are shown here.

type	Description
`lmp.data`	It is the initial state file of the calculation specified by read_data.
`lmp.in`	It is a file that specifies calculation conditions.
`lmp.log`	It is a log file. It is the same as: file: *water.log*.
`lmp.dump`	It is a trajectory file in dump format.
`lmp.restart`	It is a restart file containing information on the final state.
`lmp_final.data`	It is a data file containing information on the final state. It is generated from the restart file.
`postproc.sh`	The `lmp_tmp_final.data` generated by LAMMPS is not sufficient to run LAMMPS as is, so this script does some processing to make up for the insufficient information.
`lmp.xtc`	Trajectory file in xtc format for using the Gromacs tool for results processing.
`lmp.gro`	gro-format coordinate file to use the Gromacs tool for processing results. Convert from the data file specified as the input file
`lmp.top`	:guilabel:Specifies the density of the final step in the *Enable direct density control* feature. Convert from the data file specified as the input file
`restart.bat`	When a job is interrupted and terminates abnormally, this batch file can be executed to resume the calculation from the state

---

Hint: **Working folder**

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.
  - **The suffix varies depending on the type of solver.**
  - For example, in the case of Gromacs, if the file opened in the main window is: file: *aaa.gro* and the suffix is `_ gmx_tmp`, the working folder will be named `aaa_gmx_tmp` .
- It must be in the same hierarchy as the file opened in the main window.
- Processing continues in the working folder of the same name even when continuing jobs, but by default the backup of the working directory of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the one with the smallest number in the range where duplicate names do not exist. For example, if the working folder is `aaa_gmx_tmp`, it is `aaa_gmx_tmp1`.
  - **Directories without numbers are always up to date.**

The job is run through *Winmostar Job Manager*.

6.13.6 Open Log File

Open the LAMMPS log file (`*.log`) with a text editor.

6.13.7 Show log excerpts

Displays excerpts of key information from the log file.

6.13.8 Animation

Select the data file and dump file and animate the MD calculation trajectory. The file name of the main window does not change. For the animation display operation method, see *Animation operation area*. In the case of calculations where changes in chemical bonds occur, such as ReaxFF, checking the *Options → Enable Dynamics Bond* checkbox in the Animation Manipulation Area will determine whether or not a bond exists based on the bond distance at each step, allowing you to see how the bond changes. You can check how the bond changes.

6.13.9 Energy Plot

Select the log file and display a graph of various thermodynamic quantities such as energy, temperature and pressure. You can plot the value specified by thermo_style. Please see *Energy Plot window* for how to operate subwindow.

6.13.10 Import Last Coordinate (data)

Open `*_lmp_tmp\lmp_tmp_final.gro`. When using this function, the file name of the main window does not change.

6.13.11 Analyses

Radial Distribution Function

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the radial distribution function. See *Radial Distribution Function* for details.

Diffusion Constant/Mean Square Displacement

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar, and display the mean square displacement and the self diffusion coefficient. See *Diffusion Constant/Mean Square Displacement* for details.

Scattering Function

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the scattering function. For details, see *Scattering Function*.

Total Linear Moment

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the total linear moment. See *Total Linear Momentum* for details.

Velocity Distribution

The xtc and dump files output by LAMMPS and the gro, ndx, mdp, top, and data files automatically generated by Winmostar are selected and the velocity distribution is displayed. mdp and top files can only be generated when using general-purpose forcefields such as GAFF, so this function is not available when using parameter files. This function is not available when using parameter files, for example. See *Velocity Distribution* for details.

Velocity Correlation / Vibration Spectrum

Select the xtc file output by LAMMPS and the gro, ndx, mdp, and top files automatically generated by Winmostar to display velocity correlation functions and vibration spectra.The mdp and top files can only be generated when using general-purpose force fields such as GAFF, so this function cannot be used when using parameter files. See *Velocity Autocorr/Vibration Spectrum* for details.

Static Dielectric Moment

Select an xtc file output by LAMMPS and a gro, ndx, mdp, or top file automatically generated by Winmostar to display the distribution and histogram of relative permittivity or dipole moment.The mdp and top files can only be generated when using a general-purpose force field such as GAFF, so this function cannot be used when using parameter files. See *Radial Distribution Function* for details.

Density Profile

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the radial distribution function. Since mdp and top files can only be generated when using general-purpose force fields such as GAFF, this function cannot be used when using parameter files. See *Radial Distribution Function* for details.

Free Volume

Select the xtc file output by LAMMPS and the gro, ndx, mdp and top files automatically generated by Winmostar and display the free volume. Since mdp and top files can only be generated when using general-purpose force fields such as GAFF, this function cannot be used when using parameter files. See *Free Volume* for details.

Various autocorrelation functions (ave/correlate)

Displays the autocorrelation function created by the fix ave/correlate command, which is output when calculating thermal conductivity and viscosity using the Green-Kubo formula

Various autocorrelation functions (ave/correlate/long)

Displays the autocorrelation function created by the fix ave/correlate/long command.

Bond/Angle/Dihedral Distribution

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the radial distribution function. Since mdp and top files can only be generated when using general-purpose force fields such as GAFF, this function cannot be used when using parameter files. For details, see *Scattering Function*.

Hydrogen bonding analyses

Select the xtc file output by LAMMPS and the gro, ndx, mdp, top files automatically generated by Winmostar and analyze the hydrogen bonds between the selected groups. mdp and top files can only be generated when using generic forcefields such as GAFF. This function is not available when using parameter files. See *Radial Distribution Function* for details.

radius of inertia

Select the xtc file output by LAMMPS and the gro, ndx, mdp, top files automatically generated by Winmostar, and analyze the radius of inertia of the selected group. mdp and top files can only be generated when using a general purpose force field such as GAFF, so this function is not available when using parameter files. This function cannot be used when parameter files are used. See *Radius of Gyration* for details.

Atom/Group Distance Change

Select the xtc file output by LAMMPS and the gro, ndx, mdp, top files automatically generated by Winmostar to analyze the change in distance between specific atoms or groups of atoms. mdp and top files can only be generated when using generic forcefields such as GAFF. This function is not available when using parameter files. See *Atom/Group Distance Change* for details.

viscosity

The viscosity is calculated from the stress autocorrelation function obtained with the Multiple tau correlator (fix ave/correlate/long). The upper graph shows the normalized autocorrelation function C(t)/C(0) in a log-linear plot, the middle graph shows it in a log-log plot, and the lower graph shows the viscosity obtained from the integrated autocorrelation function. The autocorrelation function plot shows the function fitted to the lower equation in green.

$$f(x) = A_1 \exp(-(x/B_1)^{C_1}) \cos(D_1 x) + (1 - A_1) \exp(-(x/B_2)^{C_2})$$

In the lower graph, the short-time side has a large error due to insufficient integration range, while the long-time side has a large error due to insufficient sampling of the autocorrelation function. Also, the time (excluding the short-time oscillation component) that the fitted function is below the value entered for *Threshold for switching integration from raw to fitted* is displayed in the *Switch integration at*. The *Estimated Viscosity* displays the viscosity obtained by integrating the autocorrelation function with the trapezoidal formula. The numerical integration is performed over the *Switch integration at* time, with the short integration over the autocorrelation function obtained directly from the calculation and the long integration over the function fitted to the above equation. Integrating the long time side over the function fitted to the above equation reduces the effect of errors due to under-sampling. If Plot Autocorrelation Function is not checked, only the viscosity obtained from the integrated value of the autocorrelation function will be plotted. This is useful when determining the interval mean from the graph Options.

Thermal Conductivity

Calculate thermal conductivity from the autocorrelation function of the heat flow obtained with the multiple tau correlator (fix ave/correlate/long). The upper graph shows the normalized autocorrelation function C(t)/C(0) in a log-log plot, the middle graph shows a log-log plot, and the lower graph shows the thermal conductivity obtained from the integrated value of the autocorrelation function. The autocorrelation function plot shows the function fitted to the lower equation in green.

$$f(x) = A_1 \exp(-(x/B_1)^{C_1}) \cos(D_1 x) + (1 - A_1) \exp(-(x/B_2)^{C_2})$$

In the lower graph, the short-time side has a large error due to insufficient integration range, while the long-time side has a large error due to insufficient sampling of the autocorrelation function. Also, the time (excluding the short-time oscillation component) that the fitted function is below the value entered for *Threshold for switching integration from raw to fitted* is displayed in the *Switch integration at*. The *Estimated Viscosity* displays the thermal conductivity obtained by integrating the autocorrelation function with the trapezoidal formula. The numerical integration is performed over the *Switch integration at* time, where the short time side is integrated over the autocorrelation function directly obtained from the calculation, and the long time side is integrated over the function fitted to the above equation. Integrating the long time side over the function fitted to the above equation reduces the effect of errors due to under-sampling.

6.13.12 Dissipative Particle Dynamics

DPD Cell Builder

Create a simulation cell for dissipative particle dynamics.

Reset
Restore all settings to default.

Monomers Available
Select the monomer (particle) that constitutes the polymer chain.

>> Add >>
Add selected monomers.

<< Delete <<
Delete the added monomer.

Branch

Start
Specify the branch start position.

End
Specify the branch end position.

Monomers Used
A list of added monomer species and number is displayed.

Clear
Delete all listed monomer species.

>> Add >>
Add the listed polymer chain to the calculation target.

<< Delete <<
Delete the added polymer chain.

Export
Output the contents of Monomer Used to a file.

Import
Reads the contents of Monomer Used from a file.

Polymers Used
The composition and number of added polymer chains are listed.

Build
Enter dimensionless densities and build simulation cells.

Close
Close the window.

DPD Potential Editor

Winmostar Create and edit a potential file for proprietary dissipative particle dynamics.

Potential Files
Select the potential file used for dissipative particle dynamics.

New
We will create a new potential file.

Delete
Delete the selected potential file.

Mass tab

- **Species**
  The name of the monomer (particle) is displayed.
- **Mass**
  Set the mass (dimensionless).

Bond tab

- **R_0**
  Set bond (bond) potential parameter R_0 (equilibrium distance, dimensionless).
- **TO**
  Set bond (bond) potential parameter K (spring constant, dimensionless).

Nonbond tab

- **Aij**
  Enter the unbonded potential parameter Aij (dimensionless).
- **Rcut**
  Enter the unbonded potential parameter Rcut (cutoff radius, dimensionless).
- **Gamma**
  Enter the coefficient of friction (dimensionless).
- **Set**
  The set potential parameters are reflected in the list.

OK
Save the set potential parameters in the potential file and close the window.

Close
Discard the settings and close the window.

6.14 *MD* → *Gromacs* menu

It is a menu about Gromacs. Because Winmostar runs Gromacs on the Cygwin environment, in order to use this function, please set up *CygwinWM* is required.

6.14.1 Asign Force Field

Asign Force Field. The choices vary depending on the type of solver. After assigning a forcefield, use *Get Info* to check the assigned forcefield. In the case of LAMMPS, if a gro file containing velocities is open in the main window at the time this function is used, a data file containing velocities is generated. Similarly, in the case of Gromacs, if a data file with velocities is open, a gro file with velocities is generated; this is useful when you want to take over Gromacs and LAMMPS calculation data with velocities. Once you assign a force field and run the MD calculation, the bond order is automatically determined from the equilibrium length of the force field parameters. Depending on the type of force field, the bond order determined at that time may be different from the bond order before the force field assignment. Some force fields are affected by the bond order. Use *Overwrite Bonds from File* if you want to return to the bond order before force field assignment.

Automatically assign parameters

Assign new force field parameters. Structures connected to each other by bonds in the molecule display area will be recognized as a single molecule.

(General)

Specifies the force field for molecules other than proteins and water molecules. Internally, **`acpype`** is used for GAFF, GAFF2, OPLS/AA-L+GAFF, an in-house program for Dreiding, a proprietary extension of OpenBabel for UFF, and mktop for OPLS-AA. The configuration for Dreiding is described in `polymer/dreiding.lib.txt`. Check *Universal Force Field* for details on UFF.

Exception

For specific molecules, assign the user specified LJ parameters without using the force field selected in (General). In the left column of the subwindow, check the molecule you want to specify the LJ parameter and enter the LJ parameter in the right column.

Note: For example, when you want to allocate LJ parameters to solid phase atoms in a solid-liquid interface system.

(Protein)

Specify the force field of the protein. Here, the atom to which the name of the amino acid residue is assigned in the PDB or gro format is recognized as a protein. Internally, **`gmx pdb2gmx`** is used.

Warning: This function can not be used when reading the molecular structure from a file not including residue name.

(Water)

Specify the force field of the water molecule. You must specify the selected water model with *Solvate/Build Cell*. Internally we get the parameters from the library of Gromacs topology installed in Cygwin.

Add [position_restraints] for protein

If a protein exists, write information (`[position_restraints]` section) to constrain the position in the topology file with *-POSRES* on the *Advanced* tab. Ignored if protein is absent.

Add [position_restraints] for protein

For the molecule specified by the user, write information (`[position_restraints]` section) to constrain the position in the topology file with *-POSRES* on the *Advanced* tab. For example, when fixing solid phase in solid-liquid interface system.

Add [distance/angle/dihedral_restraints] for selected atoms

For the molecule specified by the user, write information to constrain distance, angle, dihedral angle to topology file by *-POSRES* on the *Advanced* tab.

Dump Now

Based on the current settings, generate a topology file.

Note:

- If you want to customize the forcefield information by editing it with a text editor, first save the file containing the forcefield information using *Dump Now* and edit the top for Gromacs or the data file for LAMMPS with a text editor.
- Next, for Gromacs, import the gro file at *File → Import File* (select *Discard and import*), then at *Assign Force Field* select :guilabel:` Select *Use parameters written in topology file* and click the *OK* button. You will then be asked for the location of the top file, so open the top file you just saved and edited.
- For LAMMPS, import the data file at *File → Import File* (select *Discard and import*), then at *Assign Force Field*, select *Use the parameters written in file opened on :guilabel:`main window* and click on the *Next >* button. If the force field information is not written in the data file, you will get a *Choose the type of force field*, choose the type of generic force field you want to use and click the *OK* button.
- Charges are taken from the structure displayed in the main window. If more than one type of charge is set in the main window (for example, if the GAMESS log file is opened and Mulliken charge and Lowdin charge are set), the following order of priority is used: (high priority) User charge > NBO charge > Lowdin charge > ESP charge > Mulliken charge (low priority). When the file is opened and the Mulliken charge and Lowdin charge are set (for example, when the file is opened and the Mulliken charge and Lowdin charge are set), the order of priority is User charge > NBO charge > Lowdin charge > ESP charge > Mulliken charge (low priority).

Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)

(for LAMMPS) Select if you want to use the potential for inorganic materials, ReaxFF or DPD. After pressing the *Next* > button, specify the type of force field you actually want to use. pair_style and Potential file must be set in [Tools]-[Preferences]-[Calculations] to allow the user to enter them freely.

Use parameters written in topology file

(For Gromacs) Select this option if you want to run MD calculations using a top file that already exists. The corresponding gro file must be opened or imported in the main window. If you edit the structure after opening or importing it, the correspondence with the top file will be broken and the calculation will not be possible. If you want to use this function after editing the structure after opening or importing it to the extent that it does not affect the force field information (for example, editing only the coordinates without changing the bonds), export the structure in gro format after editing it and open or import that file before using this function.

Use parameters written in file opened on main window

(For LAMMPS) Select this option if you want to run the MD calculation using a data file that already exists. The main window must have the data file you want to use open or imported. If you edit the structure after opening or importing the file, the correspondence with the top file will be broken and the calculation will not be possible. After pressing the *Next* > button, specify the type of force field to use.

6.14.2 Workflow Setting

Set up and run the Gromacs calculation flow in project mode. 12-Step Compression in Preset is the polymer equilibration procedure described in [Hofmann2000_2] , [Larsen2011_2] . Also, 21-Step Compression-Decompression is the polymer equilibration procedure described in [Larsen2011_2].

Preset

Loads and saves a preset of settings.

# of Jobs

Specifies the number of jobs.

Enable parameter/structure scan

This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file).

Import

Import the settings output by Export. Click the arrow to the right of the button to recall settings previously used in the same project or on Winmostar.

Export

Output configuration file.

OK

Run a calculation or generate a file with your settings. See *For project mode* for details.

Details

Set up detailed calculation conditions. The *Configure* will be launched.

Ensemble

Specifies the ensemble type. However, tcoupl is forced to nose-hover when Precision is High or Medium, and pcoupl is forced to berendsen when Precision is Low.

	Configuration
Minimize	integrator=steep tcoupl=no pcoupl=no
Minimize(NMA)	integrator=l-bfgs tcoupl=no pcoupl=no emtol=0.01 -DFLEXIBLE=True
NVT	integrator=md tcoupl=berendsen pcoupl=no
NPT	integrator=md tcoupl=berendsen pcoupl=parrinello-rahman pcoupltype=isotropic
NPT(aniso)	integrator=md tcoupl=berendsen pcoupl=parrinello-rahman pcoupltype=anisotropic
NPT(z)	integrator=md tcoupl=berendsen pcoupl=parrinello-rahman pcoupltype=semiisotropic
NVE	integrator=md tcoupl=no pcoupl=no
NPH	integrator=md tcoupl=no pcoupl=parrinello-rahman pcoupltype=isotropic

Temperature
Specify temperature.

Pressure
Specify pressure.

Simulation time
Specify simulation time.

# of snapshots
Specify the number of times to output coordinates and velocity to the trr file.

Initial velocity
If Random, the first speed is generated randomly. if From parent, the last speed of the previous job is inherited.

Free boundary condition
Calculate with free boundaries instead of periodic boundary conditions.

	Configuration
True	pbc=no coulombtype=cut-off nstlist=1 ns-type=simple cutoff-scheme=group Use buffer-tolerance=False comm-mode=angular
False	pbc=xyz coulombtype=pme nstlist=10 ns-type=grid cutoff-scheme=verlet Use buffer-tolerance=True comm-mode=linear

Precision
Sets the precision of the calculation. However, constraints is forced to hbonds when Ensemble is Minimize and none when Minimize(NMA) or NMA.

	Configuration
Low	Modify cutoff=True rlist=1 rvdw=1 rvdw-switch=0.9 rcoulomb=1 rcoulomb-switch=0.9 nstenergy=10 dt=0.002 nhchainlen=10 shake-tol=1e-5 pme-order=4 ewald-rtol=1e-6 fourier-spacing=0.12 vdw-modifier=potential-shift-verlet coulomb-modifier=potential-shift-verlet nsttcouple=10 nstpcouple=10 Enable double precision=False nstcomm=50 lincs-order=4 lincs-iter=1 buffer-tolerance=1e-6 constraints=all-bonds
Medium	Modify cutoff=True rlist=1.2 rvdw=1.2 rvdw-switch=1.1 rcoulomb=1.2 rcoulomb-switch=1.1 nstenergy=20 dt=0.001 nhchainlen=10 shake-tol=1e-6 pme-order=4 ewald-rtol=1e-6 fourier-spacing=0.11 vdw-modifier=potential-shift-verlet coulomb-modifier=potential-shift-verlet nsttcouple=10 nstpcouple=10 Enable double precision=True nstcomm=50 lincs-order=4 lincs-iter=1 buffer-tolerance=1e-6

6.14.3 Configure

Set calculation conditions of Gromacs. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. See *Run Gromacs* for the behavior when clicking *Run*. *Assign Charges Automatically* will start automatically if there is a molecule to which no charge is assigned. If no force field is assigned, *Asign Force Field* will be launched automatically. *Reset* button returns to the default state. Save the setting excluding Force Field with *Save* button. Load the setting saved with *Save* with the *Load* button.

Continue Simulation

Execute a continuous job. For details, see *Run Gromacs*.

Preset

Specify the preset of the calculation condition. Each preset changes the following keywords.

	Minimize (fast)	NVT (fast)	NPT (fast)	NVE (fast)
dt		0.002	0.002	0.002
nsteps	5000	5000	5000	5000
integrator	steep	md	md	md
gen-vel		yes	no	no
tcoupl		berendsen	berendsen	
ref-t		300	300	
pcoupl		no	parrinello-rahman	
ref-p			1,0	
pbc	yes	yes	yes	yes
comm-mode	linear	linear	linear	linear
nstcomm		50	50	50
nh-chain-length		10	10	
nsttcouple		-1	-1	
nstpcouple			-1	
constraints	hbonds	all-bonds	all-bonds	all-bonds
lincs-order		4	4	4
lincs-iter		1	1	1
shake-tol		1e-5	1e-5	1e-5
nstxout	100	100	100	100
nstvout	100	100	100	100
nstenergy	10	10	10	10
buffer-tolerance	5e-3	5e-3	5e-3	5e-3
rvdw	1,0	1,0	1,0	1,0
rvdw-switch	0.9	0.9	0.9	0.9
coulombtype	pme	pme	pme	pme
rcoulomb	1,0	1,0	1,0	1,0
rcoulomb-switch	0.9	0.9	0.9	0.9
fourier-spacing	0.12	0.12	0.12	0.12
pme-order	4	4	4	4
ewald-rtol	1e-5	1e-5	1e-5	1e-5

continues on next page

Table 3 – continued from previous page

	Minimize (fast)	NVT (fast)	NPT (fast)	NVE (fast)
Enable double precision	False	False	False	False
-DFLEXIBLE	False	False	False	False
Extend simulation from full-precision trajectory	False	False	False	False

	Minimize (medium)	NVT (medium)	NPT (medium)	NVE (medium)
dt		0.001	0.001	0.001
nsteps	10000	10000	10000	10000
integrator	steep	md	md	md
gen-vel		yes	no	no
tcoupl		berendsen	berendsen	
ref-t		300	300	
pcoupl		no	parrinello-rahman	
ref-p			1,0	
pbc	yes	yes	yes	yes
comm-mode	linear	linear	linear	linear
nstcomm		50	50	50
nh-chain-length		10	10	
nsttcouple		-1	-1	
nstpcouple			-1	
constraints	hbonds	hbonds	hbonds	hbonds
lincs-order		4	4	4
lincs-iter		1	1	1
shake-tol		1e-5	1e-5	1e-5
nstxout	200	200	200	200
nstvout	200	200	200	200
nstenergy	20	20	20	20
buffer-tolerance	1e-6	1e-6	1e-6	1e-6
rvdw	1.2	1.2	1.2	1.2
rvdw-switch	1.1	1.1	1.1	1.1
coulombtype	pme	pme	pme	pme

continues on next page

Table 4 – continued from previous page

	Minimize (medium)	NVT (medium)	NPT (medium)	NVE (medium)
rcoulomb	1.2	1.2	1.2	1.2
rcoulomb-switch	1.1	1.1	1.1	1.1
fourier-spacing	0.11	0.11	0.11	0.11
pme-order	4	4	4	4
ewald-rtol	1e-6	1e-6	1e-6	1e-6
Enable double precision	True	True	True	True
-DFLEXIBLE	False	False	False	False
Extend simulation from full-precision trajectory	False	False	False	False

	Minimize	NVT	NPT	NVE
dt		0.0005	0.0005	0.0005
nsteps	20000	20000	20000	20000
integrator	steep	md	md	md
gen-vel		yes	no	no
tcoupl		nose-hoover	nose-hoover	
ref-t		300	300	
pcoupl		no	parrinello-rahman	
ref-p			1,0	
pbc	yes	yes	yes	yes
comm-mode	linear	linear	linear	linear
nstcomm		1	1	1
nh-chain-length		1	1	
nsttcouple		1	1	
nstpcouple			1	
constraints	hbonds	hbonds	hbonds	hbonds
lincs-order		8	8	8
lincs-iter		2	2	2
shake-tol		1e-9	1e-9	1e-9
nstxout	400	400	400	400
nstvout	400	400	400	400

continues on next page

Table 5 – continued from previous page

	Minimize	NVT	NPT	NVE
nstenergy	40	40	40	40
buffer-tolerance	1e-9	1e-9	1e-9	1e-9
rvdw	1.5	1.5	1.5	1.5
rvdw-switch	1.4	1.4	1.4	1.4
coulombtype	pme	pme	pme	pme
rcoulomb	1.5	1.5	1.5	1.5
rcoulomb-switch	1.4	1.4	1.4	1.4
fourier-spacing	0.10	0.10	0.10	0.10
pme-order	6	6	6	6
ewald-rtol	1e-9	1e-9	1e-9	1e-9
Enable double precision	True	True	True	True
-DFLEXIBLE	False	False	False	False
Extend simulation from full-precision trajectory	False	False	False	False

	Minimize (vapor,fast)	NVT (vapor,fast)	NPT (vapor,fast)	NVE (vapor,fast)
dt		0.002	0.002	0.002
nsteps	5000	5000	5000	5000
integrator	steep	md	md	md
gen-vel		yes	no	no
tcoupl		berendsen	berendsen	
ref-t		300	300	
pcoupl		no	parrinello-rahman	
ref-p			1,0	
pbc	no	no	no	no
comm-mode	angular	angular	angular	angular
nstcomm		50	50	50
nh-chain-length		10	10	
nsttcouple		-1	-1	
nstpcouple			-1	
constraints	hbonds	all-bonds	all-bonds	all-bonds

continues on next page

Table 6 – continued from previous page

	Minimize (vapor,fast)	NVT (vapor,fast)	NPT (vapor,fast)	NVE (vapor,fast)
lincs-order		4	4	4
lincs-iter		1	1	1
shake-tol		1e-5	1e-5	1e-5
nstxout	100	100	100	100
nstvout	100	100	100	100
nstenergy	10	10	10	10
buffer-tolerance	5e-3	5e-3	5e-3	5e-3
rvdw	1,0	1,0	1,0	1,0
rvdw-switch	0.9	0.9	0.9	0.9
coulombtype	cut-off	cut-off	cut-off	cut-off
rcoulomb	1,0	1,0	1,0	1,0
rcoulomb-switch	0.9	0.9	0.9	0.9
fourier-spacing				
pme-order				
ewald-rtol				
Enable double precision	False	False	False	False
-DFLEXIBLE	False	False	False	False
Extend simulation from full-precision trajectory	False	False	False	False

	Minimize (vapor)	NVT (vapor)	NPT (vapor)	NVE (vapor)
dt		0.0005	0.0005	0.0005
nsteps	20000	20000	20000	20000
integrator	steep	md	md	md
gen-vel		yes	no	no
tcoupl		nose-hoover	nose-hoover	
ref-t		300	300	
pcoupl		no	parrinello-rahman	
ref-p			1,0	
pbc	no	no	no	no

continues on next page

Table 7 – continued from previous page

	Minimize (vapor)	NVT (vapor)	NPT (vapor)	NVE (vapor)
comm-mode	angular	angular	angular	angular
nstcomm		1	1	1
nh-chain-length		1	1	
nsttcouple		1	1	
nstpcouple			1	
constraints	hbonds	hbonds	hbonds	hbonds
lincs-order		8	8	8
lincs-iter		2	2	2
shake-tol		1e-9	1e-9	1e-9
nstxout	400	400	400	400
nstvout	400	400	400	400
nstenergy	40	40	40	40
buffer-tolerance	1e-9	1e-9	1e-9	1e-9
rvdw	1.5	1.5	1.5	1.5
rvdw-switch	1.4	1.4	1.4	1.4
coulombtype	cut-off	cut-off	cut-off	cut-off
rcoulomb	1.5	1.5	1.5	1.5
rcoulomb-switch	1.4	1.4	1.4	1.4
fourier-spacing				
pme-order				
ewald-rtol				
Enable double precision	True	True	True	True
-DFLEXIBLE	False	False	False	False
Extend simulation from full-precision trajectory	False	False	False	False

	Minimize (NMA)	NMA
dt		
nsteps	20000	20000
integrator	l-bfgs	nm
gen-vel		

continues on next page

Table 8 – continued from previous page

	Minimize (NMA)	NMA
tcoupl		
ref-t		
pcoupl		
ref-p		
pbc	yes	yes
comm-mode		
nstcomm		
nh-chain-length		
nsttcouple		
nstpcouple		
constraints	none	none
lincs-order		
lincs-iter		
shake-tol		
nstxout	400	400
nstvout	400	400
nstenergy	40	40
buffer-tolerance	1e-9	1e-9
rvdw	1.5	1.5
rvdw-switch	1.4	1.4
coulombtype	pme	pme
rcoulomb	1.5	1.5
rcoulomb-switch	1.4	1.4
fourier-spacing	0.10	0.10
pme-order	6	6
ewald-rtol	1e-9	1e-9
Enable double precision	True	True
emtol	0.01	
-DFLEXIBLE	True	True
Extend simulation from full-precision trajectory	False	True

# of Threads

Specify the thread parallel number.

MPI (for Remote Job)

Specify MPI parallel number. It is reflected only when executing by remote job submission.

Basic

Run Control

dt
Specify one step increment in numerical integration.

nsteps
Specify the maximum number of steps to calculate.

integrator
Specify the calculation algorithm.

Velocity Generation

gen-vel
Specify whether to generate the initial speed.

Fix random seed
When checked, gen-seed will be used.

gen-seed
Specify the initial speed random seed.

Explicitly set gen-temp
If checked, I will do the initial speed temperature here. If you do not enter ref - t will be the initial speed temperature.

Temperature Coupling

tcoupl
Select the temperature control algorithm.

tc-grps
Specifies the group to be temperature controlled (multiple settings are allowed, separated by spaces). If freezegrps is set when tc-grps=System, set tc-grps=freeze_xyz no_freeze and only no_freeze will control temperature.

ref-t
Specify the set temperature (Multiple settings can be set with a space delimiter).

year-t
Specify the time constant for temperature control (more than one can be set with a space delimiter).

Pressure Coupling

pcoupl
Select pressure control algorithm.

pcoupltype
It shows how to move cells in pressure control.

ref-p
Specify set pressure.

year-p
Specify the time constant for pressure control.

compressibility
Specify the compression ratio of the whole system.

Advanced

Boundary Condition

pbc
Select the periodic boundary condition.

Energy Minimization

emtol
Specify the maximum force which is the convergence condition of energy minimization calculation.

emstep
Specify the initial value of step width to move particles in energy minimization calculation.

Run Control

comm-mode
Specify how to remove the momentum of the whole system.

nstcomm
Specify the frequency of removing the momentum of the whole system.

Temperature/Pressure Coupling

nh-chain-length
Specify the number of stages of Nose-Hoover chain when temperature is controlled by the Nose-Hoover method.

nsttcouple
Specify the frequency of temperature control.

nstpcouple
Specify the frequency of temperature control.

refcoord-scaling
Specify the scaling of the reference coordinates of position restraint during temperature control.

Constraints

constraints
Select the constraint condition.

constraint-algorithm
Select the constraint algorithm.

continuation
Specify whether to inherit the constraint distance from the parent job.

lincs-order
Specify the order of the LINCS method.

lincs-iter
Specify the number of iterations in the LINCS method.

shake-tol
Specify the truncation error parameter used for the convergence judgment of the SHAKE method.

Misc.

print-nose-hoover-chain-variables
Specify this parameter when transferring temperature/pressure control parameters to a child job.

define -DFLEXIBLE
Select to make water molecule flexible.

define -DPOSRES
Select this to constrain the position of a specific molecule. (Include posres.itp)

Extend simulation from full-precision trajectory
If this item is checked and *Continue Simulation* is checked, the job is continued from the trr file of the previous job. If this item is not checked, the job is continued from the gro file in the final state of the previous job. For example, if you want to run normal mode analysis after the energy minimization calculation, you need to check the box.

Output

Output Control

nstxout
Specify the frequency of atomic coordinates output in steps.

nstvout
Specify the frequency of atomic velocity output in steps.

nstenergy
Specify the frequency of outputting system-wide statistics such as energy to edr file (energy file) in steps.

nstxout-compressed
Specify the frequency of atomic coordinates output in xtc format which can save file size by the step number.

compressed-x-grps
Specifies the group to output in xtc format. By default, the entire system is targeted. If you want to specify a group other than the default group, use Additional Group to add a group.

energygrps
If you want to obtain the time variation of the potential energy between specific atomic groups, specify the name of the atomic group to be used here. If you want to specify a group other than the default group, use Additional Group to add a group.

Additional Group
Adds atomic groups that can be used during MD calculations. Atomic groups must be registered beforehand in the main window with *Register Selected Group*. Add the groups you wish to specify with compressed-x-grps or energygrps. The group specified here will be added to the ndx file that is read at the time the tpr file is created by the grompp command.

Interaction

Modify cutoff radii not to exceed L/2
When checked, automatically adjusts rlist, rvdw, rvdw-switch, rcoulomb, and rcoulomb-switch so that they do not exceed half the lattice constant.

Neighbor Searching

nstlist
Specify how often to update the neighbor list.

ns-type
Specify how to create the neighbor list.

cutoff-shceme
Specify the method of selecting atoms to be included in the neighbor list.

Use buffer-tolerance
Specify the truncation error of binary potential energy, which is a parameter for automatically setting the cutoff distance of the neighbor list. When unchecked, the value of rlist is set as the cutoff distance.

rlist
Specify the cutoff distance of the neighbor list.

VdW

vdwtype
Specify the calculation method of van der Waals potential.

rvdw-switch
When Switching is selected for Van der Waals potential calculation, specify the distance at which Switching starts.

rvdw
Specify the cutoff distance of van der Waals potential calculation.

DispCorr
Select whether long-distance correction of energy and pressure accompany cutoff.

vdw-change
Select settings such as Switching/Shift when Van der Waals potential cutoff.

Electrostatics

coulombtype
Specify the calculation method of coulomb potential.

rcoulomb-switch
When Switching is selected for Coulomb Potential Calculation, specify the distance at which Switching starts.

rcoulomb
Specify the real space cutoff distance of Coulomb potential calculation.

Coulomb-change
Select the setting such as Switching/Shift at the cutoff of Coulomb potential.

Ewald

Set # of grids for fourier space
If checked, use fourier-spacing. If you do not want to use it, use fourier-nx, ny, nz.

fourier-spacing
Ewald, PME or PPPM method in wave number space mesh size.

fourier-nx, ny, nz
Ewald, PME or PPPM method to specify the cutoff distance or mesh number (x, y, z component, respectively) of wave number space.

pme-order
Specifies the order of the extrapolation function in the PME method.

ewald-rtol
Ewald, PME or PPPM method accuracy parameters.

Restraint

Set freezegrps to constrained atoms
Set freezegrps and constrain coordinates based on the optimization flags of the structure in the main window.

Automatic

Rescale velocities to..

Use it when you want to bring the system temperature closer to the target temperature in the NVE ensemble. Calculate the scaling factor from the average temperature under calculation and the temperature entered here and scale the velocity of each particle in the final structure.

Rescale box size to..

It is used when calculating with the NVE or NVT ensemble in the state close to the set pressure after calculating with the NPT ensemble. Scale the final structure to the average cell size under calculation.

Others

Other Parameters

Specify other settings based on the description of the mdp file.

Options

Restore Working Folder

Click to return *working folder* to its pre-execution status, such as when a continuous job ends abnormally.

Dump .mdp File

Create and save a Gromacs calculation condition (mdp) file with the settings in the currently opened window.

Dump All Files for Remote

This function does not run Gromacs, but only saves the files needed for Gromacs calculations. Please open the *Tools → Remote Job Submission* window before using this function.

Rerun from xtc

For the structure of the trajectory (xtc) file output from a calculation that has already been completed, only the energy is calculated using the calculation conditions set in the currently opened window, and the energy (edr) file is obtained.

Open top file

Open the top file generated by the Assign Force Field function in a text editor.

maxwarn

Allow continuation of calculation warning message Specify the maximum number of messages (0: suspend with one or more messages)

Verbose Output

Specify this when displaying the step under calculation.

Concatenate .edr and .trr files

Click to merge with the executed .edr file and .trr file. File binding is performed as postprocessing of Continue Simulation.

Unwrap Atoms (trjconv -pbc nojump)

Output the calculated .gro and .trr files at coordinates that do not wrap around at periodic boundaries (unwrapped).

Enable Double Precision

Execute MD calculation and pre-post processing with double precision version of Gromacs binary.

Overwrites any output file without making a backup in working folder

If checked, when creating a new file in the working folder, a backup will be made if there is an old file with the same name. To save disk space, it is recommended to uncheck this item if *Make a Backup of Working Folder* is checked.

Read initial temperature and pressure coupling variables from .edr file
Reads temperature/pressure control variables from the source job's edr file at the time of the continuation job.

Force use Gromacs 5.0.7 on local computer
When using CygwinWM 2025/7/1 version or later with Gromacs5.0.7 and Gromacs2024.4 installed, Gromacs5.0.7 is forced to be used where Gromacs2024.4 is used by default. In particular, if you want to perform free boundary energy minimization calculations, you must use Gromacs5.0.7 because it is not implemented in Gromacs2024.4. This setting is valid for local jobs only.

Enable detailed parallelization setting
Instead of using -nt to specify the number of total threads, the number of parallel Thread-MPI (-ntmpi) and OpenMP (-ntomp) threads can be specified individually.

# of Thread-MPI
Specifies the number of Thread-MPI parallel number.

# of OpenMP
Specifies the number of OpenMP parallel number.

Reset
Reset settings..

Import
Loading configuration file.

Export
Output configuration file.

6.14.4 Run Gromacs

Run Gromacs. The execution method differs depending on the situation.

- **(Default) If *Continue Simulation* is unchecked and *Automatically assign parameters* is checked on *Asign Force Field***
  Create a new coordinate file (extension: gro) and topology file (extension: top) before starting the job.
- **If *Continue Simulation* is unchecked and :guilabel:` Use parameters from topology file` is selected for *Asign Force Field***
  Start the job using the coordinate file (extension: gro) opened in the main window and the topology file (extension: top) specified at *Asign Force Field*.
- **When *Continue Simulation* is checked**
  The coordinate file (`gmx_mdrun_tmp.gro`) and the topology file (`gmx_tmp.top`) in the working folder linked to the coordinate file (extension: gro)) To start the job.

Following file will be generated with execution. As an example, the file/folder name when the input file is `water.gro` is also shown.

type	Description
out file `water.out`	`water.sh` standard output text file.
sh file `water.sh`	For running Gromacs and its pre/post processing Shell script.
conf.sh file `water_conf.sh`	This is a shell script from which settings that depend on the content of the calculation are extracted.
bat file `water.bat`	This is a batch file for executing `water.sh`.
Working Folder `water_gmx_tmp\`	Working folder.

The following files are generated in the working folder. Only the main files are shown here.

type	Description
`input.gro`	In the case of a new job, the gro file specified at the time of execution is copied. In case of continuous job, it becomes the file of the previous job.
`gmx.top`	In the case of a new job, the top file specified at the time of execution is copied. In case of continuous job, it becomes the file of the previous job.
`gmx.mdp`	It is a file that specifies calculation conditions.
`gmx_mdrun.tpr`	Generate from gro, top, mdp file It is an input file of mdrun.
`gmx_mdrun.ndx`	Index file for result processing.
`gmx_mdrun.edr`	Temperature, pressure, energy etc. were stored It is an energy file.
`gmx_mdrun.gro`	It is a gro file of the final structure.
`gmx_mdrun.trr`	It is a trajectory file.
`gmx_mdrun.xtc`	Compressed trajectory file.
`gmx_mdrun.log`	This is the log file of mdrun.

Hint: ** Working folder **

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.
  - ** The suffix varies depending on the type of solver. **
  - For example, in the case of Gromacs, if the file opened in the main window is `aaa.gro` and the suffix is `_ gmx_tmp`, the working folder will be named `aaa_gmx_tmp` .
- It must be in the same hierarchy as the file opened in the main window.
- Processing continues in the working folder of the same name even when continuing jobs, but by default the backup of the working directory of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the one with the smallest number in the range where duplicate names do not exist. For example, if the working folder is `aaa_gmx_tmp`, it is `aaa_gmx_tmp1`.
  - ** Directories without numbers are always up to date. **

The job is run through *Winmostar Job Manager*.

6.14.5 Open Log File (log)

Open the log file (`* _ gmx_tmp gmx_tmp_mdrun.log`) of **`gmx mdrun`** with a text editor.

6.14.6 Open Stdout File

Open the standard output (`*. Out`) of the shell script when running Gromacs with a text editor.

6.14.7 Animation

Select the gro file and trr file, and animate the MD calculation trajectory. The file name of the main window does not change. If you open a trr file while a calculation is running, only the collapsed coordinates in the simulation cell will be read. After the calculation, the **`gmx trjconv -pbc nojump`** command will convert the trr file so that the uncollapsed coordinates are read. For the animation display operation method, see *Animation operation area*.

6.14.8 Energy Plot

Selects the Gromacs output edr file and displays graphs of various thermodynamic quantities, such as energy, temperature, and pressure. Internally, the command **`gmx energy`** is executed. Please refer to the manual of gmx energy for more detailed behavior. Please see *Energy Plot window* for how to operate subwindow.

6.14.9 Import Last Coordinate (gro)

`* _ gmx_tmp \ gmx_tmp_mdrun.gro`. When using this function, the file name of the main window does not change.

6.14.10 Configure Sequential Job

Configure settings for continuous execution of Gromacs. If you want to run with settings other than the presets, enter the calculation conditions you want to run in advance with *Configure* and save it in gmxset format with the *Save* button.

6.14.11 Run Sequential Job

Run Gromacs sequentially based on the contents of *Configure Sequential Job*.

6.14.12 Analyses

Radial Distribution Function

Select a trr, tpr or ndx file output by Gromacs and display the radial distribution function. Internally, the command **`gmx rdf`** is executed. Please check the manual of gmx rdf for more detailed behavior. Radial distribution functions are computed between *Reference Group* and *Target Group*.

Definition

Atom
Set the calculation target to atomic coordinates.

Center of geometry
The target of the calculation is the geometric mean coordinates of the molecules, using Gromacs 5.0.7 in CygwinWM.

Center of mass
The target of the calculation is the position of the center of mass of the molecule, and Gromacs 5.0.7 in CygwinWM is used.

Output

RDF
Calculate radial distribution function.

Cumulative Number RDF
Calculate the integrated coordination number.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Diffusion Constant/Mean Square Displacement

Select the trr, tpr, and ndx files output by Gromacs and display the mean square displacement and self-diffusion coefficient. Internally, the :command **`gmx msd`** is executed. Please refer to the manual of gmx msd for more detailed behavior.

Type
For no, the mean-square displacement is calculated as usual; for x, y, and z, the mean-square displacement is calculated on each axis.

Diffusion Constant
Use the **`gmx msd`** command to display the self-diffusion coefficient calculated from the slope of the time-mean square displacement graph.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Scattering Function

Select a trr, tpr or ndx file output by Gromacs and display the scattering function. Internally, the :command **`gmx saxs`** is executed. Please refer to the manual of gmx saxs for more detailed behavior.

Interval
Specify the interval at which to acquire the snapshot used to calculate the scattering function. Attention is necessary because enormous calculation is necessary if it is too small.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Total Linear Momentum

Select the trr, tpr, and ndx files output by Gromacs and display the total linear momentum. Internally, the trajectory is converted to an animated gro file containing the velocities and then the histogram is calculated inside Winmostar.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File

Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame

Specify the start time when trajectory is read in ps units.

Last Frame

Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance

Edit the arguments of the gmx command before running the analysis.

Show Log

Display the log file of the gmx command output during the analysis run.

Draw

Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Velocity Distribution

Select the trr, tpr, and ndx files output by Gromacs and display the velocity distribution. Internally, the trajectory is converted to an animated gro file containing the velocities and then the histogram is calculated inside Winmostar.

Norm

Calculates the velocity distribution with respect to the absolute value of the velocity vector.

X/Y/Z

Calculates the velocity distribution for the x, y, and z components of the velocity vector.

# of bins

Specifies the number of divisions of the velocity distribution function.

Target Group

Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group

It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group

Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)

In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)

In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Velocity Autocorr/Vibration Spectrum

Select the trr, tpr, and ndx files output by Gromacs to display the velocity correlation function and the vibration spectrum. Internally, the :command **`gmx velacc`** is executed. Please refer to the manual of gmx velacc for more detailed behavior.

Velocity Autocorrelation
Output speed correlation function.

Vibration Spectrum
Output vibration spectrum.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of

atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Static Dielectric Constant

Select a trr, tpr or ndx file output by Gromacs to display the distribution and histogram of the relative permittivity or dipole moments. Internally, the :command **`gmx dipoles`** is executed. Please refer to the manual of gmx dipoles for more detailed behavior.

Dielectric constant
Plot the relative dielectric constant. The value of epsilon at the last time in the graph is the relative dielectric constant obtained from that calculation. The value is output below the graph.

Total dipole moment
Plot the time variation of dipole moments of molecules belonging to the Target Group.

Histogram of total dipole momen
Plot the distribution of dipole moments for molecules belonging to the Target Group.

Autocorrelation function of dipole moment
Plot the autocorrelation function of the dipole moments. The definition of a dipole moment is selected in Definition.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to

add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Share Viscosity

Select the trr, tpr, ndx file output by Gromacs and display the viscosity. Internally, the :command **`gmx tcaf`** is executed. Please refer to the manual of gmx tcaf for more detailed behavior.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Density Profile

Select a trr, tpr or ndx file output by Gromacs to display the density distribution. Internally, the :command `gmx density` is executed. Please refer to the manual of gmx density for more detailed behavior.

Group
The density distribution is output for the components that are checked here.

Axis
Specifies the direction in which the density distribution is calculated.

# of slices
Specify the number of points for the density distribution graph.

Definition
Specify the definition of density.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered*

Group, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Free Volume

Select a trr, tpr or ndx file output by Gromacs to display the density distribution. Internally, the :command `gmx freevolume` is executed. Please refer to the manual of gmx freevolume for more detailed behavior.

Radius of probe
Specify the radius of the virtual probe particles that are randomly inserted into the system when calculating the free volume.

# of probe insertions
Specify the number of virtual probe particle insertions.

Random seed
Specify a random seed to determine where to insert virtual probe particles.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered*

Group, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Hildebrand Solubility Parameter

Calculate the Hildebrand solubility parameter from the edr, gro file output by Gromacs. Calculation results of gas phase and liquid phase are required. Hildebrand The **`gmx energy`** command is executed to obtain the cohesion energy, density (specific volume) and compression rate necessary for calculating the solubility parameter.

Chi/DPD parameter

Calculate the Chi parameter · DPD aij parameter from the edr, gro file output by Gromacs. It is necessary to calculate the gas phase and liquid phase of each of the two components. Internally use the value calculated by *Hildebrand Solubility Parameter*.

Bond/Angle/Dihedral distribution

Select a trr, tpr, or ndx file output by Gromacs to display the distribution of distances, angles, or two-plane angles between the selected groups. Internally, the **`gmx distance`** command (distance) or the **`gmx angle`** command (angle, two plane angle) is executed. Please refer to the manuals of gmx distance and gmx angle for more detailed behavior.

Type
Select the type of value to plot (bond, angle, dihedral, improper or ryckaert-bellmemans).

Calculate for marked atoms
Calculates the distance, angle, or dihedral angle between atoms marked with a marker in the main window.

Calculate for target group
Calculate the distance, angle, or dihedral angle using the NDX file selected in the Target Group.

Calculate for
Calculates the angle or dihedral angle for the selected angletype or dihedraltype.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group

It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group

Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)

In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)

In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File

Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame

Specify the start time when trajectory is read in ps units.

Last Frame

Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance

Edit the arguments of the gmx command before running the analysis.

Show Log

Display the log file of the gmx command output during the analysis run.

Draw

Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Hydrogen bonding analysis

Selects the trr, tpr, and ndx files output by Gromacs and analyzes the hydrogen bonds between the selected groups. Internally, the **`gmx hbond`** command is executed. Please refer to the gmx hbond manual for detailed behavior.

Type

Select the type of value to plot: for Autocorrelation function, use Gromacs 5.0.7 in CygwinWM.

Cutoff angle

Specifies the cutoff value for the hydrogen-donor-acceptor angle when determining hydrogen bonding.

Cutoff distance

Specifies the cutoff value for the donor-acceptor distance when determining hydrogen bonding.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Atom/Group Distance Change

Select a trr, tpr, or ndx file output by Gromacs and analyze the change in distance between specific atoms or between specific groups of atoms. Internally, the `gmx distance` command is executed. Please refer to the manual for the gmx distance command for detailed behavior.

Definition of distance
Select a definition for the distance. For “COMs of Reference and Target Groups”, it calculates the distance between the center of gravity of the group selected in the Reference Group and the center of gravity of the group selected in the Target Group. For “Odd and even atoms in Target Group,” calculate the distance between the odd and even atoms defined in the group specified in the Target Group.

Component
Select the type of distance to plot.

Use periodic boundary condition
Apply periodic boundary conditions when calculating distances.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Root Mean Square Deviation

Select the trr, tpr, and ndx files output by Gromacs and display the RMSD (mainly for proteins). Internally, the :command **`gmx rms`** is executed. Please refer to the manual of gmx rms for more detailed behavior.

Group
Results are output for the components checked here. Normally select *Backbone*.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Radius of Gyration

Select a trr, tpr or ndx file output by Gromacs and display the rotation radius (mainly for the protein). Internally, the :command **`gmx gyrate`** is executed. Please refer to the manual of gmx gyrate for more detailed behavior.

Group
Results are output for the components checked here. Normally you will select Backbone.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

Ramachandran Plot

Select the trr, tpr, and ndx files output by Gromacs to display the Ramachandran plots for each amino acid residue. Internally, the :command `gmx rama` is executed. Please refer to the manual of gmx rama for more detailed behavior.

Residue
Here a Ramachandran plot of the selected residue is output.

Target Group
Calculate the physical quantity for molecules/atoms belonging to the selected group here. A group written in the opened ndx file can be selected here.

Reference Group
It only appears for physical quantities to be calculated for atom pairs such as radial distribution functions. The physical quantity is calculated between *Target Group* and *Reference Group*.

Edit Group
Adjust the contents of the Target Group and Reference Group.

Create Group (by Element)
In the *Create Group* window, check *Extracted Atom Names* and enter *New group Name* and press the *Create* button, the group is added to the ndx file It will be added. When you press the *Close* button, the groups added to *Target Group* and *Reference Group* are added.

Create Group (by Selecting Atoms in 3D)
In the *Create Group* window, first select the target molecule species in *Target*, then Ctrl+click or Ctrl+drag to select the atoms in the 3D molecule that you want to add to the group, in blue color. Then click *Add*. Add all the atoms you want to add to the group, and click *OK* button to add the group to the ndx file. Click *Close* button to add the group you added to the *Target Group* or *Reference Group*.

Select ndx File
Loads a Group from an ndx file. If you want to perform result analysis on an arbitrary group of atoms, select a group for analysis in the main window, register the group with *Select Registered Group*, create an ndx file with *Export Groups to Index File (ndx)* to create an ndx file and then select the ndx file with this function.

First Frame
Specify the start time when trajectory is read in ps units.

Last Frame
Specify the end time, in ps, to read trajectories. If *Maximum* is checked, the last frame is specified.

Edit Commands in Advance
Edit the arguments of the gmx command before running the analysis.

Show Log
Display the log file of the gmx command output during the analysis run.

Draw
Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

6.14.13 Modify Trajectory File

You can perform operations such as thinning, rotation, and calculation of spatial distribution functions on the trajectory data in the trr or xtc file output from Gromacs. Internally, the :command **`gmx trjconv`** is executed. Please refer to the manual of gmx trjconv for more detailed behavior. Click *Execute* button to start the process.

Output interval
Specify how many frames to output by thinning the trajectory.

Postprocess
Specify the operation after processing. If *Spatial distribution function* is selected use **`gmx spatial`**.

Target group
Specify the group to output.

Rotate and Trans
The group specified by *Reference group* is fixed so that the group specified by *Target group* is rotated and translated.

Reference group
Specify refernce in *Roate and Trans*.

Group for SDF
Specify which group to calculate SDF calculated when *Spatial distribution function* (SDF) is selected in *Postprocess*.

6.14.14 Start ER

Calculate the solvation free energy using the energy indication (ER) method.

1. Execute the calculation of the following three in Gromacs beforehand and leave each working folder. Only use equilibrium state data after finishing equilibration such as energy minimization.
   A. Solution system (1 solute molecule + many solvent molecules)
   B. Solvent system (large number of solvent molecules)
   C. Solute system (one solute molecule)
2. Drag and drop the working folder of A. Solution system on the *Solution* tab. Or, in each column of the xtc, log, top file, press ... button to read individual files.
3. Likewise select the B. Solvent system file on the *Solvent* tab.
4. Similarly select the C. Solute system file in the *Solute* tab. If an xtc file is specified, if the solute specifies a flexible model, pdb or gro file, it is treated as a rigid body model.
5. Select the molecular name of the solute in *Solute Name*.
6. If necessary, specify MPI parallel number at free energy calculation from *Options* button.
7. To implement free energy calculation in the local environment press the *Start* button. Calculation begins when you specify the folder to output the result. On Cygwin, **`ermod`** flows.
8. To implement in the remote environment, press the *Close* button once. And at *Remote job* execute *Program* with `ermod`. On the remote server, it is necessary for **`ermod`** and **`slvfe`** command to pass **`$PATH`**. (Installing ERmod on remote server is *here <https://winmostar.com/en/gmx4wm_en_linux.html>*) After finishing the calculation, press *get* button in *Remote job*, you will find `ermod_remote_*` under the folder where `winmostar.exe` is placed and the result is transferred from the remote server.

9. After calculating the free energy calculation, to display the result, select the *Import ER* menu.

Hint: If you want to analyze the data using ERmod functions, which are not supported by Winmostar, you can also follow the procedure below.

1. First, we will use Winmostar to calculate the MD for solution, solvent only, and solute only. For those procedures, please refer to the tutorial on using the ER method.
2. Follow the steps after "Generate input configuration for running ermod" in Quick Start Guide on the official ERmod homepage. Follow the steps after "Generate input configuration for running ermod". Click [Tools]-[Cygwin] in Winmostar to start the Cygwin terminal, where the installation of Gromacs, ERmod, etc. is completed. The "(ERmod directory)" in the procedure is `/usr/local/ermod` on Cygwin. The `etohsolution.top` will be the top file saved at the start of the solution calculation. Please use `solution_run.xtc` and `solution_run.log` which are stored in the working folder of MD for solution, solvent only, and solute only, respectively.

6.14.15 Import ER

The results processed by *Start ER* are displayed. After selection, specify the output destination folder specified by *Start ER*. You can specify units for displaying energy in *Unit*. Press the *Log* button to display ERmod's log file.

6.14.16 Start BAR

Calculate the solvation free energy using the Bennett Acceptance Ratio (BAR) method.

1. Calculate the solution system (1 solute molecule plus a large number of solvent molecules) using Gromacs. Leave all working folders for each step of equilibration and calculation of equilibrium state.
2. Select *Start BAR*.
3. Specify how to integrate the state (lambda = 1, Full Coupling) in which the solute is not interacting with the solvent (lambda = 0) to the interaction state (lambda = 1, Full Coupling) on the *Integration Path* tab. Enter the coupling coefficient of van der Waals potential (left) and the coupling coefficient of coulomb potential (right) in the two columns on the left of the *Insert* button and press *Insert* to add an integration path.You can delete the integration route by pressing *Delete*.
4. In *Procedure* tab, specify the simulation procedure of each state on the integration path. Specify the procedure of equilibration of solution system (lambda = 1) prepared beforehand in folder unit. Add a folder by dragging and dropping to the *Add* button or list. Delete folder with *Delete* button. The calculations performed in the last step of the list are used for free energy calculations.
5. Press *Start* to execute MD calculation for each lambda.
6. After finishing MD calculation of each lambda, to display the result, choose *Import BAR*.

6.14.17 Import BAR

Display the result of processing with *Start BAR*. After selecting the menu, specify the destination folder with *Start BAR*. The **`gmx bar`** is executed in the background and the result is displayed. Please refer to the manual of gmx bar for more detailed behavior.

> *Unit* allows you to specify the unit in which the energy is displayed. If you press *Log* button, the log file of **`gmx bar`** will be displayed. The displayed graph shows the change in free energy between the state in which the solute is not interacting with the solvent (lambda=0) and the state in which it is interacting (lambda=1).

6.15 Solid Menu

It is a menu related to first principle (band) calculation. Solid pack is required to use the functions of the solid menu.

6.15.1 Crystal Builder

Create a crystal structure. It is mainly used for the following purposes.

- Enter the space group, lattice constant, asymmetric element and create crystal structure.
- Open the CIF file on the crystal builder and replace the axes a, b, c.
- Open a CIF file containing a noninteger occupancy and allocate atoms.

File menu

New
We will create a new crystal structure.

Open
Open the CIF file.

Save As
Save the crystal structure displayed in the crystal builder in CIF format or XYZ format.

Save As P1 CIF
If checked, save it in P1 when saving in CIF format.

Edit Menu

Exchange Axis
Exchange the coordinates (x, y, z) of the axis (a, b, c) and the asymmetric element. For details, please see International Tables vol.

Discard symmetry
Discard the symmetric operation and let P1 be the space group. At this time, all symmetric elements reproduced by the existing symmetrical operation are recognized as asymmetric elements.

Assign Atoms to Non-Integer Occupancy Sites
Random atoms are generated for each site based on the item (_atom_site_occupancy) defined in the imported CIF file. If you want to create a supercell according to the occupancy rate, use this function after creating a sufficiently large supercell using the repeat function.

View menu

Show Multi-View
We will draw by triple drawing. In the three view, only the upper left window corresponds to free rotation, and the remaining three direction cameras are fixed to the a, b, c axes of the crystal and therefore will not rotate.

Always View Center
When checked, always keep the gaze point on the center of gravity

Orbit/Roll
Specify the rotation method.

Orbit
It performs free rotation.

Roll around a-, b-, c-axis
It rotates around the a, b, c axes.

Show Bond
Displays the join.

Show Element Name
It displays the element symbol.

Show Atoms on Boundary in Duplicate
Display atoms on the boundary.

Show Unit Cell
Display unit lattice.

Make Replicated Atoms Transparent
Transparent display of atoms generated by symmetrical operation.

Lattice

Crystal System
Select crystal system.

Space Group
Select space group from number or Hermann-Mauguin symbol.

Lattice Constant
Set lattice constants (fields that can be entered depend on the selected space group).

Asymmetric unit

Add atom
Add an atom that becomes an asymmetric element.

Delete atom
Delete the atom which becomes the asymmetric element selected on the list.

Element
Enter/Modify the element symbol.

X, Y, Z
We set the atomic site with the fractional coordinate (fractional coordinate).

OK
Load the created crystal structure into the main window. If you want to cancel the import, please click *Edit* → *Undo* on the main window.

Cancel
Discard the structure entered in the crystal builder and return to the main window.

6.15.2 Build Cluster Model

If *Tools → Preferences menu* has *Use New Slab Builder* checked, it works as follows.

Miller indices
Define the Miller index (hkl) of the surface.

Force orthorhombic cell
If unchecked, the first basic lattice found by the internal process that satisfies the specified Miller index will appear. If checked, the internal process is executed until a basic lattice of rectangles satisfying the specified Miller index is found, at which point the structure appears.

Supercell
Enter the number of supercells in the surface horizontal direction (a or b-axis).

Set slab width by length
Specify the thickness of the slab in angstroms, and enter the location of the lower and upper bound of the slab in the Lower bound and Upper bound.

Set slab width by repeat units
Specify the thickness of the slab in basic cell units, and enter the location of the lower and upper bound of the slab in the Lower bound and Upper bound.

Vacuum
Enter the thickness of the vacuum layer; if Vacuum is entered, the Total width is automatically changed.

Total width
Enter the length of the cell in the c-axis direction; if Total width is entered, Vacuum is automatically changed.

Position
Specify the position of the slab perpendicular to the surface.

Terminate dangling bonds width hydrogen
If checked, hydrogen atoms are added to the bonds that are broken on the slab surface. If more hydrogen is added than expected, use *Delete* or *Delete atom* after using this function to delete excess hydrogen atoms.

Do not insert vacuum
If checked, no vacuum layer is inserted. This is used when you do not want to create a slab and just want to re-create the basic lattice with a mirror index.

Maximum slab width internally generated
Specifies the maximum thickness of the slab to be generated by the internal process if the basic grid is not found at the specified Miller index, such as in the case of a high-index surface. The value (absolute value) set in Lower bound or Upper bound must be less than half of this value.

OK button
Creates a slab model and displays it in the main window.

If *Tools → Preferences menu* does not check *Use New Slab Builder*, it works as follows. Calling this function with a (bulk) crystal CIF file loaded will create a slab. Internally, it uses pymatgen or an in-house routine that simulates pymatgen. First, click the *Generate Slab* button, and then click the *OK* button.

Miller indices
Define the Miller index (hkl) of the surface.

Minimum slab size
Enter the cell size in the face vertical (c-axis) direction.

Supercell
Enter the number of supercells in the surface horizontal direction (a or b-axis).

Force c-axis to be perpendicular to a and b axes
Ensure that the c-axis is perpendicular to the a and b axes.

Convert hexagonal to orthorhombic
Convert Hexagonal to Orthorhombic.

Generate Slab button
This button creates a candidate surface structure based on the items above.

Surface configurations
Select a surface structure from among the candidates.

Slab, Vacuum, Total width
Enter the size of the surface vertical. If you enter ont of *Vacuum* or *Total width*, the other will be determined automatically.

Position
Specify the position of the slab perpendicular to the surface.

OK button
Creates a slab model and displays it in the main window.

Warning: In order to use this feature, you need *CygwinWM setup*.

6.15.3 Generate Supercell

Duplicate the cell displayed in the main window and create a super cell. Enter the number of repetitions in *a* , *b* , *c* and click the *OK* button.

6.15.4 Build Cluster Model

Cut out nanoclusters from the crystal structure. The atoms of the original unit cell are opaque and atoms outside the unit cell are translucent.

View menu
It is the same as *Crystal Builder*.

Center
Specify the cluster center point in fractional coordinates. With an atom selected on the graphic screen, click Set to specify the selected atom position as the center point.

Cluster Radius
Specifies the radius of the cluster in angstroms.

Hydrogen
Modifies hydrogen on cluster surface.

OK
Perform the processing.

6.15.5 Convert Lattice (Primitive-Conventional)

Converts between primitive cells-conventional cells for cells displayed in the main window. Uses spglib in the background.

6.15.6 Convert lattice to equivalent rectangular cells

Convert to equivalent rectangular cells for cells displayed in the main window. Useful for converting hexagons to rectangular cells. Uses atomsk in the background.

> **Warning:** In order to use this feature, you need *CygwinWM setup*.

6.15.7 Transform Unit Cell

The rotation matrix is used to deform the unit grid vectors in each of the a, b, and c axes. Since each element of the rotation matrix is an integer, the transformed cell is also a unit cell. This is useful when you want to re-transform the unit cell lattice vectors.

6.15.8 Refine Lattice

This function detects the symmetry of a cell displayed in the main window with a set tolerance, and then slightly adjusts the coordinates to conform to that symmetry, which may help avoid symmetry-related problems in Quantum ESPRESSO and other applications. It uses spglib in the background.

6.15.9 Quantum ESPRESSO

See *Solid → Quantum ESPRESSO menu*.

6.15.10 OpenMX

See *Solid → Quantum ESPRESSO menu*.

6.15.11 FDMNES

See *Solid → FDMNES menu*.

6.16 *Solid → Quantum ESPRESSO* menu

It is a menu related to Quantum ESPRESSO.

6.16.1 How to set up Quantum ESPERSSO

To install Quantum ESPRESSO, install CygwinWM version 2023/04/05 or later, which contains `pw.exe`, etc. in `/opt_win/QuantumESPRESSO*/bin/` of CygwinWM. and so on in `/opt_win/QuantumESPRESSO*/bin/`. To use Quantum ESPRESSO from Winmostar, use *Tools → Preferences menu*. If you use CygwinWM 2023/04/05 version or later, you do not need to configure. First, under *program path → Quantum ESPRESSO*, select the Quantum ESPRESSO `pw.exe` that you want to use. Next, under *Calculation → mpiexec (QE)*, select *MPICH* or *Select* and select the `mpiexec.exe` of the MPI you want to use. If you are using Quantum ESPRESSO in CygwinWM, select `/opt_win/MSMPI/Bin/mpiexec.exe` under CygwinWM. Then, under *Calculation → Options for mpiexec (QE)*, enter the arguments for **`mpiexec.exe`**. If you use Quantum ESPRESSO in CygwinWM, enter **`-np % WM_NUM_PROC%`**. Finally, select the version of `pw.exe` that you selected in *Calculation → Version of QE to use*, or *7.1* if you are using Quantum ESPRESSO in CygwinWM. If you want to add a pseudo-potential file, click *Tools → Preferences menu → Calculation → Solid → QE pseudo-potential folder → Open QE pseudo directory* and add the pseudo Add the pseudo-potential file to the opened folder. The pseudopotential file extension must be upf (case insensitive). You can also create and select a new pseudo-potential folder. If you want to add MOL files for RISM calculations, click *Tools → Preferences menu → Calculation → Solid → Folder for QE MOL files → Open* and add MOL files to the opened folder. The pseudopotential file extension must be mol (case-insensitive); you can also create a new folder for MOL files and select it. Instructions for installing Quantum ESPRESSO on a remote machine can be found at *Installing Winmostar and solvers*.

6.16.2 Workflow Setup

Set up and run the Quantum ESPRESSO calculation flow in project mode.

Preset
Import and saves a preset of settings.

# of Jobs
Specify the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation. For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File → Project → Scan Results* to tabulate the calculation results.

Import
Import the settings output by Export. Click the arrow at the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Runs a calculation or generates a file with your settings. See *For project mode* for details.

Details
Set detailed calculation conditions. The *Configure* will be launched.

Task
Select the type of calculation.

	Setting details
Energy	calculation=scf ion_dynamics=none cell_dynamics=none tprnfor=False tstress=False nosym=False nstep=50 Use cell_factor=False electron_dynamics=none pot_extrapolation=none wfc_extrapolation=none Unit for atomic position=angstrom
NSCF	calculation=nscf ion_dynamics=none cell_dynamics=none tprnfor=False tstress=False nosym=False nstep=50 Use cell_factor=False electron_dynamics=none pot_extrapolation=none wfc_extrapolation=none Unit for atomic position=angstrom
Optimize(Atom)	calculation=relax ion_dynamics=bfgs cell_dynamics=none tprnfor=True tstress=False nosym=False nstep=50 Use cell_factor=False electron_dynamics=none pot_extrapolation=none wfc_extrapolation=none Unit for atomic position=angstrom
Optimize(Atom&Cell)	calculation=vc-relax ion_dynamics=bfgs cell_dynamics=bfgs tprnfor=True

Charge
Specifies the charge for the entire system.

# of bands
Specify the number of bands.

Spin
Set up the spin polarization calculation. Polarized (Manual) allows you to set the initial magnetization moment more flexibly for magnetic material calculations because Use Spin Density as is false and each element can have only one initial magnetization moment.

	Setting details
Non-polarized	nspin=1
Polarized	nspin=2 Use Spin Density as=True
Polarized(Manual)	nspin=2 Use Spin Density as=False

Cutoff energy
Sets the cutoff energy (ecutwfc) of the wave function.

Manually specify cutoff energy
If not checked, Cutoff energy is automatically specified from Precision.

K points
Specify how to calculate K points.

Pressure
Specify pressure.

Phonon(DFPT)
Set up phonon calculations using DFPT(ph.x).

	Setting details
Disabled	Run phonon=False epsil=False lraman=False asr=no ldisp=False
Gamma	Run phonon=True epsil=True lraman=True asr=crystal ldisp=False
Dispersion	Run phonon=True epsil=False lraman=False asr=crystal ldisp=True

Use Bravais-lattice index

If checked, input file will be created with other than ibrav=0. Check this box because it is necessary to set special points from ibrav when calculating band structure and phonon bands.

Pseudopotential

Specify a pseudopotential file. changing Type will narrow down the Functional and Pseudo files. changing Functional will narrow down the Pseudo files. Changing Functional will narrow down the Pseudo files. See Pseudopotential in *Configure* for instructions if the desired choice does not appear.

Properties

Calculate properties checked to match when calculating.

Precision

Set calculation precision.

	Setting details
Extra-low	conv_thr=1d-5 etot_conv_thr=1d-3 forc_conv_thr=1d-2 press_conv_thr=1.0 degauss=0.02 tr2_ph=1d-10 Spacing=0.44(metal) 0.63(nonmetal) ecutwfc=30(metal) 25(nonmetal)
Low	conv_thr=1e-6 etot_conv_thr=1d-4 forc_conv_thr=1d-3 press_conv_thr=0.5 degauss=0.02 tr2_ph=1e-11 Spacing=0.44(metal) 0.63(nonmetal) ecutwfc=40(metal) 30(nonmetal)
Medium	conv_thr=2d-7 etot_conv_thr=4d-5 forc_conv_thr=5d-4 press_conv_thr=0.25 degauss=0.02 tr2_ph=1e-12 Spacing=0.31(metal) 0.50(nonmetal) ecutwfc=50(metal) 35(nonmetal)
High	conv_thr=1d-7 etot_conv_thr=2d-5 forc_conv_thr=3d-4 press_conv_thr=0.125 degauss=0.02 tr2_ph=1e-14 Spacing=0.25(metal) 0.44(nonmetal) ecutwfc=55(metal) 40(nonmetal)
Extra-high	conv_thr=5d-8 etot_conv_thr=1d-5 forc_conv_thr=1d-4 press_conv_thr=0.05 degauss=0.01 tr2_ph=1e-16

Metal

Enable smearing. (occupations=smearing) Also adjusts the contents of Precision (above).

6.16.3 Configure

Set the calculation condition of Quantum ESPRESSO. To set up the calculations immediately after setting *Run* button, once to return to the main window please press :guilabel:` OK` button. See *Run* for behavior when clicking *Run*. Return to the default state with *Reset* button. Save the setting except Force Field with *Save* button. Load the setting saved by *Save* with the *Load* button. If the Quantum ESPRESSO keyword displayed in the *Keyword Editor* and the contents set in this function window are different, you will be asked if you want to load the keyword from the Keyword Editor. When invoking this function, if the structure displayed in the main window can be changed to a primitive cell, *Convert Lattice (Primitive-Conventional)* is executed automatically.

Output Directory

Specify the output destination folder (outdir) of the data, and at the same time specify the new/continued execution of the job.

Create

Create a new folder to output data to. outdir will be set to the new folder.

Continue

Continue with the last executed QE job that is loaded on the main screen. outdir is set to the outdir of the last executed job.

Select

Specify the folder specified in the dialog that opens as the output destination and continue the job from the data in that folder. outdir will be set to what you specify here.

Preset

Select preset for setting. Each preset changes the following keywords

	SCF	SCF+Ba +DOS	SCF+Ba (Fermi surf)	Relax	Relax (variable cell)	BOMD	CPMD	Phonopy
calculatio	scf	scf	scf	relax	vc-relax	md	cp	scf
Use nbnd	False	True	True	False	False	False	False	False
K_POIN	gamma	automatic 4 4 4 1 1 1	automatic 4 4 4 1 1 1	gamma	automatic 4 4 4 1 1 1	gamma	gamma	gamma
tstress	False	False	False	False	False	True	False	False
Set ibrav and celldm	False	True	True	False	False	False	False	False
occupatio			smearing					
ion_dyna				bfgs	bfgs	verlet	none	
cell_dyna					bfgs			
tprnfor	False	False	False	True	True	True	True	True
tstress	False	False	False	False	True	False	False	True
Use cell_facto	False	False	False	False	True	False	False	False
pot_extra						second_orde		

Use MPI

Specify whether to execute parallel calculation using MPI when executing QE. Enter the number of MPI processes in the horizontal field.

Basic Tab

restart_mode

When from_scratch is set, the job is started without using information from previous jobs; when restart is set, the job is started using information from outdir; when Automatically set, in project mode, from_scratch is used for new jobs and restart is used for other jobs. Automatically set is used in project mode for new jobs from_scratch, and restarts for all other jobs. In file mode, from_scracth is used when Output Directory=Create, and restart is used for other jobs.

calculation

Select the type of calculation.

# of bands

The selection in parentheses displays the number of valence electrons when pseudopotentials are used. If the valence number fails to calculate automatically, it is displayed as N/A.

Do not specify

nbnd is set automatically.

Specify nbnd

Explicitly specify the number of bands.

Specify nbnd(Relative)

Specified relative to the number of valence bands.

Use nbnd

Specify the number of bands. If not checked, it will be set automatically.

K_POINTS

Choose how you want to specify the k-point from the pull-down menu and specify the k-point in the QE format in the text box below. If you want to use k-point information generated by a website such as SeeK-path, select the type of K_POINTS (e.g. crystal) and then paste the k-point coordinates and points into the text box below it. After selecting the type of K_POINTS (e.g. crystal), paste the coordinates of the k-points and the number of points into the text box below it. The number of k points (nks) written to the input file will be automatically filled in.

gamma

Calculated at the Γ point only.

automatic

Use Monkhorst-Pack method. Enter "(number of divisions in kx direction) (number of divisions in ky direction) (number of divisions in kz direction) (shift flag in kx direction) (shift flag in ky direction) (shift flag in kz direction)" (separated by spaces). The shift flag is 0 for no shift (k points contain Γ points) and 1 for shift (k points cross Γ points).

automatic(by spacing)

Use Monkhorst-Pack method. The number of divisions in each direction is set by the Spacing parameter (*Spacing parameter*).

automatic(by spacing,slab)

Use Monkhorst-Pack method. The number of divisions in each direction is set by the Spacing parameter (*Spacing parameter*). However, the number of vertical slab divisions detected automatically is set to 1.

Others

Please refer to the pw.x manual or doc/brillouin_zones.pdf under the QE installation folder for details.

Set default k-path
The default k-point path of the Bravo lattice (ibrav) detected for the crystal displayed in the main window is acquired from UserPref/kpath_default.txt and set.

nosym
Specify whether to use spatial symmetry.

noinv
Specify whether time reversal symmetry is used or not.

Set ibrav = … and celldm
If the primitive cell is displayed in the main window and checked, set the appropriate ibrav and celldm. If it is not checked, set ibrav = 0 and set CELL_PARAMETERS.

ecutwfc
Specify the cutoff energy of the plane wave when calculating the wave function.

Ecut for US/PAW
Sets how ecutrho is specified when selecting an Ultrasoft or PAW pseudopotential file.

Specify ecutrho/ecutwfc
Set ecutrho from the ratio of ecutrho to ecutwfc and the value of ecutwfc.

Specify ecutrho
Directly set the value of ecutrho.

ecutrho
Specify cutoff energy of plane wave at electron density and potential calculation.

tot_charge
Specify the charge of the entire system in the simulation cell.

occupations
Specify smearing for metals and tetrahedron for DOS calculations.

ion_dynamics
Specify the algorithm to change ion (nucleus) position.

cell_dynamics
Specify algorithm to change simulation cell.

tprnfor
I will calculate the force.

tstress
Calculate the pressure tensor.

Advanced tab

conv_thr
Specify tolerance of energy at SCF calculation.

etot_conv_thr
Structural Optimization (relax) Specify the energy tolerance for calculation.

forc_conv_thr
Structural Optimization (relax) Specify the force tolerance during calculation.

press_conv_thr
Specify tolerance of pressure when cell structure optimization (relax - vc) calculation is calculated.

electron_maxstep
Specify the maximum iteration number of the SCF calculation.

nstep
Specify the maximum number of steps for structure optimization (relax) calculation and the number of steps for MD calculation.

upscale
Specify coefficients for automatically decreasing conv_thr during structure optimization (relax) calculation.

diagonalozation
Specify diagonalization algorithm.

diago_david_ndim
Specifies the size of the workspace when diagonalized with the Davidson algorithm.

spline_ps
Interpolate pseudopotentials with cubic spline, useful for GIPAW calculations.

la2F (for pw.x)
Outputs a file with written eigenvalues for electron-phonon interaction calculations in pw.x.

smearing
Specify the method of occupancy smoothing (smearing).

degauss
Specify the parameter of occupancy smoothing.

mixing_beta
Specify the mixture ratio of old and new KS orbitals in SCF calculation. The closer to 1, the greater the ratio of predicted values.

mixing_mode
Specify the mixture algorithm of old and new KS orbitals.

vdw_corr
Van der Waals (dispersion) Specify how to correct forces.

Use input_dft
When checked, overwrite the setting of the functional to the setting written in the pseudopotential file.

nqx1/2/3
Specifies the number of k-point sampling when calculating the Fock operator. If Default, use the same value as K_POINTS.

cell_dofree
Specify the degree of freedom (direction) for moving the simulation cell.

Use cell_factor
Explicitly specify the construction parameter of the pseudopotential table. Sometimes it is better to set a larger value for vc - relax (structure optimization calculation with cell size change).

Spin/DFT+U tab

nspin
Set up spin polarization calculation.

Use tot_magnetization
When checked, specify the magnetization of the whole system here. If you do not check it, specify starting_magnetization.

starting_magnetization
Gives the initial value of the magnetization of each atom species. Use “Use Spin Density as

starting_magnetization" if you want to calculate antiferromagnets, since in this case all atoms of the same element have the same value.

noncolin
Specifies whether or not non-colinear calculations are performed. If checked, nspin is not output to the input file. nspin is not output, but nspin=2 must be set on the same tab to set starting_magnetization.

lspinorb
Pseudopotential file with spin orbit interaction can be used during calculation of non-colinear.

Use Spin Density as starting_magnetization
Use the value of Spin Density set in the main window as-is as starting_magnetization. If checked, the above starting_magnetization is ignored. Use this feature when atoms of the same element have different starting_magnetization, such as in antiferromagnets.

lda_plus_u
Perform LDA + U calculation.

Hubbard_U/alpha
Specify the U and alpha parameters of Hubbard for each atom type.

Phonon tab

Run Phonon Calculation as Postprocess
Perform a phonon calculation. Specifically, ph.x is run after pw.x is run. To enable this item, you must select scf, nscf or relax for Calculation. If you want to run ph.x after the SCF or Relax calculation is finished, you can run it with Calculation=nscf, which will immediately finish pw.x and immediately start ph.x processing. The ph.x and other input/output files are created in the working folder.

tr2_ph
Specify the censored error of phonon calculation.

alpha_mix(1)
Specify mixing factor.

epsil=.True.
Calculate the dielectric constant obtained from phonon calculation.

lraman=.True.
Include calculation of Raman spectrum.

electron_phonon
Specifies the method of electron-phonon interaction calculation.

el_ph_sigma
Specifies the interval of double-delta smearing during electron-phonon interaction calculations.

el_ph_nsigma
Specifies the number of double-delta smearing during electron-phonon interaction calculations.

Use fildvscf
Output files used in electron-phonon interaction calculations when running q2r.x.

la2F = .true. (for q2r)
Check in Electron Phonon Interaction Calculations

asr(for dynmat)
Specifies how the Acoustic Sum Rule is given in the post-processing (dynmat.x) after phonon calculation. It does not affect the phonon calculation itself.

lperm=.True.(for dynmat)
The contribution of the Gamma point to the dielectric constant is calculated in the post-processing (dynmat.x) after the phonon calculation.

ldisp=.true.
Calculate phonon dispersion. In order to acquire phonon band structure, phonon density of states you need to specify this.

nq1,nq2,nq3
Specify the number of K points when computing phonon variance.

Use spacing
Use Monkhorst-Pack method. The number of divisions in each direction is set by the Spacing parameter (*Spacing parameter*).

NMR/EFG tab

Run GIPAW calculation (gipaw.x) as postprocess
Run a GIPAW calculation. Specifically, gipaw.x is run after pw.x is run. The gipaw.x input and output files will be created in your working folder. To see the details of the results of the GIPAW calculation, open gipaw.out or gipaw2.out directly in a text editor.

job
Specify what you want the GIPAW calculation to output. If you choose 'nmr & efg', gipaw.x will be invoked twice, with job=nmr and job=efg, respectively.

conv_threshold
Specify the truncation error for diagonalization.

diagonalozation
Specify diagonalization algorithm.

q_gipaw
Specifies the magnitude of the infinitesimal wavenumber to use when calculating with linear response theory.

verbosity
Specifies the level of output to the log.

use_nmr_macroscopic_shape/nmr_macroscopic_shape
Specifies whether the chemical shift values should be corrected to account for the macroscopic shape of the sample.

spline_ps
Specifies whether pseudopotentials should be spline complement.

q_efg
Specifies the quadrupole moment of the nucleus.

hfi_nuclear_g_factor
Specifies the g-tensor of the nucleus.

Enter q_efg
This is an input aid for q_efg. You can quote from the default or user-prepared q_efg tables.

Open q_efg table
Open q_efg table.

Dynamics tab

Simulation Package
Specify the calculation package to be used for MD calculation. For cp.x, use the CPMD method.

DT
Specify the time step of MD calculation with atomic unit.

tempw
Specify the target temperature when temperature control is specified by MD calculation.

press
Specify the target pressure when specifying pressure control in MD calculation.

ion_temperature
Specify the temperature control method of ion (nucleus) in MD calculation.

ion_velocities
Specify the initial velocity of ion for MD calculation.

gangbang
Specify the allowable value of temperature during temperature control.

pot_extrapolation
Born-Oppenheimer Specify the extrapolation method of the potential when using MD.

wfc_extrapolation
Specify the extrapolation method of wave function when Born-Oppenheimer MD is used.

electron_dynamics
Specify the algorithm to change the KS trajectory when Car - Parrinello MD is used.

electron_velocities
Specify the initial speed of electrons when Car - Parrinello MD is used.

emass
Car-Parrinello Specify the virtual mass of electrons when using MD.

emass_cutoff
Car-Parrinello Specifies the cutoff value of the virtual mass of electrons during MD calculation.

orthogonalization
Specify the method of matrix calculation (orthonormalization).

Dipole Corr tab

tefield
A sawtooth type external electric field is applied.

dipfield
Use dipole correction.

edit
Sets the direction in which the tefield and dipfield are applied.

emaxpos
The location where the external electric field is at its maximum value when applying tefield and dipfield is given in fractional coordinates (in the range of 0 to 1).

eopreg
The size of the region where the external electric field decays when applying tefield and dipfield is given in fractional coordinates.

eamp
Gives the magnitude of the external electric field when applying the tefield and dipfield.

ESM tab

assume_isolated=esm
Check if you use ESM (Effective Screening Medium) method.

esm_bc
Specify the type of boundary condition used in the ESM method.

esm_efield
Specify the electric field.

esm_w
Sets the offset for the location where the ESM will be placed.

lfcpopt
Calculation of constant chemical potential (constant mu) will be carried out. The initial system charge is specified by tot_charge on the Basic tab.

the fcp_m
Set the target value of Fermi energy in constant calculation of chemical potential.

Enter Relative Potential
Supports input of Target Fermi Energy. First, specify the log file for calculation at voltage 0 and acquire Fermi energy at voltage 0. Next, input the applied voltage. From these two pieces of information, calculate Target Fermi Energy.

RISM(1) tab

trism=.True.
Enable RISM calculations. Check here to run ESM-RISM calculations, and check *assume_isolated = esm* on the *ESM* tab. To use this feature, you need to install a separate version of Quantum ESPRESSO with the ESM-RISM feature enabled.

closure
Select the closure to use for RISM calculation

tempw
Specify the initial velocity of ion for MD calculation.

ecutsolv
Specify the cutoff energy of the plane wave when calculating the wave function.

solute_lj
Specify the LJ parameter of the solute (DFT region). If *none* is selected, enter the LJ parameter in *solute_epsilon* and *solute_sigma* below

noinv
Specify the number of molecular species of the solvent.

SOLVENTS
Select the unit of *Density* from the pull-down menu and specify the density (concentration) of each solvent molecule type and the name of the MOL file. MOL files must be in the folder specified by *Directory for MOL Files* below.

Directory for MOL Files
Specify a folder containing MOL files that can be selected with *SOLVENTS*.

RISM(2) tab

laue_expand_right/left
Specify the position of the far end of the solvent region in the ESM-RISM calculation.

laue_starting_right/left
Specify the starting position of the solvent region in the ESM-RISM calculation.

laue_buffer_right/left
Specify the location of the solvent buffer area in the ESM-RISM calculation.

Run only 1D-RISM
If checked, run 1drism.x instead of pw.x. No DFT calculations will be performed. Useful if you only want to know the correlation function between solvent atoms and the chemical potential between solvents.

rism3d_conv_level
Specify parameters for dynamically changing the truncation error of 3D-RISM calculation at each step of SCF calculation.

rism1d/rism3d_maxstep
Specify the maximum number of 1D and 3D-RISM iterations.

rism1d/rism3d_conv_thr
Specify the truncation error for 1D and 3D-RISM.

mdiis1d/3d_size
Specify the convergence parameter of RISM calculation by MDIIS algorithm.

mdiis1d/3d_step
Specify the convergence parameter of RISM calculation by MDIIS algorithm.

Others tab
Fill in the other settings in QE's input file format (FORTRAN namelist format). An example of entry is displayed by pointing the pointer.

Preview tab
A preview of the configuration keywords will be displayed.

Options Tab

Verbosity
Specify the amount of information output by QE.

atomic_position unit
Specify the unit of ATOMIC_POSITIONS and CELL_PARAMETERS.

Use max_seconds
If checked, processing of QE will be interrupted after the number of seconds entered here.

Options for executable
Gives the arguments of the command to run pw.x or pw.exe. For example, you can specify -nk, -nb, -nt, or -nd to control parallelism.

Dump all files for remote
Output files necessary for job execution under Linux environment. The same file as the file generated by the remote job submission function is output.

Open k-path file
Open the configuration file (UserPref/kpath_default.txt) that describes the k-point path specified by default for each type of ibrav (bracket lattice). If UserPref/kpath_default.txt does not exist, it is copied from wmx/kpath_default.txt.

QE Version
Specifies the version of the QE to which the input file of the output QE corresponds. The output format of some keywords (&fcp, HUBBARD, etc.) varies with the version.

Properties tab

Calculate these properties after pw.x

Select post processing to be executed immediately after executing pw.x. Various parameters of the processing selected here are specified in the Parameter/Value column on the right.

Pseudopotential tab

Mass

Specify the mass of each element.

Default

Set standard mass.

Light

Set the mass of all elements to 1. It is used for the purpose of promoting structural relaxation of ions.

Manual

In the list below, for each element, the user individually sets the mass.

Pseudopotential

Select a pseudopotential file from among those that are common to all elements in the system.

(Type)

Select the type of pseudopotential.

(Functional)

Selects the type of functionality. Choose from the choices narrowed down by (Type).

(File)

Select a pseudopotential file. Choose from the choices narrowed down by (Type) and (Functional). If you choose (Manual), the user sets the pseudopotential individually for each element in the list below.

Pseudopotential files are searched in the folder specified in the pseudo Directory. Preference is given to the first entry in `qe_pseudo_priority_list.txt` in the user configuration folder.

Reload pseudo Files

The pseudo-potential file placed in the folder specified by pseudo Directory is read again.

pseudo Directory

Specify the folder where the pseudopotential file will be placed. If the case of *pseudo in QE#39;s directory*, use the pseudo folder under the installation directory of QE. If the case of *(select…)*, use the directory selected in the dialog.

Open Pseudo Directory

Open the folder specified in pseudo Directory.

Download Pseudo Files

Download the pseudopotential file and install it.

Open Priority List

Open UserPref/qe_pseudo_priority.txt. If it does not exist, it is copied from wmx/qe_pseudo_priority.txt.

Reset

Reset settings.

Import

Loading configuration file.

Export

Output configuration file.

Spacing parameter

The Spacing parameter is used to determine the number of k-point divisions N in each direction, independent of the system size.

$$N = \max(1, \mathrm{ceiling}(|\vec{b}_i|/\mathrm{Spacing}))$$

$\vec{b}_i$ (where i is the index for each direction $0, 1, 2$) is the reciprocal lattice vector $\vec{a}_i\vec{b}_i = 2\pi\delta_{ij}$ for the lattice vector (basic translation vector) $\vec{a}_i$.

6.16.4 Run

Run Quantum ESPRESSO. The execution method differs depending on the situation. When CPMD is selected **`cp.x`**, otherwise it executes **`pw.x`**.

- (Default) When *Output Directory* = *Create*, create a new working folder and execute the calculation.
- If the case of *Output Directory* = *Continue*, use outdir of the input file open in the main window as the working folder then.
- If the case of *Output Directory* = *Select*, use the selected folder as the working folder (outdir).

Following file will be generated with execution. As an example, the file/folder name when the input file is `si.pwin` is also shown.

type	Description
pwout file `si.pwout`	Calculation log file.
bat file `si.bat`	It is a batch file for running Quantum ESPRESSO.
Working Folder `si_qe_data\`	Working folder.

The following files are generated in the working folder. Only the main files are shown here.

type	Description
Pseudopotential file `*.UPF`	The pseudopotential files used in the calculations are copied here and the ESPRESSO_PSEUDO environment variable is set in the working folder.
`pw_bands.in`	This is an input file for executing bands calculation in post processing.
`pw_bands.out`	This is the log file of `pw_bands.in`.
`pw_dos.in`	Input file for executing dos calculation in post processing.
`pw_dos.out`	`pw_dos.in` log file.
`ph.in`	Input file for running phonon calculations with **`ph.x`** in post-processing.
`ph.out`	This is the log file of `ph.in`.

Hint: ** Working folder **

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.
  - ** The suffix varies depending on the type of solver. **
  - For example, in the case of Gromacs, if the file opened in the main window is `aaa.gro` and the suffix is `_gmx_tmp`, the working folder will be named `aaa_gmx_tmp`.
- It must be in the same hierarchy as the file opened in the main window.
- Processing continues in the working folder of the same name even when continuing jobs, but by default the backup of the working directory of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the one with the smallest number in the range where duplicate names do not exist. For example, if the working folder is `aaa_gmx_tmp`, it is `aaa_gmx_tmp1`.
  - ** Directories without numbers are always up to date. **

Job is run through *Winmostar Job Manager*.

6.16.5 Open Log File (pwout)

Open the log file with a text editor.

6.16.6 Show Extracted Log

Excerpts of key information from the log file are displayed.

6.16.7 Animation

Optimization, BOMD(pwout, out)

From the information of the log file, animation such as structure optimization, BOMD calculation etc. is created and displayed. For CPMD use *CPMD(pos)*. See *Animation operation area* for animation display operations. From the animation operation area, you can calculate radial distribution function, self-diffusion coefficient, mean square displacement, displacement of each atom, etc.

CPMD(pos)

Specify CPMD's pos and cel files and display animation. To display the result of pw.x, use *Optimization, BOMD(pwout, out)*. See *Animation operation area* for animation display operations. From the animation operation area, you can calculate radial distribution function, self-diffusion coefficient, mean square displacement, displacement of each atom, etc.

6.16.8 Energy Plot

SCF Energy Change (pwout)

Select the log file and display a graph of total energy. For CPMD use *CPMD Energy Plot (evp)*.

Property
Select the values to be displayed in the graph.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

CPMD Energy Plot (evp)

Specify the evp file of CPMD and display time variation of various energies.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

6.16.9 Analyses

Density od States

Specify the working folder (outdir) and the SCF calculation log file and display the density of states. Fermi energy is acquired from the log file of SCF calculation. dos.x runs in the background. The range of energies where the density of states near the Fermi energy is zero is calculated internally, and the values of the band gap, VBM (upper end of the valence band) and CBM (lower end of the conduction band) energies are calculated and displayed.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Projected DOS

Specify the working folder (outdir) and the SCF calculation log file and display projected density of state(PDOS). Fermi energy is acquired from the log of SCF calculation. Projwfc.x runs in the background.

Check atom using viewport
The molecular structure read from the log file is displayed in 3D. The orbitals of the atoms selected by clicking there are checked in the list of orbitals.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Band Structure

Specify the working folder (outdir) and SCF calculation log file and display the band structure. Calculation must be completed with calculation = bands in advance. Fermi energy is acquired from the log file of SCF calculation. Bands.x runs in the background.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Lowdin Charge

Specify the working folder (outdir), calculate and display the Lowdin charge. Projwfc.x runs in the background.

Lowdin Charge

Specify a working folder (outdir) to calculate and display the Bader charge. You must generate a cube file of all electron densities beforehand using the PAW method. The bader program is playing in the background.

Electron Density

Specify working folder (outdir) and display isoelectric density surface. In the background, pp.x flows, and a cube file is generated. Refer to *Surface Setup / Cubgen window* for how to operate subwindow.

Spin Density

Specify working folder (outdir) and display isoelectric density surface. In the background, pp.x flows, and a cube file is generated. Refer to *Surface Setup / Cubgen window* for how to operate subwindow.

Potential Energy

Specify a working folder (outdir) and display the isopotential energy surface. In the background, pp.x flows, and a cube file is generated. Refer to *Surface Setup / Cubgen window* for how to operate subwindow.

Potential Energy Distribution

Specify the working folder (outdir) and the log file of the SCF calculation to display the potential energy distribution in the z-axis direction (excluding exchange correlation energy). Fermi energy is acquired from the log of SCF calculation. The difference between the Fermi energy and the maximum value of the potential energy ,excluding exchange-correlated energy, distribution is displayed as an estimate of the work function. Pp.x and average.x flow in the background.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Fermi Surface

Specify the log file for SCF calculation and bands calculation and display the Fermi surface. For Fermi surface display, use *FermiSurfer <https://mitsuaki1987.github.io/fermisurfer/index_ja.html>*. Specify the k point division number for bands calculation in *# of K Points* and press the *Calc* button to display the Fermi surface.

Dielectric Function

Specify the working folder after calculating the dielectric function and display the dielectric function.

Direction
Specify the direction of the dielectric function to be acquired.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

NMR

Specify a working folder after GIPAW calculation to display NMR spectra. See *NMR Window* for subwindow operation.

IR/Raman

Specify the working folder after phonon calculation and log of SCF calculation and display IR and Raman spectrum. Refer to *IR Spectrum Window* for how to operate the subwindow.

Phonon Band Structure

Phonon Specifies the working folder after the variance calculation and displays the phonon dispersion curve.

ASR
Specify the type of Acoustic Sum Rule to be applied.

K Points
Specify the path of the dispersion curve to be acquired. In each line, describe the x, y, z components in units of 2pi/a, and next to it describe the number of divisions up to the next point. (Enter a total of 4 columns with a space separator)

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Phonon Density of States

Phonon Specifies the working folder after distributed calculation and displays the phonon density of states.

ASR
Specify the type of Acoustic Sum Rule to be applied.

K Points
Phonon DOS Specifies the division number of K points during DOS calculation.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Charge/Energy Profile (esm1)

Specify the esm1 file output by ESM calculation (assume_isolated = esm) and display the charge or energy distribution in the z-axis direction. You can also plot the difference between the two esm1 files.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

1D-RISM RMS Change

Plot the change in RMS of the 1D-RISM calculation performed at the beginning of the RISM calculation (trism = .True.).

Draw
Displays a graph.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

3D/Laue-RISM RMS Change for Last Step

Plot the change of RMS of 3D-RISM or ESM-RISM calculation in the last SCF step when RISM calculation (trism = .True.) is executed.

Draw
Displays a graph.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Solvent Pair Distribution Func. (1drism)

Interatomic correlation function (radial distribution function) of RISM region is calculated using 1 drism file outputted by RISM calculation (trism =. True.).

Obtain Chemical Potentials
The chemical potential between solvent molecules is output in csv format.

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

Solvent Charge/Energy Profile (rism1)

Calculate the solvent density, energy, and charge in the direction in which the DFT region-RISM region contacts (vertical direction of the interface) by using the rism1 file output by RISM calculation (trism = .True.).

Draw
Display the graph. The result analysis program is executed as necessary.

Close
Close the window.

For how to operate the graph drawing area, see *How to operate the graph*.

6.16.10 Generate MOL File

Creates a MOL file for the solvent used in the RISM calculation (trism=.True.). To set LJ parameters from a LAMMPS data file, open the data file in the main window and check *Use parameters in displayed file* in the main window. The created file should be placed in the folder specified by *Directory for MOL Files* on the *RISM (1)* tab of the Configure window of the MOL file.

6.16.11 Nudged Elastic Band

Workflow Setup/Keyword Setup

Set up and run the conditions for the NEB calculation; use `neb.x` to run the NEB. Please set in the state that the structure optimization calculation of each of the start state and the end state has been completed.

6.16.12 Run

Run Quantum ESPRESSO NEB calculation in file mode.

Open Log File (pwout)

Open the NEB calculation log file in a text editor.

NEB error change

Displays errors in each iteration of the NEB calculation.

Animation

Specify the output file of the NEB calculation and display the changes in energy and atomic structure along the reaction coordinates after the NEB calculation convergence. If you want to see the energy change at each iteration of the NEB calculation continuously, use *Energy Plot*. For the animation display operation method, see *Animation operation area*.

Energy Plot

Specify the output file of the NEB calculation and display the change in energy along the reaction coordinates. You can visualize the appearance at each iteration of the NEB calculation. Use *Animation* if you want to visualize the atomic structure.

6.16.13 BoltzTraP

BoltzTraP calculates thermoelectric characteristics based on the output of nscf calculation in QuantumESPRESSO.

Configure & Run

Set the calculation conditions for pre-post processing using BoltzTraP and execute pre-processing. *Create .intrans File* button

> Read nscf calculation output file (*.pwout) of Quantum ESPRESSO and generate BoltzTraP setting file (*.intrans). Assuming that the output file is mg2si_nscf.pwout, a working folder named mg2si_nscf is created in the same level. mg2si_nscf.intrans is generated in mg2si_nscf. If the intrans file is successfully created, read the contents of the file and reflect it in the input fields of the following keywords.

Fermilevel (Ry)
Fermi energy read from pwout file is set.

energy grid
Specify the interval of the set energy.

energy span
Specifies the range of band energies to consider in calculations around the Fermi level.

number of electrons
Specify the number of electrons in a unit cell.

lpfac
Specify the factor for complementing the band energy by Fourier expansion.

efcut
Specify the calculation range by changing the chemical potential.

Tmax
Specify the upper limit of the set temperature.

temperature grid
Specify the interval of the set temperature.

energy of bands
Specify the energy width of the band obtained from DOS.

Calculate expansion coeff
If checked, compute expansion coefficients (CALC). If not checked, read expansion coefficients from file (NOCALC).

Start BoltzTraP button

Recreate the intrans file based on the setting conditions and execute BoltzTraP. At this time, the following files and folders are created. The main files in the working folder (mg2si_nscf) at the end of the calculation are described below.

type	Description
intfans file `mg2si_nscf.intrans`	BoltzTraP input file.
.trace file `mg2si_nscf.trace`	This file contains information on energy and temperature dependence of thermoelectric properties calculated by BoltzTraP. The BoltzTraP Import Result menu reads this file and performs visualization.

Cancel button

Close Configure & Run window without doing anything.

Import Result

The following thermoelectric properties calculated by BoltzTraP are read and visualized.

- Seebeck coefficient
- Electrical conductivity
- Electrical thermal conductivity
- Power factor
- Figure of merit

To display the energy dependence of the characteristic value at each temperature, select T [K] from the combo box and select the target temperature from the list. If you want to display the temperature dependence of the characteristic value for each energy, select E-Ef [eV] from the combo box and select the target energy from the list.

6.16.14 Phonopy

Calculations using Phonopy are performed in the following three steps.

1. Create a supercell based on a given crystal structure (project mode) or Quantum ESPRESSO input file (file mode).
2. Execute Quantum ESPRESSO for all generated super cells.
3. Create a ForceSets file from the Quantum ESPRESSO output file to calculate Phonon bands, DOS, thermophysical properties, etc.

Create a supercell

Generate a supercell for the Phonopy calculation for the crystal structure displayed in the molecule display area in the "Project" mode. Depending on the type of crystal, multiple structures may be generated. To run Quantum ESPRESSO calculations on these structures, use *Workflow Setup* with Enable scan calculation.

Configure & Run

In file mode, set the calculation conditions for pre- and post-processing using Phonopy and execute the pre-processing.

***Open* button**

Read the input file (*.in, *.pwin) of Quantum ESPRESSO. Post processing in Phonopy requires stress information. Therefore, the file to be read must include the tprnfor and tstress keywords. The input file of Quantum ESPRESSO for Phonopy can be set by using Quantum ESPRESSO Configure Preset=Phonopy.

DIM

Specify the number of times the supercell repeats in the x, y, and z directions, separated by a space.

MP

Specify the reciprocal lattice when calculating Phono DOS and thermodynamic properties in Phonopy, separated by a space.

ATOM_NAME

Specify the elements included in the unit cell separated by a space. It is automatically entered when the input file is opened with the *Open* button.

Start button

Execute Phonopy based on the setting conditions, and create a super cell that is pre-processing.
At this time, the following files and folders are created.

type	Description
bat file `si.bat`	Batch file to execute the preprocessing of Phonopy.
sh file `si.sh`	Shell script file for executing the preprocessing of Phonopy.
si_ph_data folder `si_ph_data`	Working folder.

The following files are generated in the working folder si_ph_data.

type	Description
mesh.conf file `mesh.conf`	Used to calculate density of states and thermodynamic properties in post processing of Phonopy.
band.conf file `band.conf`	Used when calculating band structure in Phonopy post processing.
header file `header.in`	Keyword information other than the structure information specified in si.pwin is described.
supercell file `supercell-*.in`	Supercell information generated by Phonopy is described in Quantum ESPRESSO input file format. Since multiple supercell patterns are generated, * is replaced by numbers such as 1, 2, and so on.
tmp file `tmp-*.in`	Combines header.in and supercell-*.in.

Cancel button

Close Configure & Run window without doing anything.

Edit .conf File

In file mode, opens the conf file in a text editor. Use this if you want to edit the keywords set in the keyword configuration screen.

Quantum ESPRESSO Continuous Execution

In File mode, Quantum ESPRESSO is executed on all super cells generated in the Keyword Setup and Execution screen. If you use this menu, Quantum ESPRESSO will run in the local environment.

Run Phonopy

Performs Phonopy post-processing in file mode. At this time, the following files are created in the working folder :file: si_ph_data .

type	Description
sh file `phonopy.sh`	Shell script to execute Phonopy post processing
band.yaml file `band.yaml`	Information on the band structure calculated by post processing of Phonopy is output.
dos.dat `dos.dat`	Information on the density of states calculated by post processing of Phonopy is output.
thermal_properties.yaml file `thermal_properties.yaml`	Information on thermodynamic properties calculated by Phonopy post processing is output.

Band Structure

Displays the band structure based on band.csv included in the working folder.

Density od States

Displays the density of states based on toal_dos.csv included in the working folder.

Thermodynamic properties

Displays thermodynamic properties based on thermal_properties.csv included in the working folder.

6.17 *Solid* → *OpenMX* menu

Menu related to OpenMX

6.17.1 How to configure OpenMX

VPS and PAO files to be loaded in Winmostar's workflow and keyword settings are loaded from the path specified by the OPENMX_DATA_PATH environment variable in CygwinWM. In addition, for remote jobs, the same version of OpenMX as OpenMX on CygwinWM must be installed on the remote server, and the same environment variable OPENMX_DATA_PATH as on CygwinWM must be set on the remote server. When using OpenMX3.8 or earlier with DFT_DATA13, copy omxprm_dft_data13.txt from the wm_systemwmx folder to the UserPref folder as omxprm.txt, and the recommended settings for DFT_DATA13 will be used by default for the VPS and PAO files. DFT_DATA13 is used by default for VPS and PAO files.

6.17.2 Workflow configuration

Configure and run the OpenMX calculation flow in project mode.

Preset
Import and saves a preset of settings.

# of Jobs
Specifies the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It makes it possible to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Clicking on *Config* opens the configuration window for the scan calculation. For a parameter scan, select %WM_SCAN1% for the *Target Variable* and enter the parameters you want to set for %WM_SCAN1% in each line of the *Values*. Then enter %WM_SCAN1% in the parameters you want to set in the workflow settings window or in the keyword settings window. For structure scans, select %WM_STRUCT% for the *Target Variable* when the animation appears in the molecule display area (e.g. by opening an SDF file). After the scan calculation is finished, use *File* → *Project* → *Scan Results Display* to tabulate the calculation results.

Import
Load the settings output by Export. Click on the arrow to the right of the button to recall settings previously used in the same project or on Winmostar.

Export
Outputs the configuration to a file.

OK
Runs a calculation or generates a file with the settings. See *For project mode* for more information.

Details
Set detailed calculation conditions. The *Configure* will be launched.

Task
Specifies the type of calculation.

	Settings
Energy	MD.Type=nomd
Optimize(Atom)	MD.Type=Opt
Optimize(Atom&Cell)	MD.Type=RFC5
BOMD	MD.Type=NVE

Charge
Specifies the charge for the entire system.

Spin
Set up spin polarization calculations.

K points
Specifies how the K point is calculated.

Pressure
Specify pressure.

Functional
Specifies a functional.

Properties
Calculate the physical properties checked in conjunction with the time of calculation.

Precision
Sets the calculation accuracy.

	Settings
Extra-low	SCF.criterion=5e-6 MD.Opt.criterion=5e-3 KSpacing=0.44(metal) 0.63(nonmetal) SCF.EnergyCutoff=80(metal) 80(nonmetal)
Low	SCF.criterion=5e-7 MD.Opt.criterion=5e-4 KSpacing=0.44(metal) 0.63(nonmetal) SCF.EnergyCutoff=120(metal) 120(nonmetal)
Medium	SCF.criterion=1e-7 MD.Opt.criterion=2.5e-4 KSpacing=0.31(metal) 0.50(nonmetal) SCF.EnergyCutoff=160(metal) 160(nonmetal)
High	SCF.criterion=5e-8 MD.Opt.criterion=1.5e-4 KSpacing=0.25(metal) 0.44(nonmetal) SCF.EnergyCutoff=300(metal) 200(nonmetal)
Extra-High	SCF.criterion=2.5e-8 MD.Opt.criterion=5e-5 KSpacing=0.08(metal) 0.11(nonmetal) SCF.EnergyCutoff=600(metal) 400(nonmetal)

Metal

Enable smearing. Set SCF.ElectronicTemperature to 800 if enabled, 300 if disabled, and also adjust the contents of Precision (above).

6.17.3 Configure

Set the OpenMX calculation conditions. Click the *Run* button to execute the calculation immediately after setting, or the: guilabel:` OK` button to return to the main window. See *Run* for behavior when clicking *Run*. The *Reset* button returns to the default state. Click the *OK* button to reflect the settings and return to the main window. *Cancel* button closes the window without doing anything. When calling this function, if the structure displayed in the main window can be changed to a primitive cell, *Convert Lattice (Primitive-Conventional)* is automatically executed.

Preset
Select a settings preset.

Use MPI
Specify whether to perform parallel computation using MPI when running OpenMX. Enter the number of MPI processes in the horizontal column.

Use OpenMP
Specify whether to perform parallel computation using OpenMP when running OpenMX. Enter the number of OpenMP threads in the horizontal column.

Basic tab

Restart
Set to On to take over the final state of the job being taken over.

Restart Directory
Specify the rst folder of the job to take over if other than Restart=Off.

XcType
Specify exchange correlation potential. You can specify “LDA”, “LSDA-CA”, “LSDA-PW”, or “GvG-PBE”. Here, “LSDA-CA” is the Ceperley-Alder local spin density function, and “LSDA-PW” is the Perdew-Wang local spin density function with zero density gradient in the GGA format. “GGA-PBE” is a GGA functional proposed by Perdew et al.

EigenvalueSolver
Specify the calculation method for eigenvalue problems with “scf.EigenvalueSolver”. O (N) divide-and-conquer method is “DC”, O (N) Krylov subspace method is “Krylov”, numerically exact low-order scaling method is “ON2”, cluster calculation is “Cluster”, band calculation is specified “Band”.

Specify Kgrid by spacing
Set Kgrid with the Spacing parameter (*Spacing parameter*).

Kgrid
In OpenMX, the first Brillouin zone in k-space is separated by an equidistant mesh. At that time, when “Band” is specified with the “scf.EigenvalueSolver” keyword, the number of grids (n1, n2, n3) for discretizing the first Brillouin zone in k-space must be specified with the “scf.Kgrid” keyword. Specify as “n1 n2 n3” to discretize the reciprocal lattice vector in k space.

energycutoff
Specifies the cutoff energy that defines the integration grid spacing. This integration grid is used to calculate matrix elements for the difference electron Coulomb potential and exchange correlation potential, and to solve the Poisson equation using the Fast Fourier Transform (FFT).

System.Charge
Specifies the charge for the entire system.

ElectronicTemperature
Set the electronic temperature (K).

MD.Type

Specifies the type of molecular dynamics calculation or structure optimization. Currently available options are: No MD (“ Nomd ”), structural optimization of atomic coordinates (“ Opt ”), Structural optimization (“RFC5”), including unit cell flexibility, NVE Ensemble MD (“NVE>”), NVT ensemble MD (“NVT_VS”) by speed scaling method, NVT ensemble MD (“NVT_NH”) by the Nose-Hoover method.

Advanced(1) tab

criterion

Specify the convergence condition for the SCF calculation (in Hartree). The SCF iteration ends when the condition dUele < scf.criterion is met. Here dUele is the absolute difference in band energy between the current SCF iteration and the previous iteration. The default value is 1.0e-6 (Hartree units).

maxIter

Sets the maximum number of SCF iterations. The SCF iteration loop ends with the number of times specified by this keyword even if the convergence condition is not met.

Mixing.Type

Specify the electron density mixing method to generate the electron density (or density matrix) that is input to the next iteration step of the SCF calculation. Simple mixing method (“Simple”), Guaranteed-Reduction Pulay method (“GR-Pulay”), RMM-DIIS method (“RM-DIIS”), Kerker method (“Kerker”), or RMM-DIISK method (“RMM- DIISK”) or RMM-DIISH method (“RM-DIISH”) can be specified. OpenMX’s simple mixing method has been improved to reference the convergence history to speed up the convergence. When using “GR-Pulay”, “RMM-DIIS”, “Kerker” or “RMM-DIISK”, the SCF calculation can be accelerated by paying attention to the following points. Some convergence is required before mixing begins in a way that conforms to the Pulay method. Therefore, use a slightly larger “scf.Mixing.StartPulay” value. A good value for “scf.Mixing.StartPulay” is 10-30. For metal systems, use a high “scf.ElectronicTemperature” value. When “scf.ElectronicTemperature” is small, numerically unstable behavior is often seen. Increase the value of “scf.Mixing.History”. In most cases, “scf.Mixing.History = 30” is a reasonable value. Among the mixing methods described above, “RMM-DIISK” is the most robust.

Init.Mixing.Weight

Specify the initial mixing ratio used in the Simple, GR-Pulay, RMM-DIIS, Kerker, RMM-DIISK, and RMM-DIISH methods. Valid range is 0 <Init.Mixing.Weight < 1

Min.Mixing.Weight

Specifies the lower limit of the mixing ratio in simple and Kerker mixing methods.

Max.Mixing.Weight

Specifies the upper limit of the mixing ratio in simple and Kerker mixing methods.

Mixing.History

In the GR-Pulay method, RMM-DIIS method, Kerker method, RMM-DIISK method and RMM-DIISH method, the input electron density (Hamirutonian) in the next iteration step of SCF is estimated based on the electron density of the past SCF iteration (Hamiltonian).). The “scf.Mixing.History” keyword specifies the number of past SCF iteration steps used for this estimation. For example, if “Mixing.History” is set to 3, the 6th SCF iteration takes into account the 5th, 4th, and 3rd step electron density in the past.

Mixing.StartPulay

Specify the SCF step that starts the GR-Pulay, RMM-DIIS, Kerker, RMM-DIISK, and RMM-DIISH methods. SCF steps up to the start of these methods use simple or Kerker mixing.

lapack.dste

Select the LAPACK routine.

ProExpn.VNA

Set the neutral atom potential VNA to" ON "when expanding with the projection operator, otherwise set to" OFF ". When set to" OFF ", the matrix elements of the VNA potential are calculated using a discrete grid in real space.

HoppingRanges

Defines the radius (Å) of the sphere centered on each atom. In the DC method and the O (N) Krylov subspace method, a cluster is formed by selecting the atoms contained in this sphere.

KrylovH.order

Specifies the Krylov subspace dimensions for the Hamiltonian of each cut cluster.

KrylovS.order

If you set" Exact.Inverse.S = off "in the keyword below, the inverse matrix of the overlap integral is approximated using the Krylov subspace method. At this time, specify the dimension of the Krylov subspace method of the overlap matrix for each cut cluster.

Exact.Inverse.S

When set to" on ", the inverse of the overlap matrix of each clipped cluster is evaluated strictly. Please refer to the keyword" KrylovS.order "above when setting to" off ".

Recalc.Buffer

If set to" on ", the buffer matrix is recalculated for each SCF iteration. If" off ", the buffer matrix is calculated in the first SCF step and fixed in subsequent SCF iterations.

Expand.Core

When set to" on ", the core region consists of atoms in a sphere with a radius of $1.2 \times r_{min}$. Where $r_{min}$is the distance between the central atom and the nearest neighbor. This core region defines the set of vectors used in the first step when generating the Krylov subspace. If" off ", the central atom is considered the core region.

Advanced(2) tab

maxIter

Specify the maximum number of iterations for MD and structural optimization calculations.

Opt.criterion

If you choose a structure optimization method with the" Type "keyword, set the convergence condition (Hartree/Bohr) with the keyword" Opt.criterion ". Structural optimization ends when the maximum absolute value of the force applied to the atom is smaller than the value specified here.

Opt.DIIS.History

When performing structure optimization using "DIIS", "EF", or "RF", the "Opt.DIIS.History" keyword is used to specify the past step number to be referred to for structure optimization.

Opt.StartDIIS

Specify the step to start structural optimization with "DIIS", "EF", and "RF" with the "Opt.StartDIIS" keyword. The steepest descent method is used in the previous steps before starting the DIIS-type structural optimization.

Opt.EveryDIIS

Specifies how often to switch between structural optimization by "DIIS", "EF", or "RF" and structural optimization by the steepest descent method; this setting is ignored when MD.Type=Opt.

Spin/DFT+U tab

SpinPolarization

Specifies the non-spin or spin polarization of the electron system. Specify "ON" to perform spin polarization calculations and "OFF" to perform non-spin polarization calculations. In addition to the two aforementioned options, specify the option “NC” to perform a non-colinear DFT calculation. For spin polarization calculations, the initial spin density is set according to the spin density (interpreted as the difference between the number of Up and Down spin electrons) set for each atom in the main window. The spin density can be set with *Charge/Spin Density* and so on.

SpinOrbit.Coupling

Specifies spin-orbit interaction.

Constraint.NC.Spin

Specifies whether to perform constrained DFT calculations for non-colinear spin orientations.

Constraint.NC.Spin.V

Specifies the strength of the constraint in constrained DFT calculations for noncollinear spin orientations.

Hubbard.U

Set to“ ON ”for LDA + U and GGA + U calculations.

Hubbard.Occupation

In the LDA + U method, you can choose from three occupancy operators: “onsite”, “full” and “dual”.

Restart.Spin.Angle.Theta

Specify the Euler angles (theta, phi) of the spin orientation needed to calculate the magnetic anisotropy energy by the second variational method.

Restart.Spin.Angle.Phi

Specify the Euler angles (theta, phi) of the spin orientation needed to calculate the magnetic anisotropy energy by the second variational method.

MD tab

TimeStep

Specify time step (fs).

Applied.Pressure

Specify pressure (GPa).

NH.Mass.HeatBath

If you select “NVT_NH” for the “Type” keyword, this keyword sets the mass of the heat bath. Units are unified atomic mass units (units where the mass of the main isotope of a carbon atom is 12.0).

TempControl

Specify the temperature of atomic motion in MD and NVT ensembles. If’ NVT_VS “is selected, the temperature of atomic motion can be controlled as shown in the example below.

```
<MD.TempControl
  3
  100   2  1000.0  0.0
  400  10   700.0  0.4
  700  40   500.0  0.7
MD.TempControl>
```

The description starts with “<MD.TempControl” and ends with “MD.TempControl>” .The first number “3” indicates the number of lines for the temperature specification that follows. There are three lines in the example. The first column of the following row indicates the number of MD steps, and the second column specifies the MD step interval for speed scaling. In the example, speed scaling is performed every 2 steps up to the 100th step, every 10 steps between 100 and

400 steps, and every 40 steps between 400 and 700 steps. Columns 3 and 4 specify temperature (K) and scaling parameter alpha, respectively. For details, refer to the "Molecular Dynamics" chapter. On the other hand, for NVT_NH, the temperature of atomic motion can be controlled with the following description.

```
<MD.TempControl
  4
  1    1000.0
  100  1000.0
  400   700.0
  700   600.0
MD.TempControl>
```

The description starts with "<MD.TempControl" and ends with "MD.TempControl>". The first number "4" refers to the number of lines that follow the temperature specification. In this example, there are 4 lines. The first and second columns of the subsequent rows specify the number of MD steps and the temperature of the atomic motion, respectively. The temperature between the specified MD steps is linearly complemented.

Others tab
Enter any OpenMX parameter.

Preview tab
A preview of the configuration keywords will be displayed.

Options tab

level.of.stdout
Specify the level of output information to the standard output. If" 0 "is specified, the minimum information is output. If "1", additional information is output in addition to the minimum output. "2" is an option for developers.

level.of.fileout
Specify the level of output information to the output file. If "0" is specified, the minimum information is output (no Gaussian cube and grid file output). "1" is the standard output information level. If "2", additional information is output in addition to the standard output.

Atoms.Coord.Unit
Specify the unit of the atomic coordinate.

Edit and confirm Atoms.SpeciesAndCoordinates
Edit Atoms.SpeciesAndCoordinates directly.

Properties tab

dispersion
Set to" ON "to evaluate band dispersion.

Use default path
Sets the path of k points for evaluating band variance based on the automatically determined Bravais lattice type.

DOS.fileout
Set to ON to evaluate the total density of states (DOS) and projected partial density of states (PDOS).

Erange
Specify the energy range (lower limit and upper limit) for DOS calculation separated by single-byte spaces.

Kgrid
Specify (n1, n2, n3) grid points to discretize the first Brillouin zone for DOS calculations.

MO.fileout
If you want to output molecular orbitals to a file, specify “ON”.

num_HOMOs
Specify the number of highest occupied molecular orbitals (HOMO) to output.

num_LUMOs
Specify the number of lowest unoccupied molecular orbitals (LUMOs) to output.

Nkpoint
If “fileout”is set to “ON” and “EigenvalueSolver” in the SCF tab is set to “Band”, specify the number of k points to output MO with the “Nkpoint” keyword.

Species tab

Atom
Specify the name of the atomic species.

Basis
Specify the number of primitive trajectories and the number of reduced trajectories.

PAO
Specify the file name without extension of pseudo-atomic base orbit.

VPS
Specify file name without pseudopotential extension.

Reset
Reset settings.

Import
Loads a configuration file.

Export
Outputs a configuration file.

6.17.4 Run

Execute OpenMX The following files are generated upon execution. As an example, the file/folder name when the input file is: file:` dia.mxin` and System.Name is wm is shown.

Type	Description
bat file `dia.bat`	A batch file for running OpenMX. Run dia.sh via CygwinWM.
sh file `dia.sh`	A shell script file for running OpenMX.
log file `dia.log`	log file of dia.sh
mxout file `dia.mxout`	Calculation output file. A copy of wm.out in the working folder.
Working folder `dia_mx_data\`	Working folder

The following files are generated in the working folder. Only the main files are shown here.

Type	Description
`tmp.dat`	File to specify calculation conditions. A copy of dia.mxin.
`tmp.std`	This is a redirected file of OpenMX standard output.
`wm.out`	History of SCF calculation and structure optimization, Mulliken charge, total energy and dipole moment are preserved.
`wm.xyz`	The final geometric structure obtained by MD or structural optimization is preserved.
`wm.bulk.xyz`	"scf.EigenvalueSolver = Band" will output the atomic coordinates including the copied cell atoms.
`wm.md`	Atomic coordinates for each MD step are saved.
`wm.md2`	Atomic coordinates in the last MD step are saved. An atom is specified using the specified atomic species symbol.
`wm.ene`	Calculated values for each MD step are saved. The contents of each saved value can be checked in the" iterout.c "routine.
`wm.Band`	Band dispersion data file is saved.
`wm.Dos.val`	Eigenvalue data file for calculating density of states.
`wm.Dos.vec`	Eigenvector data file for calculating density of states.
`wm.tden.cube`	The total electron density in Gaussian cube format is stored.

Hint: **Working folder**

- A working folder is a folder with the suffix of the name of the file opened in the main window.
  - ** The suffix depends on the type of solver. **
  - For example, for Gromacs, if the file opened in the main window is `aaa.gro` and the suffix is `_gmx_tmp`, the name of the working folder is `aaa_gmx_tmp`.
- It must be on the same level as the file opened in the main window.
- Although processing continues in the working folder with the same name for continued jobs, by default, a backup of the working directory of the previous job is created immediately before the continuous job is executed.
  - The name of the backup will be the lowest number in the range where there are no duplicate names. For example, if your working folder is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
  - ** Unnumbered directories are always up to date. **

Job is run through *Winmostar Job Manager*.

6.17.5 Open Log File (mxout)

Open the log file with a text editor.

6.17.6 Show log excerpts

Displays excerpts of key information from the log file.

6.17.7 Animation (md)

Create and display animations such as structure optimization and molecular dynamics calculations from md file information. Please refer to *Animation operation area* for how to operate the animation. From the animation operation area, you can calculate the radial distribution function, self-diffusion coefficient, mean-square displacement, and displacement of each atom.

6.17.8 energy change

SCF energy change (std)

Select the std file and display a graph of the residuals. Please refer to *How to operate the graph* for how to operate the graph drawing area.

6.17.9 Analyses

Density of of States

Specify the working folder (`dia_mx_data\`) and display the density of states. Calculation must be completed with Dos.fileout = on Please refer to *How to operate the graph* for how to operate the graph drawing area.

Partial DOS

Specify the working folder (`dia_mx_data\`) and display the partial density of states (PDOS). Calculation must be completed with Dos.fileout = on Please refer to *How to operate the graph* for how to operate the graph drawing area.

Band Structure

Specify the working folder (`dia_mx_data\`) and display the band structure. Calculation must be completed with Band.dispersion=on

Density/Spin/Energy Distribution

Specify the cube file and display the electron density, spin density, and energy distribution. See *Surface Setup / Cubgen window* for how to operate subwindows.

Fermi Surface

Specify the working folder (`dia_mx_data\`) and display the fermi surface. Use *FermiSurfer <https://mitsuaki1987.github.io/fermisurfer/index_ja.html>* to display the Fermi surface. In *# of K Points*, specify the number of k-point divisions when calculating bands, and press the *Calc* button to display the Fermi surface.

6.18 *Solid* → *FDMNES* menu

It is a menu related to FDMNES. The method of installing FDMNES is described in *Installing Winmostar and solvers*.

6.18.1 Configure

Set the calculation condition of FDMNES. To set up the calculations immediately after setting *Run* button, once to return to the main window please press *OK* button. See *Run* for behavior when clicking *Run*. Return to the default state with *Reset* button.

Target Atom
Specify the atom (Absorber) of the XANES spectrum measurement target. Clicking the *Set Atom* button will set the atom with the marker in the main window. .

Edge
Select the electron shell of the XANES spectrum you want to obtain.

Range
Specify the range of the XANES spectrum you want to acquire.

Cluster Radius
Specify the radius of the cluster created by expanding the simulation cell (supercell) inside FDMNES. The larger this value is, the closer the bulk state is, but the processing speed decreases.

Method
Select the calculation method.

Convolution
Obtain convoluted broadened spectrum with Lorentz function.

Calc LDOS
The local density of states (LDOS) is output into a file whose file name suffix is _sd*.txt.

Definition for Energy
Specify the horizontal axis (energy) definition when displaying XANES spectrum.

6.18.2 Run

Run FDMNES. Following file will be generated with execution. (Only major files are shown) As an example, the file/folder name when the input file is `cu.fdmnes` is also shown.

type	Description
log file `cu.log`	Calculation log file.
bat file `cu.bat`	It is a batch file for running FDMNES.
conv file `cu_conv.txt`	XANES This is a text file containing data such as spectra.

The job is run through *Winmostar Job Manager*.

6.18.3 Opem Log File (log)

Open the log file with a text editor.

6.18.4 Analyses

XANES Spectrum

Select the conv file (`*_conv.txt`) and display the XANES spectrum.

6.19 *Solids* → *VASP* menu

Menu about VASP.

6.19.1 How to set up VASP

For VASP execution from Winmostar, only remote jobs are supported. In the template script for the remote job, pass the PATH environment variable through the VASP binaries (vasp_std, vasp_gam, vasp_ncl, etc.) and specify the PATH_POTCAR_PAW_LDA, PATH_POTCAR_PAW_GGA, PATH_POTCAR_PAW_PBE variables to specify the directories in which the LDA, GGA, and PBE POTCAR files are grouped, respectively. The VASP binary to be used for the actual calculation can be selected in the Details of the VASP Workflow Configuration or in the VASP Executable of the Basic tab of the VASP Keyword Configuration. If you want to use different executables on Winmostar, you must pass them through the PATH with their aliases (vasp_gam, vasp_std, vasp_ncl, etc.). vasp_std is implicit in the Test Connection function for remote jobs. It is assumed that files are placed under the directories specified by PATH_POTCAR_PAW_LDA, PATH_POTCAR_PAW_GGA, and PATH_POTCAR_PAW_PBE in a directory structure named (element name)/POTCAR. If only POTCAR.Z is placed under the directory with the element name, POTCAR will be automatically extracted.

6.19.2 Workflow Setup

Configures and executes the OpenMX calculation flow in project mode.

Preset
Recalls and saves a preset of settings.

# of Jobs
Specify the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It is possible to run multiple calculations where only certain parameters differ (parameter scan), or to run calculations on multiple structures with the same parameters (structure scan). Click *Config* to open the configuration window for the scan calculation. For a parameter scan, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*. Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window. For structure scans, select %WM_STRUCT% for the *Target Variable* when the animation appears in the molecule display area (e.g., with an SDF file open). After the scan calculation is finished, use *File* → *Project* → *Parameter/Structure Scan Result* to tabulate the calculation results.

Import
Loads the settings output by Export. Click the arrow to the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Outputs the configuration to a file.

OK

Runs a calculation or generates a file with your settings. See *For project mode* for details.

Details

Set up detailed calculation conditions. *Configure* will be launched.

Task

Specifies the type of calculation.

	Settings
Energy	IBRION=-1 ISIF=0 NSW=0
Optimize(Atom)	IBRION=1 ISIF=0 NSW=50
Optimize(Atom&Cell)	IBRION=1 ISIF=3 NSW=50
BOMD	IBRION=0 ISIF=0 NSW=50

Functional

Select the pseudopotential and functional to use.

Cutoff energy

Specify the value if you want to explicitly set the cutoff energy.

Manually specify cutoff energy

explicitly sets the cutoff energy.

Precision

Sets the calculation accuracy.

	Settings
Medium	PREC=Normal
High	PREC=Accurate

6.19.3 Keyword Settings

Set the calculation conditions for VASP. After setting, press the *Run* button to run the calculation immediately, or press the *OK* button to return to the main window once you are done. :guilabel:See *Run* for behavior when *Run* is clicked. *Reset* button to return to the default state. The *OK* button applies the settings and returns you to the main window. The *Cancel* button closes the Window without doing anything. When invoking this function, if the structure displayed in the main window can be converted to a primitive cell, then *Convert Lattice (Primitive-Conventional)* will be executed automatically.

Basic tab

VASP Executable
Specifies the name of the VASP executable binary to be used in the calculation.

PREC
Batch setting for calculation accuracy.

NBANDS
Specifies the number of KS orbitals to use in the calculation.

K-point
In the case of “by KSPACING and KGAMMA”, KSPACING and KGAMMA keywords are used to set the K points. If “by KPOINTS file” then the KPOINTS file is used to set the K points.

KSPACING
Specifies the density of the K point.

KGAMMA
Specifies whether point K contains the Gamma point.

KPOINTS file
Enter the information to be included in the KPOINTS file.

ISYM
Specifies symmetry handling.

ENCUT
Specifies the cutoff energy of the wave function.

NELECT
Specify the number of electrons.

ISMEAR
Specify smearing method.

IBRION

Specify the mode of calculation. (SCF calculation, MD calculation, structural optimization calculation, etc.)

ISIF

Specify whether force and pressure calculations, atomic positions, and cells should be updated.

Advanced tab

EDIFF

Specify the censoring error for SCF calculations.

EDIFFG

Specifies the censoring error for structural optimization calculations.

NELM

Specify the maximum number of iterations for SCF calculation.

NELMIN

Specify the minimum number of iterations for SCF calculation.

NSW

Specifies the maximum number of iterations for structural optimization calculations.

TIME

Specifies time increments in some algorithms.

ALGO

Specify algorithm for SCF calculation.

NSIM

Specify the number of bands to be optimized simultaneously when using the RMM-DIIS method.

INIWAV

Specifies how the initial value of the orbit is generated when ISTART=0.

SIGMA

Specify smearing width.

IVDW

Specifies the method of dispersion force correction.

GGA

Specify LDA or GGA function.

LHFCALC

Specify the range-separation parameter for the strict-exchange term.

HFSCREEN

Specify the range-separation parameter for the strict-exchange term.

PRECFOCK

Specifies the FFT grid to be used in the calculation of the exact exchange term.

VOSKOWN

Specifies whether or not Vosko-Wilk-Nusair interpolation is used.

ADDGRID

Specify if you want to use an additional grid for Augmentation Charge.

LASPH

Specifies whether to include non-spherical components related to the electron density gradient in the PAW sphere.

LREAL
Specifies whether the projection operator is evaluated in real or inverse space.

Spin tab

ISPIN
Specify for spin polarization calculation.

MAGMOM
Specifies the initial spin of each atom.

Output tab

NWRITE
Adjusts the amount of information output to the OUTCAR file.

LWAVE
Specify whether to output wave function information in a WAVECAR file at the end of the calculation.

LCHARG
Specify whether charge density information should be output to the CHGCAR file at the end of the calculation.

LPARD
Specifies whether to evaluate partial charge densities resolved at the band or k points.

IBAND
Specifies the band used to evaluate partial charges.

EINT
Specifies the energy interval at which partial charges are evaluated.

LORBIT
Specifies the projection method and whether to output to a PROCAR or PROOUT file.

LORBMOM
Specify whether or not to output orbit moments.

LVTOT
Specify whether all potentials should be output to the LOCPOT file.

LVHAR
Specify whether Vionic(r)+Vhartree should be output to the LOCPOT file.

LELF
Specify whether to output ELFCAR files.

EMIN
Specifies the lower limit of the DOS energy range for output.

EMAX
Specifies the upper limit of the DOS energy range for output.

NEDOS
Specifies the number of grids when evaluating DOS.

LEPSILON
Specify whether to calculate the dielectric matrix, piezoelectric tensor, or Born effective charge from the DFPT calculation.

MD tab

MDALGO
Specifies the time evolution algorithm for MD calculations.

POTIM
Specify the time increment for MD calculations or the update step width for structural optimization calculations.

TEBEG
Specify default temperature.

TEEND
Specify final setpoint temperature.

SMASS
Specify the method of temperature control or the mass parameters of the heat bath.

LANGEVIN_GAMMA
Specifies friction parameters for the Parrinello-Rahman pressure bath.

LANGEVIN_GAMMA_L
Specify friction parameters for Parrinello-Rahman pressure bath.

PMASS
Specifies the mass parameter of the Parrinello-Rahman pressure bath.

MLFF tab

ML_LMLFF
Specify whether to use a machine learning force field.

ML_ISTART
Specify whether to train and predict machine learning force fields, etc.

ML_LEATOM
Specifies whether to output energy from the machine learning force field.

ML_MB
Specifies the maximum number of local reference placements in the machine learning force field.

ML_CTIFOR
Specifies the threshold in Bayesian error estimation of forces obtained from machine learning force fields.

ML_IWEIGHT
Specifies how to set the force, energy, and pressure weightings when training machine learning force fields.

ML_WTIFOR
Specifies the force weighting when training machine learning force fields.

ML_WTSIF
Specifies the pressure weighting when training machine learning force fields.

ML_WTOTEN
Specifies the energy weighting for learning machine learning force fields.

Others tab

Other settings for INCAR
Enter any other parameters you wish to include in the INCAR file.

Preview tab

INCAR
This is a preview of the INCAR file that will be generated with the current configuration.

Pseudopotential tab

Pseudopotential
Specifies the type of pseudopotential to use.

Options tab

Dump all files for remote
Outputs files required for job execution in a Linux environment. The output file is the same as the file generated by the remote job submission function.

Restore Working Folder
Click to restore the working folder to its pre-execution state, for example, when a continuation job terminates abnormally.

6.19.4 Run

Runs VASP. Local jobs are not supported, so *Submit Remote Job* will be launched in file mode. The following files will be generated upon execution. As an example, the file/folder names when the input file is `test.poscar` are listed.

type	Description
sh file `test.sh`	This is a shell script file to run VASP. It does not contain any job-dependent settings.
conf.sh file `test_conf.sh`	This is the configuration file that is read by the shell script to run the above VASP. It contains a collection of job-dependent settings.
outcar file `test.outcar`	Log file. This is a copy of OUTCAR in the working folder.
Working folder `test_vasp_data\`	Working folder.

The following files are generated in the working folder. Only the major files are shown here.

type	Description
`INCAR`	File specifying calculation conditions.
`KPOINTS.ori`	This is the configuration file for point K.
`OUTCAR`	Logfile.

Hint: **working folder**

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.
  - **Suffixes vary depending on the type of solver. **
  - For example, in Gromacs, if the file open in the main window is `aaa.gro` with the suffix `_gmx_tmp`, the working folder is named `aaa_gmx_tmp`.
- Must be placed in the same level as the file that is open in the main window.
- Processing flows in the working folder of the same name even for continuation jobs, but by default, a backup of the working folder of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the lowest numbered to the extent that there are no duplicate names. For example, if your working folder is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
  - **Unnnnumbered directories are always up-to-date. **

Job will be run through *Winmostar Job Manager*.

6.19.5 Show Log (OUTCAR)

Open the log file in a text editor.

6.19.6 Animation(OSZICAR)

Create and display animations for structural optimization, molecular dynamics calculations, etc. from information in OSZICAR files. See *Animation operation area* for animation display operations. From the animation operation area you can calculate the radial distribution function, self-diffusion coefficient, mean-square displacement, displacement of each atom, etc.

6.19.7 Energy Change

SCF energy change (XDATCAR)

Select a log file to view a graph of energy changes during SCF calculations. See *How to operate the graph* for instructions on manipulating the chart drawing area.

6.20 Tool menu

6.20.1 Preferences

Open the Preferences window. For details, see *Tools → Preferences menu*.

6.20.2 Save/Delete Fragment

Save Fragment

Same as *Save Fragment*.

Delete Fragment

Same as *Delete Fragment*.

6.20.3 Enter a structural formula

Same as *Structural Formula*.

6.20.4 Conformation Search (Balloon)

Conformation search with Balloon. Click the *Search* button to start the process. In the *Options* field, enter the options for the Balloon. An intermediate file will be generated in the working folder named `*_balloon_tmp`. This feature works as follows

1. Conformation search without GA for the initial structure Ballon options: -v 1 -c 10 –noGA -i 300 –randomSeed 51277
2. For the lowest energy structure of 1, a conformation search using GA Ballon options: -v 1 -b -k -c 400 –full -R 0.25 –nGene 20 –random 51277
3. Conformation search without GA for 4 structures with low energy of 2 Ballon options: -v 1 -c 25 –noGA -i 300 –randomSeed 51277
4. Select 100 from the low energy structures of 3
5. If *Cluster similar structures* is checked, cluster 100 structures and aggregate similar structures below RMSD tolerance and display them in Winmostar (However, due to the simplicity of clustering, the candidates may not be reduced efficiently)

Warning: This function is affected by the join order.

6.20.5 Point Group Analysis

Determine point group symmetry of modeled molecules. This function is mainly used for the following purposes.

(1) Perform point cloud analysis of modeled molecules.

(2) Based on the determined point cloud information, distortion of the molecular structure is resolved. (Symmetrization)

(3) Conversion of symmetric unit <=> asymmetric unit can be performed.

For organic molecules that do not contain metals, it is easier for point cloud analysis to succeed if cleaned structures are used. We analyze and visualize point cloud analysis using the following functions.

Analyze
Start point cloud analysis.

Accuracy
Specify analysis accuracy of point cloud analysis. Increasing the accuracy will make the judgment of symmetry severe, and lowering will make the judgment sweeter.

Shoenflies
The symmetry of the molecule is indicated by the Shoenflies symbol.

i
Point symmetry elements are listed.

On the Axis
The rotationally symmetric elements are listed.

Sn Axis
Recurrence symmetry elements are listed.

Mirror
Mirror symmetry elements are listed.

Select
All symmetric elements listed are selected and displayed on the graphic screen.

Deselect
All symmetric elements listed will be deselected and will be hidden on the graphic screen.

Select All
All symmetric elements are selected and displayed on the graphic screen.

Deselect All
All symmetric elements are deselected and hidden on the graphic screen.

After completing point group analysis, symmetrization of molecular structure and switching between asymmetric unit and symmetric unit becomes possible by the following operation. However, it is limited only to point group symmetry other than C1.

Symmetrize
Based on the predicted point cloud information, we eliminate the distortion of the structure (deviation from perfect symmetric structure).

Show
When Symmetric Unit is checked, symmetric unit is displayed. When Asymmetric Unit is checked, only asymmetric unit is displayed. (If you go to the GAMESS Configure with only the asymmetric unit displayed, you can inherit the point cloud information and create the input.)

Text area in the lower right

Displays the coordinate information of the molecule in XYZ format.

6.20.6 Molecular Surface Area & Volume

Calculate the molecular surface area, volume and oval shape. We use the program of Mr. Nagao of Hakodate National College of Technology to calculate the surface area and volume of the molecule. (Teruo Nagao, Improvement of molecular surface area and volume calculation program, bulletin of Hakodate National College of Technology, No. 27, p 111 - 120, 1993.)

(1) van der Waals Moleuclar Surface (VMS): Surface when atoms are replaced by spheres of van der Waals radius

(2) Accessible Molecular Surface: Surface of the solvent molecule when traced with a solvent molecule around the VMS surface

(3) Molecular Surface: Contact surface and reentrant surface traced by solvent molecules around VMS surface (also called Solvent-excluded surface or Connolly surface)

Molecular volume is the volume of the interior set of spheres of vdw radius centered at each atom. Ovality (Ovality) is calculated by the following formula. Molecule surface/Minimum surface area = S/4pi(3V/4pi)**(2/3) Minimum surface area = 4pi(3V/4pi)**(2/3) (surface area of a true sphere having the same molecular volume)

6.20.7 Aspect Ratio

Calculate the aspect ratio of a molecule. The aspect ratio is defined as the ratio L/D of the length L to the diameter D of the cylinder of the smallest diameter that encloses all spheres of vdw radius centered at each atom.

6.20.8 Radius of Gyration

Calculates the radius of inertia of a molecule. The calculated radius of inertia value is saved to a file in the background. The name of the saved file can be toggled with *Tools → Preferences menu*.

6.20.9 Dipole Moment

When there is point charge information in the displayed molecular structure, the dipole moment calculated from the point charge is calculated and displayed. In the case of multiple types of charges, the dipole moment is calculated and displayed for each type of charge.

6.20.10 Sterimol Parameters

Calculate the Sterimol parameter for the substructure selected for the group on the main window.Click *Calculate* button to start the calculation.

6.20.11 Unit Normal Vector of Ring Structure

This function displays unit normal vectors of ring structures, which are necessary for NICS calculations, etc. Please group-select a target ring structure then call this function. For example, in the case of a benzene ring, the six carbons that make up the benzene ring are group-selected. The output vector is calculated as follows

1. Creates a list of two atoms with covalent bond among the grouped atoms.
2. For each two atoms in the list created in 1, compute a vector perpendicular to the plane stretched by those two atoms and the three points of the geometric center of the group selection.
3. The average of the vectors calculated in 2 is finally displayed in this function.

6.20.12 Voronoi polyhedral volume

List the Voronoi polyhedron volume for each atom.

6.20.13 Job Manager

Start Winmostar Job Manager that manages local jobs.

6.20.14 Submit Remote Job

Open a window to run and manage remote jobs in file mode. See *Each function of the Submit Remote Job window* for details.

6.20.15 emote Server

Operate remote servers for each profile in project mode.

Configure

Configure profile settings.

6.20.16 Cygwin

Start the terminal window (terminal) of *CygwinWM*.

6.20.17 Log Viewer

Displays the end of a text file (such as a solver's log file) that is updated in real time. Drag and drop text files into the window.

6.20.18 Unit Converter

Opens a unit conversion tool specialized for atomic and molecular systems.

6.20.19 Search String

It searches character strings in various log files and outputs the hit line to Excel or text file.

6.20.20 Superimpose Molecules

Multiple molecules are superimposed and displayed. It is useful for checking the similarity of multiple molecular structures.

1. *Import from Main Window* or *Import from File* button to load the molecular structure you want to display and add it to the list of *Structures*. You can also drag and drop to load them directly from Explorer.
2. In the *Structures* list, click on the filename you want to highlight and the molecule will be highlighted in blue.
3. Delete selected molecule with *Delete* button, *Reset* button to delete all molecules.
4. You can align the orientation of each molecule with *Rotate to align 3 atoms* button. Clicking on 3 atoms for each molecule specifies the first point as the origin, the second point on the X axis, and the third point on the xy plane.
5. If the molecular structures are close, adjust the *X* , *Y* , and *Z* values in the *Offset* to shift the overlapping plane.
6. If there are only two molecules in the list of *Structures*, the *RMS-Fit All* button will automatically rotate the molecules so that the RMS (root mean square of the coordinates) between the two molecules is minimized. Also, the *RMS* will show the RMS between the two molecules.
7. You can display it with *Winmostar Viewer* by pressing *Open Viewer* button.

6.20.21 Aggregate multiple files into SDF format

Aggregate and save multiple files into a single SDF file. Aggregate all files contained within the selected folder. Only files that can be opened with *Open File* are read. (Judged by the extension.)

6.20.22 Animation

Switch to animation

Using this function while no animation is displayed will switch to one frame of animation being displayed.

Discard animation

Using this function while animation is displayed will leave only the current frame and switch to no animation being displayed.

Add a frame

Duplicates the current frame and adds a new frame to the animation.

Delete current frame

Delete current frame for animation

Separate each molecule into different frames

Separates each molecule into different frames, useful for counterpoise calculations, etc.

6.20.23 Structure scan

Generate and animate a structure with slightly different coordinates and cell sizes.

Transform cell only along the selected axis
Stretch or compress the cell in the direction of the axis selected in *Axis*. If *Variable* is Length change, the value is the incremental length (in angstroms); if it is Normal strain, the value is the strain. A value of 0 in either case means that the cell size is the same as the original cell size. If *Change Atomic Position with keeping fractional coordinates* is checked, the coordinates of each atom will change with keeping the fractional coordinates fixed, if unchecked, the coordinates of each coordinate will remain unchanged.

Transform cell by shear strain
Shear strain on cell.

Transform cell similarly
Deforms the cell in a similar manner. Specify the strain in each axis as a value (e.g., a value of 0.1 will multiply the volume by $(1 + 0.1)^3 = 1.331$, a value of -0.1 will multiply the volume by $(1 - 0.1)^3 = 0.729$). The coordinates of each atom vary while the fractional coordinates are fixed. Use this when you want to calculate volume strain.

Translate group along selected axis/vector
Translates the coordinates of the selected group in the direction of the axis selected by *Axis*. The value is the distance to translate (in angstroms).

Min
Specify the minimum value.

Max
The maximum value of the *Max* value is displayed. The *Max* is automatically set from *Min*, *Interval* and *# of steps* and cannot be specified directly.

Interval
Specifies the interval between values.

# of steps
Specifies the number of values.

Show Preview
You can see a preview of the animation with your settings.

OK
Generate animation.

6.21 *Tools* → *Preferences* menu

We make various settings of Winmostar.

Basic Tab

Language
Select a language.

License code
Set the license code.

Internal UNIX environment
Choose whether to use cygwin for internal UNIX environment or Windows Subsystem for Linux (Bash on Ubuntu on Windows).

Use internal editor at [File]-[Open in Text Editor]
If checked, use *Edit-> Direct Editor* function up to V8 when you click *File* → *Open in Text Editor*. If not, use the program set in Editor with *Preferences* → *Program Path*.

Use old function adopted up to V8 for unzip
In the remote job, specify the code used to get and unzip the zip file of the working folder from the remote server. Old-style code generates errors when decompressing huge files (hundreds of MB or more).

Use old format adopted up to V9 when saving xyz file
When saving in xyz file format, save as xyz file without header which was the default before V9.

Output cell shape to save Xyz file
Output cell shape when saving in xyz file format.

Automatically adjust bond length and hydrogen after reading ChemDraw MOL format.
Automatically adjusts the bond length and hydrogen after reading the MOL format of ChemDraw.

Output residue number to save Xyz file
Output the residue number at the end of each line when saving in xyz file format.

Maintain project display area when opening files
Specifies whether the project display area is automatically hidden or maintained when switching to file mode.

Number of recently used files/projects
Specify the number of recently used files/projects.

Use external viewer to display Cube files
Use an external viewer (such as VESTA) instead of Winmostar Viewer to open Cube files. The program selected in the Cube Viewer in the program path will be used.

CIF file parse
Specifies the library to use for reading CIF files. Gemmi is the method implemented since V11.6.0. pymatgen was the method used prior to V11.5.X.

Use legacy filename for [Tools]-[Radius of Gyration]
Toggle the name of the output file between V11.6.0 or earlier format or V11.6.1 or later format in [Tools]-[Radius of Gyration].

Edit tab

Bonding Factor
Set the threshold for judging the presence or absence of covalent bond from interatomic distance.

Keep Z-Matrix connectivity while modifying structure
If checked, make sure that the Z-Matrix join relationship does not change when editing molecular structure.

Convert aromatic ring to single + double bond for MOL file
When storing the MOL file, change the aromatic ring to a combination of single bond and double bond before outputting.

Bonding exceptions
Use this function when you do not want to create bonds between specific elements in the function to automatically generate bonds. First press the *Add* button. Then select the two elements you want to exclude the join in the two pull-down menus below the list and press the *Apply* button. After that, applying *Regenerate All Bonds* etc will break the bond between the specified elements. To restore, select the line you want to unset from the list andpress the *Delete* button.

Move markers to pasted atoms.
If checked, move the marker to the pasted atom when using *Paste*.

Simple Structural Optimization Methods
Choose the method you want to use with *Quick Optimization*.

Force field, cutoff, threshold (OpenBabel)
Specify the parameters when the simple structural optimization method is OpenBabel.

Max # of atoms to show atom list
Set the maximum number of atoms to display coordinates in Coordinate Viewer.

Max # of atoms to show atom list
Set the maximum number of atoms to display coordinates in Coordinate Viewer.

Max # of atoms to generate Z-Matrix
Set the maximum number of atoms to automatically generate Z-Matrix.

Max # of atoms to generate bonds
Set the maximum number of atoms to automatically generate Z-Matrix.

Show [CH3], [C2H3] and [C6H5] buttons
Install a fragment selection shortcut button on the toolbar. (similar to V10 and earlier)

Show toolbar captions
Show captions such as “solver”, “element”, “fragment”, etc. in the toolbar.

When right-clicked on viewport

Show context menu
Displays a context menu when right-clicking in the molecule display area.

Replace with fragment
Replace with fragment when right-clicking in molecular display area. (as before V10).

Alphabetically sort fragment list
Sort the list of fragments alphabetically. (as before V10).

Calculation tab

General

Run MOPAC using Job Manager
When checked, use *Winmostar Job Manager* when executing MOPAC. If it is not entered, Winmostar will be in a wait state until calculation by MOPAC is completed, and the output result of MOPAC will be automatically loaded into the main window. It can also be set from *Use Job Manager*.

Run the other solvers using Job Manager
Specify whether to use *Winmostar Job Manager* to execute programs other than MOPAC.

max # of Jobs
Sets the maximum number of jobs for the Job Manager.

Timeout
Set the time-out period of time-consuming processing.

Use old format adopted up to V9 when saving xyz file
If checked, use the directory name with "wm_" appended to the user name for the work folder Remote Job Submission.

QM

Forcibly sleep after GAMESS run
If this is checked, GAMESS will be forced to sleep for the specified number of seconds after executing GAMESS on the local machine. This function is useful when you want to check the contents of a log immediately after calculation.

mpiexec (NWChem)
Specifies the mpiexec to use for parallel computation in NWChem local jobs. For *MPICH*, the mpiexec specified in the *program path* is used. For *Select*, any mpiexec can be specified.

Options for mpiexec (NWChem)
mpiexec (NWChem) where *Select* is the argument for the mpiexec command. Where `%WM_NUM_PROC%` is entered, the parallel number is automatically assigned at runtime. (For example, if you enter `-np %WM_NUM_PROC%` in *Options for mpiexec (NWChem)* to calculate 2 parallelisms, mpiexec will actually run with the argument `-np 2`.)

# of procs for RESP charge calculation (GAMESS)
Specify the number of parallels for automatic calculation of RESP charges using GAMESS.

Keywords for automatic RESP charge calculation (GAMESS)
Sets the keyword for automatic calculation of RESP charges using GAMESS. By default, the keyword to perform a single point calculation with HF/6-31G* is used.

MD

Modify charges from AmberTools to adjust total charge
When calculating AM1/BCC, Gasteiger, and RESP charges using acpype or AmberTools, the charge of the entire molecule is set to a strictly integer value. In this case, the value of the charge of the first atom in the molecule is slightly modified.

Retain residue and atom names during force field assignment
Sets whether residue and atom names are retained during force field assignment.

Case sensitive when generating top file
Specifies whether or not the top file that internally writes force field parameters is case-sensitive in the detection of atomic name/type name matches when it is generated. This affects all processes that use force field parameters, not just Gromacs.

mpiexec (LAMMPS)
Specifies the mpiexec to use for parallel computation in LAMMPS local jobs. For *MPICH*, the mpiexec specified in the *program path* is used. For *Select*, any mpiexec can be specified.

Options for mpiexec (LAMMPS)
mpiexec (LAMMPS) where *Select* is the argument for the mpiexec command. Where `%WM_NUM_PROC%` is entered, the parallel number is automatically assigned at runtime. (For example, if you enter `-np %WM_NUM_PROC%` in *Options for mpiexec (LAMMPS)* to calculate 2 parallelisms, mpiexec will actually run with the argument `-np 2`.)

Using double precision in MD results analysis
Sets whether `gmx` (single precision) or `gmx_d` (double precision) should be used for result analysis with Gromacs.

Update elements when top file is loaded
When reading a top file in Gromacs force field assignment, set whether elements are read from the top file and reflected in the model.

Version of LAMMPS to be used
Specifies the version of LAMMPS to which the output LAMMPS input file corresponds. The output format of some keywords (e.g. thermo_style) will vary depending on the version.

Version of Gromacs to be used
Specifies the version of Gromacs to which the output Gromacs input file corresponds. The output format of some keywords (such as tau_p) varies depending on the version..

LAMMPS Potential Folder
Set about the LAMMPS potential folder.

Open potential directory
Open LAMMPS potential folder in Explorer.

Consolidating the same parameter type in LAMMPS data files
Sets whether the same parameters Bond type, Angle type, Dihedral type, and Improper type are merged in the output LAMMPS data file.

Allow LAMMPS pair_style, Potential file input
In the force field assignment function, allow users to freely input pair_style and Potential file.

Solid

Distance tolerance for Spglib
Sets the tolerance for automatic crystal symmetry detection in Spglib

Warn calling Spglib if # atoms is more than
Sets the minimum number of atoms to skip Spglib execution.

Default extensions
Set the extension set by default when creating input files for each solver.

Open k-path file
Open a file that sets the default k-point path for calculating band structure in Quantum ESPRESSO and OpenMX. Set per ibrav in Quantum ESPRESSO.

mpiexec (QE)
Specifies the mpiexec to use for parallel computation in Quantum ESPRESSO local jobs. For *MPICH*, the mpiexec specified in the *program path* for MPICH2 is used. For *Select*, any mpiexec can be specified.

Options for mpiexec (QE)
mpiexec (QE) where *Select* is the argument for the mpiexec command. Where

`%WM_NUM_PROC%` is entered, the parallel number is automatically assigned at runtime. (For example, if you enter `-np %WM_NUM_PROC%` in *Options for mpiexec (QE)* to calculate 2 parallelisms, mpiexec will actually run with the argument `-np 2`.)

Version of QE to be used
Specifies the version of the QE to which the input file of the output QE corresponds. The output format of some keywords (&fcp, HUBBARD, etc.) is diffrent with the version

QE pseudo directory
Setup about pseudopotential folders for Quantum ESPRESSO.

Open QE pseudo directory
Open Quantum ESPRESSO pseudopotential folder in Explorer.

Download pseudo files
Automatically download pseudopotential files from the web server to the Quantum ESPRESSO pseudopotential folder.

Open priority list
Sets the order of the list of Pseudo potential choices in the Quantum ESPRESSO Keyword Settings window. Asterisks can be used as wildcards.

QE MOL directory
Specify a folder to contain the solvent files for the RISM-compatible version of Quantum ESPRESSO.

Use Pymatgen for Slab Builder
Specifies whether pymatgen is used in the function to create slabs of the old specification. If not, use the in-house routines.

Use New Slab Builder
If checked, the function to create a slab with the new specification is used; if unchecked, the function to create a slab with the old specification is used.

View Tab

Color set
Select the color set from Winmostar, GaussView, Jmol, Rasmol, and Old Winmostar.

Color

Selected atom
Change the color of the atom type of the selected particle.

Bond
Change the color of the bond.

Background
Change the color of the background.

Background (Viewer)
Change the background color of Winmostar Viewer.

Text
Change the color of the character on the molecule display window.

Color bonds with color of atoms
Colors the bonds with the color of the atoms.

VDW radius of selected atom
Change the VDW radius for the element of the atom with marker in Viewport.

Diameter of bond
Specifies the diameter of the bond.

Font size on Keyword Editor
Specify the font size of the Keyword Editor.

Scrolling speed
Adjust the speed of zoom in/out by the mouse wheel in Viewport.

'Min # of atoms to switch to wire model while zooming'
Sets the minimum number of atoms to be changed to the wire model during zooming.

'Time to return from wire model after zooming [msec]'
Sets the time in milliseconds to return from the wire model after zooming.

Depth cue
Adjusts the fog density used for depth expression.

Depth cue density
Adjusts the fog density used for depth expression.

Maximum # of atoms for depth cue
Enable depth cue if the number of atoms is greater than the specified value.

View center after opening file
Check *View Marked Atom* autoatically when opening a file.

'Interval to show hint [msec]'
Set the wait time in milliseconds for hints to appear when hovering the mouse cursor over various controls.

'Font size for hint'
Sets the font size of the hints that appear when the mouse cursor hovers over various controls.

Items to be drawn
Check the items to be displayed in Viewport. You can also be set from *View* → *Items*.

Scaling factor of charge
Adjust the size of the charge display when displaying charges in *Label/Charge*. You can also be set from *View* → *Items*.

Program Path Tab
Specify the install path of various programs. For MOPAC and GAMESS, multiple program paths can be specified. In project mode only (1) is used. In file mode, you can use *QM* → *MOPAC* and *QM* → *GAMESS* in the run menu. The program invoked by the *Run* button in the file mode keyword setup window is the program path set in (1). For Quantum ESPRESSO, select `pw.exe` out of several executables. %APPDIR% is an alias character indicating the Winmostar installation folder and %CYGWINDIR% is the CygwinWM installation folder.

6.22 Window menu

Move between various subwindows. For **Animation** window and the **Energy Plot** window etc., you can open it again after you close it from this menu.

6.23 Help menu

6.23.1 manual

Display this manual on the local machine.

6.23.2 Web manual

Launch the web browser and display this manual on the web.

6.23.3 winmostar.com

Launch the web browser and display the HP of Winmostar.

6.23.4 Periodic Table

Open the html file of the period table under Winmostar installation folder.

6.23.5 Installation Test

Check the items you want to test and click the *Start* button to run the various solver operation tests. If the tests are successful, you will see `All tests passed.` Under the operating environment of some security countermeasure software, installation of some files in CygwinWM may be obstructed when installing CygwinWM, so you can check it easily with this function.

6.23.6 Check CygwinWM

Click *Check Now* button to check the installation of *CygwinWM*. In this function, check only existence of file. If you clear the check, you will see `Successfully finished. Close this window.` Under the operating environment of some security countermeasure software, installation of some files in CygwinWM may be obstructed when installing CygwinWM, so you can check it easily with this function.

6.23.7 Open Preferences Folder

Open the UserPref folder under the Winmostar installation folder.

6.23.8 Debug Mode

Switch to debug mode.

6.23.9 Reset Job Manager

Reset Winmostar Job Manager status.

6.24 Animation operation area

In the list on the left side of the window, the number of steps, energy, power, etc. of each frame are displayed. Clicking each line in the list will display the frame corresponding to that line in the main window. At the bottom of the window, the values of the selected column in the list are displayed in a graph *Column* pull-down menu. It is also possible to analyze results directly from this function for animated (trajectory) data, check *Options* → *Tools* for details.

Reload
Re-load the animation file.

Options

Export

Current Frame
Saves the current frame as a different name.

All Frames Separately
Outputs all the frames to a separate file. For example, it is useful when you want to divide the molecular structure of an SDF file into individual files and save and edit them. To re-aggregate split files into SDF files, use *Aggregate multiple files into SDF format*.

GIF Animation
Write a GIF animation file.

JPEG Images
Export serial number JPEG file. You can also operate from the *Export* button.

XYZ File (Multiframe)
Writes out a xyz file containing all frames.

MOL2 File (Multiframe)
Writes out a mol2 file containing all frames.

SDF File (Multiframe)
Outputs all the frames to a separate file.

WMM File (Multiframe)
Writes out a WMM file containing all frames.

Animated GRO File
Output animation gro file. It can be used for linking with VMD etc.

CSV (Values)
Outputs the numbers displayed in the list in csv format.

Tools

Invert Trajectory
Invert the trajectory. This is useful when you want to combine trajectories for forward and reverse IRC calculations around the saddle point.

Skip Frames
Thin trajectories are thinned at regular intervals. This is useful when you want to reduce the size of long trajectories and reduce the processing speed of the analysis.

Translate All Atoms

Translate every atom in every frame. This function is useful when you want to fine-tune the position of an atom when visualizing calculated data.

Set Origin as Lower Bound Edge of Cell

Set the starting point in each direction of the simulation cell for each frame to the origin. This feature is useful in combination with the *Translate All Atoms* feature.

Append Trajectory

Connects animations from other files to the current animation. This is useful when you want to join trajectories of forward and reverse IRC calculations around a saddle point.

Mean Square Displacement/Diffusion Constant

Calculates mean-square displacement and self-diffusion coefficient. See *Diffusion Constant/Mean Square Displacement* for details; some solvers, such as Gromacs, do not enable this menu, but may provide an equivalent function in the solver's menu. Some solvers will ask you how many steps each frame of the animation is output every other step and the time per step of the simulation (time ticks, delt t). If you are not sure of the value you entered, check the maximum value on the horizontal axis of the displayed mean-square displacement and if it matches the simulation time, you are good to go.

Radial Distribution Function

Calculate the radial distribution function. See *Radial Distribution Function* for details. Some solvers such as Gromacs do not enable this menu, but equivalent functions may be provided in the solver menu.

Displacement of Selected Atoms

Change in Number of Molecules for Each Molecular Species

Plot the molecular number change for each molecular species.

Rotational Autocorrelation Function

Calculate the rotational correlation function using the Legendre polynomial P2 of the second degree of the vector defined between the two atoms. The first vector is defined between the first and second atoms of the group to be analyzed, the second vector between the third and fourth atoms… The object of analysis is determined in the following way The average of the rotational correlation function for each vector is plotted.

Intramolecular Vector Autocorrelation Function

Calculate the autocorrelation function of vectors defined between two atoms. The first vector is defined between the first and second atoms of the group to be analyzed, the second vector between the third and fourth atoms… The object of analysis is determined in the following way The average of the autocorrelation function for each vector is plotted. It can be used to obtain the end-to-end vector autocorrelation function of a polymer.

Draw Path

The trajectory of each atom in the selected group is displayed as a line in the molecule display area.

Extract Trajectory for Selected Group

In the main window, create a trajectory file extracting only the atoms selected from the group.

Auto

Operates on the structure of each frame when executing file output functions such as *File → Export All Frames Separately*. The operations are performed in the menu sequence.

Check All/Uncheck All

Check/Uncheck all items from *Deleting Hydrogen* to *Quick Optimization*.

Deleting Hydrogen
Removes a hydrogen atom from the structure of each frame. This is equivalent to *Delete All Hydrogens*.

Extracting One Molecule
For each frame structure, only one molecule is left in the structure.

Adjusting Coordinate
Automatically adjusts the bond length for each frame structure. The same operation is performed as *Adjust All Bond Lengths*.

Adding Hydrogen
Hydrogen is automatically added to each frame structure. This is equivalent to *To all atoms*.

Quick Optimization
Performs a simple structural optimization for each frame structure. This is equivalent to *Quick Optimization*

Running MOPAC
Execute MOPAC for each frame structure.

Enable Dynamic Bond
Automatically generates joins for each snapshot every time. It is useful for MD calculations in which chemical bonds are recombined (first principle MD, CPMD, ReaxFF, DCDFTBMD, etc.).

Speed
Adjust the playback speed.

Loop
If it is checked, the loop will be played.

Open Viewer
Display the currently open animation using *Winmostar Viewer*.

Frame
Manipulate and adjust the display position.

Plot Column
Specify the columns to be displayed in the graph display section at the bottom of this window. You can also enter a value directly.

Custom Plot
Opens a window where you can flexibly plot list contents, interatomic distances, angles, lattice constants, etc.

6.25 Energy Level Diagram window

We display energy of molecular orbital in numerical value and diagram. By clicking in the list of numerical values or in the diagram, its molecular orbital is selected and is reflectted in *Selected MO* of *MO Plot window*. The HOMO level number is displayed in *HOMO:*, and the HOMO-LUMO gap is displayed in *HOMO-LUMO Gap:*.

slider
Adjust the origin and magnification of the diagram.

***Excel* button**
Save the energy value in a CSV file and open it in Excel.

***Close* button**
Close the window.

6.26 Surface Setup / Cubgen window

Adjust the display of volume data such as molecular orbit, electrostatic potential, various cube files.

***File* → *Open* menu**
Select the cube file you want to draw.

***File* → *Export VRML* menu**
Output in VRML format.

***File* → *Export VRML & Open VRML Viewer* menu**
Output in VRML format and open the file in a VRML viewer, which can be configured in the preferences.

***File* → *Open VRML Viewer* menu**
Displays the current file in the VRML viewer.

***File* → *Open Winmostar Viewer* menu**
View the current file in Winmostar Viewer.

***File* → *Close* menu**
Close this window.

***Quantity* pulldown menu**
Specify the value of the isosurface to draw.

- **MO**
  3D distribution of molecular orbitals selected by *Selected MO*.
- **Surface**
  Molecular surface drawn at a distance of VDW radius (not exact)
- **ESP(Population Charge)**
  ESP(Population Charge) is a three-dimensional distribution of electrostatic potential calculated from the point charge after Population analysis. It works faster than *ESP*. If more than one type of charge exists, ESP charge (high priority) > Lowdin charge > NBO charge > User charge > Mulliken charge (low priority) is used in that order.
- **ESP(Population Charge)/Surface**
  Display *ESP(Population Charge)* information on the molecular surface. When multiple types of charges are present, it behaves like ESP (Population Charge).
- **MO/Surface**
  Display *MO* information on the molecular surface.
- **Density**
  It is a three-dimensional distribution of electron density.
- **ESP**
  Three-dimensional distribution of electrostatic potential calculated directly by electronic state calculation.

Hint: You can display the ESP on the surface of the molecule corresponding to *ESP/Surface* by following the steps below. (Not supported for MOPAC.)

1. Check *Dump cube file* and select *Density* with *Quantity*.

2. Pressing the *Draw* button creates a file called `*_den.cube`.
3. Select *ESP* with *Quantity*.
4. When the *Draw* button is pressed, a file called `*_esp.cube` is created. This processor may take several minutes.
5. If you open `*_den.cube` in the main window of Winmostar, a window called *Cube Plot* will open.
6. Click the … button next to *File 2* to open `*_esp.cube`.
7. Click *Draw* button

Hint: If you have the Cubegen program included with Gaussian for Windows, you can speed up the display of *ESP*. In the *Cubegen* window that appears when you open a Cube file, check the *Use Gaussian's cubegen* checkbox.

The following items can only be selected for the Cubegen window.

- **Spin**
  This is the three-dimensional distribution of the spin density (density difference between alpha and beta spins).
- **Alpha**
  This is the three-dimensional distribution of the alpha spin density.
- **Beta**
  This is the three-dimensional distribution of the beta spin density.
- **CurrentDensity=X**
  3D distribution of current density induced by a magnetic field, where X is the direction in which the magnetic field is applied, rewrite and run Y or Z as needed.
- **ShieldingDensity=XX1**
  This is the three-dimensional distribution of the magnetic shielding density. The first X after = is the direction in which the magnetic field is applied, the second X is the direction of the induced field, and the third number is the number of the atom for which the shielding density is calculated; rewrite and execute as needed.

Selected MO
Specify the number of the molecular orbit to be drawn. Selecting a molecular orbital with *Energy Level Diagram window* will set the value in this location.

***Show Diagram* button**
Energy Level Diagram window is displayed.

***alpha/beta* button**
Select a spin.

***Draw Style* pulldown menu**
Display the isosurface in grid (Mesh) or solid (Solid) model.

Transparency
Specify transparency. (0: opaque, 1: transparent)

Isosurface Value
Specify the value of the isosurface to draw.

Points
Specify the number of grid points on each side.

Scale
Specify the scaling factor that specifies the range to be drawn.

***Draw boundary* check box**
Draw a line on the boundary of the cube file. It is mainly used for band calculation such as Quantum ESPRESSO, OpenMX.

***Draw contour Map* check box**
Draw a contour line on the specified section.

***Dump cube file* check box**
When you press the *Draw* button, cube file is output at the same time as drawing.

***Draw* button**
Draw the volume data using *Winmostar Viewer*.

***Close* button**
Close this window.

6.27 IR Spectrum Window

Display IR and Raman spectra. The list on the left shows the frequency, the IR intensity, the Raman intensity, and on the graph on the right they are displayed after they are broadened. In GAMESS, you can display both spectra simultaneously by reading additional Raman spectrum with the IR spectrum read. When you click on the graph, the row of the peak close to that position is selected in the list.

Freq. Scaling
Select the frequency scaling factor to compensate for systematic errors. From the pull-down menu, select the method/basis function value used for calculation. You can edit the list of scaling factors by pressing the *Edit* button.

Raman
Select Raman Activity / Depolar (P) / Depolar (U).

IR
Display IR spectrum.

Animation
Animate the vibration state of the selected peak.

Vector
Vibration status of the selected peak is displayed.

Magnitude
Adjust amplitude in animation display and length in vector display.

X Range
Specify the range of the horizontal axis.

Reverse
The horizontal axis is inverted and displayed.

Y Scale
Change the scale of the vertical axis.

Reverse
The vertical axis is inverted and displayed.

Broadening
Set the full width at half maximum of broadening.

Export
Select the format to output the file.

Export csv (Discrete) & Open Excel
Outputs and opens a csv file for a discrete spectrum. See Export csv (Discrete) for the contents of the csv file.

Export csv (Discrete)
Outputs csv files for discrete spectra. The csv file outputs the spectrum number, wavenumber, IR intensity, Raman intensity (only if present), polarization resolving factor for plane polarized incident light (only if present), polarization resolving factor for unpolarized incident light (only if present), VCD intensity (only if present), and wavenumber after applying scaling factors csv file.

Export csv (Broadened) & Open Excel
Outputs and opens a csv file for the broadened spectrum, see Export csv (Broadened) for the contents of the csv file.

Export csv (Broadened)
Outputs a csv file for the broadened spectrum. csv file contains data number, fraction, broadened IR intensity, broadened Raman intensity (only if present), polarization resolving factor of broadened plane-polarized incident light (only if present), Broadened unpolarized incident light polarization resolving factor (only if present), broadened VCD intensity (only if present), and wavenumber after applying the scaling factor are output. The number of points output is fixed at 1000.

Export Image
Save the graph as GIF or JPEG.

Copy Image
Copy the graph to the clipboard.

Close
Close this window.

6.28 UV-Vis Spectrum window

Display visible ultraviolet spectrum. The numerical value of each spectrum is displayed in the list on the left and the broadened spectrum is displayed in the graph on the right.

***View* menu**

***Draw Peak* menu**
Draw the spectrum before broadening in the graph.

***Draw Curve* menu**
Draw the broadened graph in the graph.

Export
Select the format to output the file.

Export csv (Discrete) & Open Excel
Output and open csv file for discrete spectra.

Export csv (Discrete)
Output csv file for discrete spectra.

Export csv (Broadened) & Open Excel
Output and open a csv file for the broadened spectrum.

Export csv (Broadened)
Outputs a csv file for the broadened spectrum.

Copy Image
Copy the graph to the clipboard.

Broadening
Set the width of broadening.

Close
Close the window.

6.29 NMR Window

The NMR spectrum is displayed.

Element
Select the atoms for which you want to display the NMR spectrum.

Reference
Specify references for calculating chemical shifts. When *Element* is All, no choice appears. The list of references is managed in the wm_nmr.ref file in the UserPref folder. You can add a reference with *Edit* button.

Shielding
Reference displays the value of the selected reference.

Selected
Click in the spectrum graph to display the value of the selected spectrum.

Degeneracy Tolerance
It is a threshold when grouping by assuming that spectrum is degenerate.

Export
Select the format to output the file.

Export csv & Open Excel
Output the csv file and open it.

Export csv
Output csv file.

Copy Image
Copy the graph to the clipboard.

Close
Close the window.

6.30 Energy Plot window

Time change of thermodynamic quantity such as various energy, temperature, pressure etc. of molecular dynamics calculation is displayed. The UI appearing by the solver is different. Select the item with *Energy Terms* and click the *Draw* button to display the graph. For how to operate the graph drawing area, see *How to operate the graph*.

Uncheck All on Launch
If checked, Energy Terms will be unchecked each time this function is launched. If unchecked, the checked items in Energy Terms will be saved. It will only appear in certain solvers.

Block Average
Plot the block averaged value with the size specified by *Size*. It is useful for plotting physical quantities with large instantaneous fluctuations.

Normalize by Nmol
We standardize the energy by the number of molecules. To obtain the number of molecules, select the coordinate file.

Plot Each Data Set on Separate Graphs
If checked, each item will be plotted on a separate graph. If unchecked, each item will be plotted simultaneously on a single graph.

Calc Ave
Output the mean value of each item as a text file. If *Calc Stdev and drift* is checked, the standard deviation and drift (difference between the minimum and maximum values of a line obtained by linear regression of time series data) are also output. In the case of Gromacs, we execute `gmx energy`, and physical properties derived from fluctuations such as specific heat and bulk modulus are also output.

Draw
Draw a graph. For Gromacs, execute `gmx energy`.

Close
Close the window.

6.31 How to operate the graph

Operation in graph drawing area

Left drag
Move the graph in translation. You can restore it with *Refresh* button.

Drag right
Enlarge the graph. You can restore it with *Refresh* button.

Show Setting

Autoscale
Set the drawing range automatically.

Min/Max
When you uncheck *Autoscale* checkbox, specify the drawing area directly.

Logarithm
It displays it in logarithm. The drawing range must be greater than 0.

Refresh
Reset drawing of the graph.

Options

Copy Image
Copy the graph to the clipboard as an image.

Export csv & Open Excel
Output csv file and open Excel.

Export csv
Output a csv file.

Copy Columns
Copy selected data in a format that can be pasted into Excel.

Export Gnuplot File
Output Gnuplot file.

Calculate Average
Calculates and displays the average value of the displayed data over a specified range.

Add Cumulative Average
Add a plot of the integrated mean of the displayed data.

Add Batch Average
Add a plot of batch averages (moving averages) of the displayed data. The graph will be smoothed.

Calculate Histogram
Calculate and display a histogram of the displayed data.

Calculate Differences from First/Last Value
Calculates and displays the difference from the first or last value for the displayed data.

Calculate First Differences
Calculates and displays the first difference of the displayed data.

Calcualte Integrated Values
Calculates and displays the integral value of the displayed data.

Calculate Average between Series
Displays data averaged across multiple data (series) displayed.

Fit Curve
Fits the displayed data to a function. In Type, the type of function is selected. In Equation and List of Parameters, the function and coefficients to be fitted are displayed. If the Type is Custom, enter the function and coefficients in the Equation and List of Parameters fields. Equation can be entered in Python format, and Numpy can be called with np.In List of Initial Parameter Values, enter the initial values of the coefficients, separated by commas. Enter the range of coefficients in the List of Parameter Value Ranges as a tuple (for example, enter "(lower limit of argument 1, lower limit of argument 2, lower limit of argument 3),(upper limit of argument 1, upper limit of argument 2, upper limit of argument 3)" when there are three coefficients). Check Specify Range to specify the range to be fitted. If "Specify 2nd Range" is checked, additional fitting will be performed in a range other than the one specified in Specify Range. Fitted Parameters displays the coefficients after fitting, and clicking Fit executes the fitting.

Shift/Scale Data
Shifts the displayed data by a constant multiple or by a constant amount; you can choose whether to change the data on the x- or y-axis. You can also divide or shift by the value of a specific data point.

Change Range for Cyclic Variable
For periodic variables such as dihedral angles, change their display range.

6.32 Winmostar Viewer

Winmostar Viewer is software attached to Winmostar specialized for drawing, displaying molecular orbital etc. It is also possible to display only specific ingredients in a multicomponent system like MD.

6.32.1 How to use the mouse

Left button + drag	Rotate the viewpoint. As you drag and release the mouse button it will continue to rotate.
Right button + up and down drag	Zoom In/Out.
Left button + right button + drag	It moves vertically and horizontally.

6.32.2 Menu operation

File menu

Open
Read gld and MOLDA format files.

Export GLD
Save the currently open GLD format file with a name.

Export MOLDA
Save the structure displayed in the window in MOLDA format.

Export JPEG (Current frame)
Save the contents displayed in the window as a JPEG file.

Export JPEG (Current frame,Stereo)
Save the left and right screens for stereoscopic viewing as a JPEG file.

Export JPEG (Sequence)
Save the animation as a sequentially numbered JPEG file.

Export GIF (Animation)
Save the animation as a GIF animation.

Launch StereoPhoto Maker
Start StereoPhotomaker.

Exit
Quit Winmsotar Viewer.

View menu

Representations
Perform detailed drawing adjustment *Representations window* is displayed.

Perspective
I use perspective.

Background Color
Specify the color of the background.

- **Winmostar Viewer**
  Make the background color dark blue.
- **Winmostar**
  Make the background color the default background color of Winmostar.
- **Black**
  Make the background color black.
- **White**
  Set the background color to white.

Model
Select the model to display.

- **Ball-and-Stick Model**
  Display the spherical bar model.
- **Space-Filling Model**
  Display space filling model.
- **Stick Model**
  Displays the bar model.
- **Wire Model**
  Display wire model.
- **Show SPace-Filling Model Overlapping**
  Display superimposed spatial priority models translucently.

Show Animation Control Panel
Animation operation panel is displayed.

Copy Image
Copy the image displayed in the window to the clipboard.

Help menu

Help
It shows how to use the mouse.

About Winmostar Viewer
Display version.

Debug
Displays debugging information such as memory usage.

6.32.3 Animation operation panel

When you display animation in Winmostar 3D, the UI for animation operation appears in the upper left corner of Winmostar 3D window.

slider
Move the frame.

Once
When playback reaches the last frame, playback stops.

Loop
When playback reaches the last frame, return to the first frame and repeat playback.

Round
Repeat playback in round trip.

Close
Close this panel.

6.32.4 Representations window

Orbit/Rotation
Specify the rotation method when rotating the viewpoint with left drag.

Orbit
Rotate freely.

X, Y or Z
Rotate around the horizontal direction within the window, the vertical direction within the screen, or the direction perpendicular to the screen.

Periodic Boundary Condition
Specify how to display molecules that are outside the cell.

None
Display the original coordinates as they are.

Atom
It displays the structure so that it fits within the cell in atomic units.

Mol
Displays the structure so that the structure fits within the cell in molecule units.

Molecule
From the *1* in the middle of this window *9* is assigned to each molecule.

Composition
Assign *9* from *1* in the middle of this window to each molecular species (with the same molecular weight).

1 - 9
The checked items are displayed. In the pull-down menu *BS*, *SF*, *ST*, *WI* are Ball-stick model (default), Space filling , Stick (rod) model, wire model.

Rainbow
It displays in different colors for each molecule.

Gold
The molecule is displayed in gold color.

Stereo
It displays stereoscopically.

Enantiomer
Display the original structure and its mirror image.

Para
Display in parallel method.

Cross
It displays by the intersection method.

Anag
It displays with anaglyph. (Red and blue glasses are used)

Shift
Specify the distance between molecules.

red
Specify the size of the molecule to rotate.

H
If checked, hydrogen atoms are displayed.

Dummy
When checked, dummy atoms are displayed.

Backbone
If checked, only the backbone will be displayed. (For proteins)

Atom
Sets the display magnification of atoms.

Bond
Sets the display magnification of the join.

Z-Clip
Specify the clipping position in the Z direction.

Surface Style
Specify how to display isosurface such as molecular orbital.

- **Mesh**
  We display the isosurface in mesh (lattice) model.
- **Solid**
  Displays the isosurface in a solid model.
- **SmoothSolid**
  Display the isosurface in a smooth solid model.

Trans
Specify the transparency of the isosurface. (0: opaque, 1: transparent)

Contour Map Position
When mesh (scalar field) information such as molecular orbital is read, draw contour map (contour line) against the checked surface. The position of the contour map can be adjusted with the slider.

6.33 Winmostar Job Manager

Winmostar Job Manager (JM) runs as an auxiliary program to Winmostar, scheduling jobs for the various solvers.

MaxCores

Maximum number of cores on which the job will run on the local machine. By default it is set to the number of cores on the machine. A larger value will allow many jobs to run in parallel at the same time, but setting it to more than the number of cores on the local machine will not increase efficiency.

6.33.1 Basic actions

When Winmostar executes a job on the local machine in file mode (called *local job*) or in project mode, the JM window shown below is launched and the job is registered in the first queue. In file mode, the *Status* of queued jobs is first *WAIT* (waiting to be executed), and then the jobs are registered in order, *Priority* and *RUN* in sequence considering the number of execution cores. The job switches to the next job, and the job is started. The *Status* of a finished job changes to *END*.

JM is automatically started when executing a local job with Winmostar, but it does not end automatically, so if you want to exit it is the `x` (close) button *File → Exit* It ends from. When you exit JM, the following jobs in the: guilabel: *WAIT* state will not start.

If you want to start JM at an arbitrary timing such as stopping JM by mistake, click *Tools → Job Manager* on the Winmostar main unit.

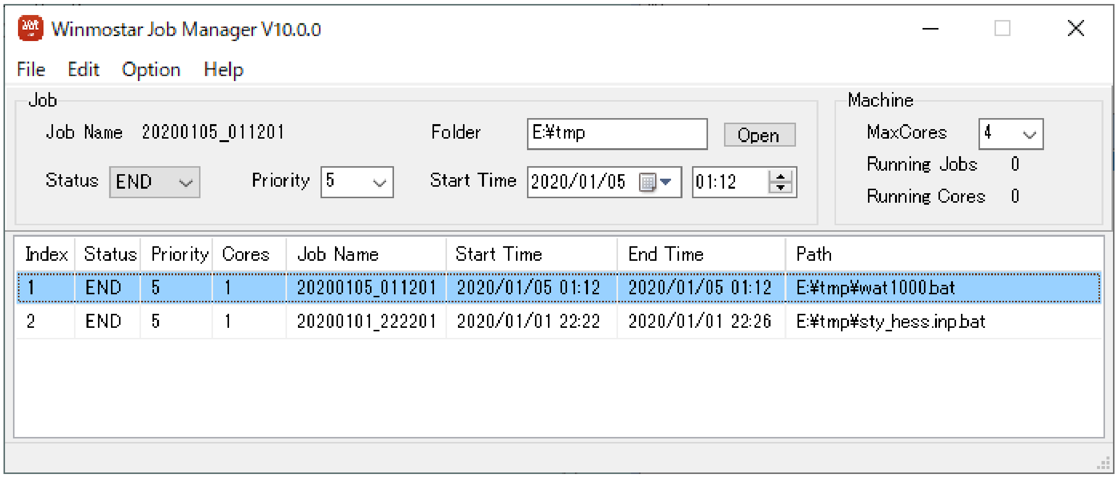
Hint: If you start the Windows Task Manager and go to the *Performance* tab, the number of cores of your machine will be displayed in the *Number of logical processors* field.

Jobs are basically executed in the order of old jobs in the *WAIT* state, but you can adjust their order by changing *Priority*. *Priority* has a lower value job execution with higher priority. For remote jobs, the timing of when they are submitted varies with *Priority*, and the actual order of execution on the remote server is determined by the scheduling software such as qsub.

The number of executed cores is set to the value set by the keyword of the solver to be used. For example, the value of %nproc= for G03W, and the value of NCPUS for GAMESS. G03W requires a parallel calculation version, and there is a limit of up to 4 cores.

JM has been adjusted not to start twice, and if you start Winmostar multiple times, the job will be registered for one JM.

JM can manage up to 200 jobs (queues) . If exceeded, old queues are deleted. Even if the running job is deleted from the queue, the job processing itself will continue.



Job Name 20200105_011201

Folder E:¥tmp

Status END

Priority 5

Start Time 2020/01/05 01:12

MaxCores 4

Running Jobs 0

Running Cores 0

Index	Status	Priority	Cores	Job Name	Start Time	End Time	Path
1	END	5	1	20200105_011201	2020/01/05 01:12	2020/01/05 01:12	E:¥tmp¥wat1000.bat
2	END	5	1	20200101_222201	2020/01/01 22:22	2020/01/01 22:26	E:¥tmp¥sty_hess.inp.bat

Note: For MOPAC, you can select whether to use JM in the Preferences of Winmostar itself. If you do not use JM, calculation results are automatically loaded into Winmostar's main window after MOPAC calculation, but if you use JM, the user must explicitly load the calculation result on Winmostar after the job is finished .

6.33.2 About power saving setting

During JM startup, JM prevents automatically entering standby (sleep) or hibernation mode depending on the time setting. Please note that it does not have a function to automatically restore like a TV recording software after entering the standby state etc. by manual operation.
When *AutoShutdown* is checked, all jobs are automatically shut down after entering the *END* state.

CHAPTER

SEVEN

REMOTE JOB

With the remote job submission function, it is possible to execute a solver on a Linux machine (**remote server**) different from the machine on which Winmostar is installed.

7.1 Supported remote environments

Winmostar supports the job scheduler listed in *Recommended remote servers*.

- Torque, OpenPBS, PBS Professional (PBS)
- Sun Grid Engine (SGE), Univa Grid Engine (UGE), Altair Grid Engine (AGE)
- Slurm Workload Manager (SLURM)
- FUJITSU Software Technical Computing Suite (PJM)

If the corresponding job scheduler is not installed on the remote server, you can execute the remote job in the following way.

1. Select `Run` with *Queue* setting.
2. Prepare commands and scripts that mimic commands such as **`qsub`**, **`qstat`** and specify the prefix of these commands with *Prefix for Queuing Commands* if necessary.

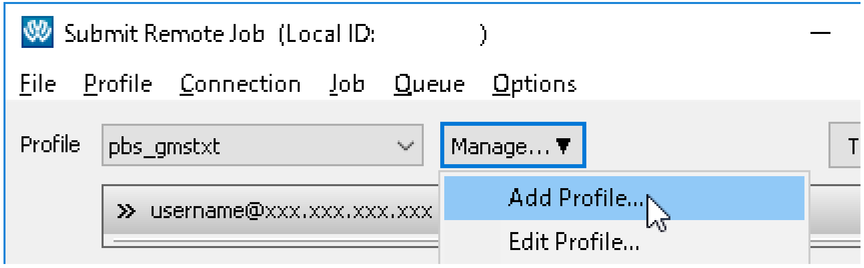
It is also assumed to run basically in a bash shell on a remote server. It is possible to run in other shells, but it may require more time and effort to change the scripts.

7.2 Remote Job Setup Procedures in file mode

See *Basic Operation Flow* for remote job setup procedure in project mode. See *Basic Operation Flow* for the overall flow of steps to run the simulation. For details of each function, see *Each function of the Submit Remote Job window*.

1. Install and configure the job scheduler and solver on the server where you want to run the calculations. At this stage, you must be able to SSH into the server without Winmostar and start the solver on the terminal. If you are planning to install it now, please refer to *here*. If you want to run jobs without using job scheduling (not recommended when running many jobs), you do not need to set up a job scheduler and should select `Run` in the *Queue* setting later.
2. Click *Submit Remote Job* button | toolbar_submit | on the tool bar.

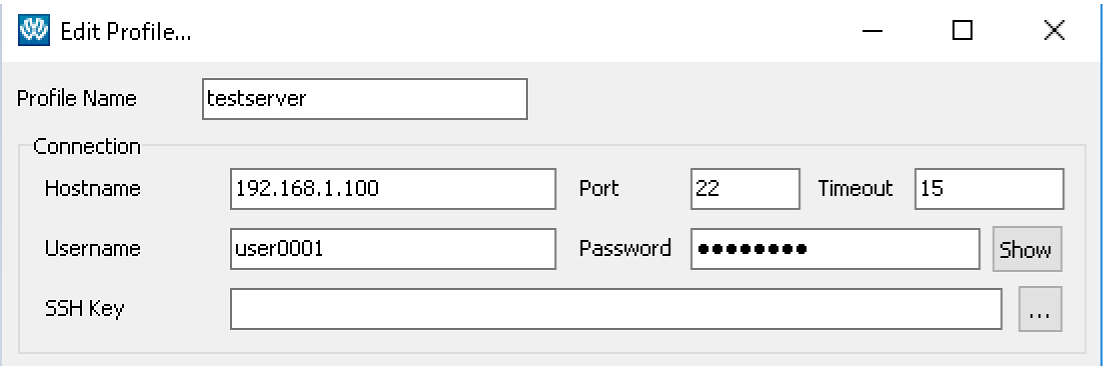
3. *Submit Remote Job* window, if you want to use a profile that is already configured, select the profile to use in *Profile*. If you are setting up a new profile, select *Manage…* → *Add Profile*.



Profile: pbs_gmstxt

» username@xxx.xxx.xxx.xxx

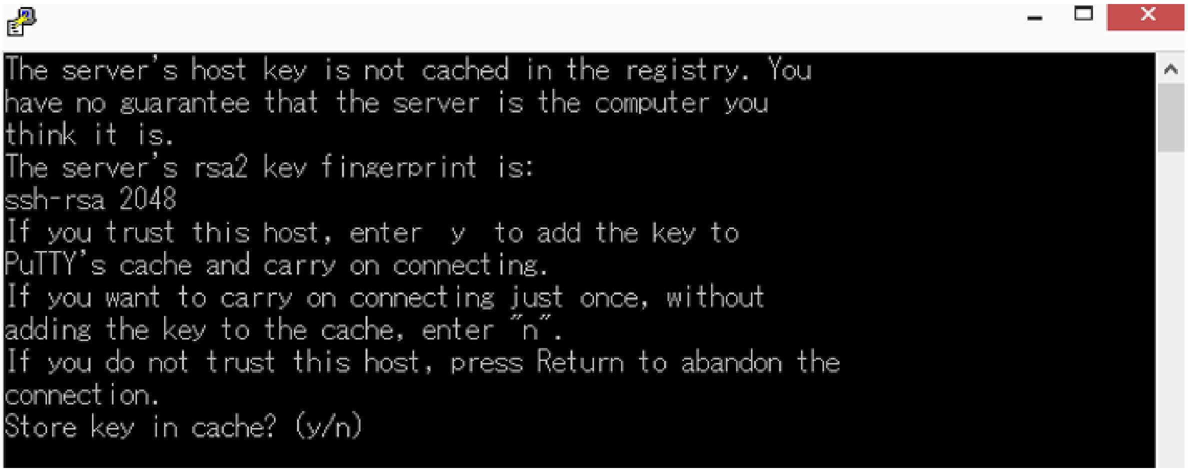
4. Enter the following contents on the top of window of *Edit Profile*.
   - Profile Name
   - Connection
     - Hostname
     - Port (normally 22 is used)
     - Timeout (Use default value if you do not know)
     - Username
     - Password (enter passphrase for private key, password otherwise)
     - SSH Private Key (only needed when using private key)



Profile Name: testserver
Hostname: 192.168.1.100
Port: 22
Timeout: 15
Username: user0001
Password: ●●●●●●●●●
SSH Key:

Please ask us to make multi-stage SSH connection to TSUBAME, FOCUS, etc.

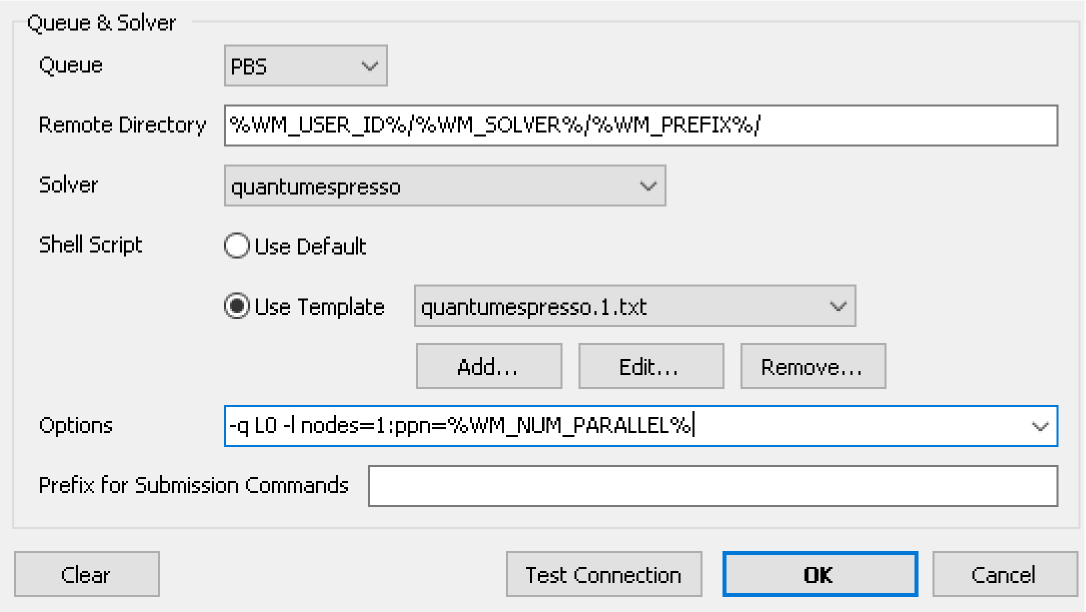
5. To test the SSH connection, click the *Test Connection* button under the *Edit Profile* window. Check the *SSH Connection Only* checkbox and click OK. When a black terminal window opens and `Store key in cache? (y/n)` may be displayed at the first connection. In that case, enter `y`.



```
The server's host key is not cached in the registry. You
have no guarantee that the server is the computer you
think it is.
The server's rsa2 key fingerprint is:
ssh-rsa 2048
If you trust this host, enter  y  to add the key to
PuTTY's cache and carry on connecting.
If you want to carry on connecting just once, without
adding the key to the cache, enter "n".
If you do not trust this host, press Return to abandon the
connection.
Store key in cache? (y/n)
```

If the connection is successful, the message "Test completed successfully" will be displayed. If the user settings or other settings are incorrect, please review the one previous setting as the message "The test ended abnormally". Even if you entered the correct password on the spot, please re-enter it in the *Edit Profile* window. If you see `ERROR: Connection timed out or an error occurred.` at the bottom of the *Submit Remote Job* window, please reconsider the connection settings. If a private key is used, the connection may not be possible due to different key formats. See *SSH public/private key authentication* for more information. If you cannot connect even though there are no problems with your input, you may be able to connect by switching the version of the library (libssh) used for SSH connections inside Winmostar. Go to [Tools] - [Preferences] - [Calculations] - [Use older version of libssh2 (1.8.2) for SSH connections] and switch the check box.

6. Enter the following contents at the bottom of the window of *Edit Profile*.
   - Queue & Solver
     - Queue
     - Options (command arguments for submitting jobs such as **`qsub`**)



Queue: PBS

Remote Directory: %WM_USER_ID%/%WM_SOLVER%/%WM_PREFIX%/

Solver: quantumespresso

Shell Script: ○ Use Default ● Use Template quantumespresso.1.txt

Options: -q L0 -l nodes=1:ppn=%WM_NUM_PARALLEL%

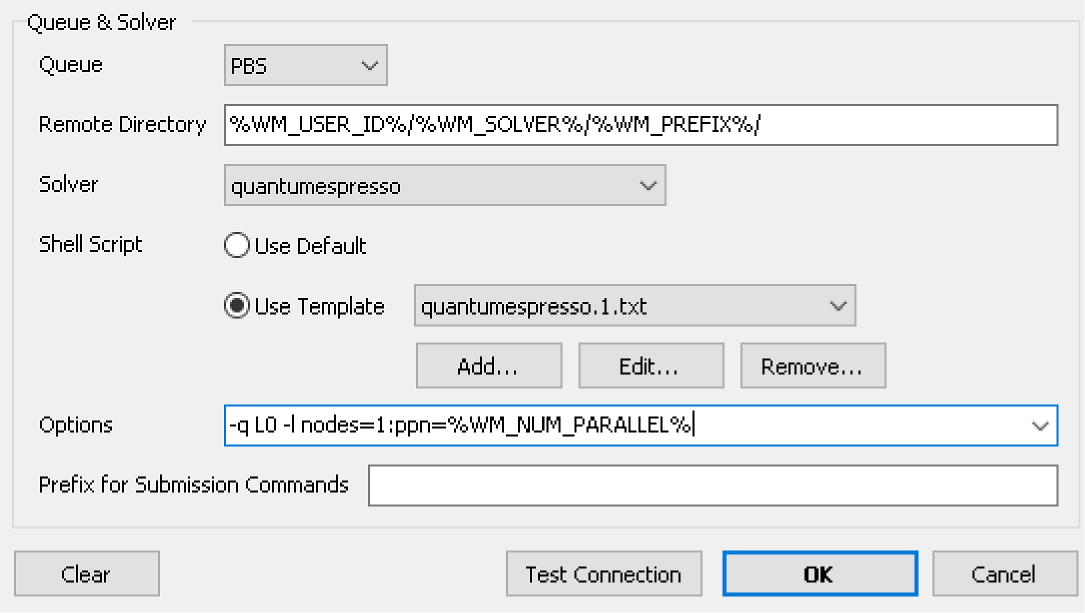
Prefix for Submission Commands:

First select *Queue* for the job scheduler installed on the server you are connecting to. Next, enter the command arguments to submit the job, such as **`qsub`** or **`sbatch`**, in the *Options* field. The information about the resource to be allocated is set here. In order to improve convenience, it is recommended to enter in the template file and in *Options* aliases in which settings such as parallel number and file name depending on each job are assigned at job execution . For details, see *Alias string available for remote job function*.

7. To test the scheduler's operation, click the *Test Connection* button under the *Edit Profile* window. If the remote server's queue is full and jobs are not flowing immediately, wait until the queue is free or continue. Check the "SSH Connection and Job Scheduler" checkbox. Enter the maximum waiting time for the Job Scheduler as well, and click *OK*. If the connection is successful, the message "Test completed successfully" will be displayed. If the setting is incorrect, the message "Connection test failed" will be displayed, so please review the one previous setting. You can check the details of Test Connection at *Test Connection* If the queue is full, the test will also terminate abnormally, in which case, please wait until the queue is empty.

8. Enter the following contents at the bottom of the window of *Edit Profile*.

   - Queue & Solver
     - Solver
     - Shell Script

   Queue & Solver

   Queue: PBS

   Remote Directory: %WM_USER_ID%/%WM_SOLVER%/%WM_PREFIX%/

   Solver: quantumespresso

   Shell Script: ○ Use Default

   ● Use Template: quantumespresso.1.txt

   Options: -q L0 -l nodes=1:ppn=%WM_NUM_PARALLEL%

   Prefix for Submission Commands:

   First select *Queue* as the job scheduler installed on the server to be connected and select solver to use on it with *Solver*. Next, click *Use Template* of *Shell Script*. If you do not have a template for the selected solver, enter the name of the template and the template will be opened in a text editor. If you have, select the template file you want to use in the pull down menu next to *Use Template* and click on the *Edit* button below it to open the template file in a text editor. Commands such as **`module load ...`**, **`source ...`**, **`export PATH = ...`** and other commands such as **`mpirun`**, enter the settings for using the solver selected on that server. Template scripts include **`` module load ... ` , :command:`source ... ` , :command:`export PATH=... ` , and :command:`mpirun ``** to use the selected solver on the server. Place them between **`# Insert commands here`** and **`# Do not modify the followings`** in the template script as much as possible. In order to improve convenience, it is recommended to enter in the template file and in *Options* aliases in which settings such as parallel number and file name depending on each job are assigned at job execution . For details, see *Alias string available for remote job function*.

9. To test the solver's operation, click the *Test Connection* button under the *Edit Profile* window. If the remote server's queue is full and jobs are not flowing immediately, wait until the queue is free or continue. Check the "Run Tests for SSH Connection, Job Scheduler, and (Solver Name)" checkbox. Set the "Maximum Wait Time for Job Scheduler [s]" to the appropriate value. Then click *OK*. If the connection is successful, the message "Test completed successfully" will be displayed. If the setting is incorrect, the message "Connection test failed" will be displayed, so please review the one previous setting. You can check the details of Test Connection at *Test Connection* If the queue is full, the test will also terminate abnormally, in which case, please wait until the queue is empty.

10. Press the *OK* button to close the *Edit Profile* window.
11. *Close* button to close the *Submit Remote Job* window. When prompted “Do you want to save the remote server configuration?” Click *Yes*.

7.3 Remote Job Operation Procedures in File Mode

See *Basic Operation Flow* for instructions on operating remote jobs in project mode.

- In the *Submit Remote Job* window, click the *Queue* → *Show Usage of Each Queues* menu and make sure the remote server information is displayed at the bottom of the window.
- If you want to start a job in file mode, click the *Send & Submit* button. The operation here is the same as for a normal local job.

  The ID of the submitted job is displayed at the bottom of the window. ID is used to kill the job. The directory in which the job was executed on the remote server can be set in *Remote Directory* of *Profile* → *Edit Profile*, and the one actually used is displayed on the *Remote Directory* field of *Submit Remote Job*. When a job is started on a remote server, standard output is output to the file `winmos.o` and standard error is output to the file `winmos.e`.

- If you want to check the status of jobs submitted in file mode, use *Queue* → *List Submitted Jobs*. If all jobs are complete, you will see `---`.

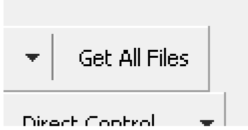
  If the submitted job ends too soon, `---` will be displayed even if you submit it.

- To check the status of a specific job on a remote server, please do the following.
  - *ls* button
  - *cat* button
  - *grep* button
  - *tail* button
  - *Get & Open* … button

  The target job is displayed in the *Remote Directory* field. For the default setting, open the input file of the job you want to target in the main window and select the profile when you submitted the job.

- If you want to run the result analysis of a job finished on a remote server in file mode on your local machine, click the *Get All Files* button.

  The target job is displayed in the *Remote Directory* field. For the default setting, open the input file of the job you want to target in the main window and select the profile when you submitted the job. After file acquisition, result analysis can be performed by the same operation method as local job.

7.4 Each function of the Submit Remote Job window

File menu

Revert All Changes
Discard the changes and reload the server configuration file.

Restore Setting File
Restore the server configuration file to the factory condition.

Import Setting File
It loads the server configuration file and adds the profile contained in it to the list of existing profiles.

Restore Setting File
Restore the server configuration file to the factory condition.

Close
Close this window.

Profile Menu

Add Profile, Duplicate Profile, Remove Profile
Add, duplicate, and delete server connection profiles. The same operation is possible from the *Manage* button in the window.

Edit Profile
Edit the profile of the server connection. Some settings can be edited directly in the Submit Job window.

Profile name
Specify the profile name displayed in the Submit Job window.

Hostname
Specify the host name or IP address of the remote server.

Port
Specify the port number used for connection.

Timeout
Specify the time (unit: second) for automatically disconnecting the connection when there is no response from the remote server.

Username
Specify the login ID (user name) to the remote server.

Password
Specify the password of the login ID. If you click [View], password hiding will be canceled.

SSH Key
Set the SSH key as needed.

Queue
Select the type of job scheduler running on the remote server to be connected.

Solver
Select the program to use in this profile. You can also change it in the window.

Shell Script
Check *Use Default* to execute calculations using the default shell script, or *Use Template* to customize the shell script. If you check *Use Template*, select a template file to use in the pull-down menu beside it, and if you want to add, edit or delete a template file *Add*, *Edit Remove* button. You can use *Alias string available for remote job function* in the template file. The template file is saved in `UserPref` in Winmostar installation folder. You can also change it in the window.

Options
Set arguments to be given after job submission command (qsub etc.). You can use *Alias string available for remote job function* for this item. You can also change it in the window.

Remote Directory
Specify the working folder of the remote server. If it is empty (Local User ID)/(program name)/(file name) is the working directory from the home directory. The Local User ID is the user name under Windows in operation and is displayed in the title of the Submit Remote Job window. If the Local User ID contains double-byte characters or half-width spaces, the directory name is internally converted to single-byte alphanumeric characters. If you enclose it with a single quotation like :command: *'/ work/dir'*, create `(Local User ID)/(program name)/(file name)` from the specified directory. Also, if you enclose two single quotations like `''/work/dir''`, a directory with (Local User ID) will not be created. You can use *Alias string available for remote job function* for this item.

Prefix for Queueing Commands
When executing commands such as qsub, if you need the prefix of those commands, set them here. Normally it is empty.

Test Connection
Test SSH connection, details of the Test Connection can be found at *Test Connection*.

Connection Menu

Test Connection and File Transfer
The same operation is possible with the *Test Connection* button in the window.

Job Menu

Send Local Files & Submit Job
Generate an input file required for calculation, transfer it to the remote server by SFTP, and submit it to the job scheduler. After submitting, the ID of the job is displayed. Generate the input files needed for the calculation, transfer them to the remote server via SFTP, and then submit them to the job scheduler. The ID of the submitted job is displayed at the bottom of the window; the ID is used to cancel (KILL) the job. The same operation is possible with the *Send & Submit* button in the window.

Submit Job
It generates an input file necessary for calculation and transfers it to the remote server by SFTP.

List Files at Remote Directory
Get the list of files in Remote Directory. The same operation is possible with the *ls* button in the window.

Display Remote File
Retrieve the contents of the selected file in Remote Directory. The same operation is possible with the *cat* button in the window.

Display Last Part of Remote Log File
Get the end of the log file in Remote Directory. The same operation is possible with the *tail* button in the window.

Search String in Remote Log File
Search strings in the log files in Remote Directory. The same operation is possible with the *grep* button in the window.

Restert Terminated Job
If a remote job is forcibly interrupted by the job scheduler, etc., this function restarts the calculation.

Force Job Finalization
If all files are not generated due to abnormal termination of calculation, and *Get All Remote Files* does not operate normally, executing this function forcibly terminates the process, and *Get All Remote Files* can be executed.

Get Remote File and . . .

Get a specific file in Remote Directory and visualize it. The same operation is possible with the *Get File & . . .* button in the window.

Queue menu

A concrete command name in the selected job scheduler is displayed in parentheses in each menu name.

List Submitted Jobs

Get a list of jobs registered in the job scheduler. The same operation is possible with the button with the same command name in the window.

Kill Submitted Job

Suspends the job registered in the job scheduler. You must enter the ID of the job displayed immediately after submitting. The same operation is possible with the button with the same command name in the window.

List Submitted Jobs in Detail

Get a detailed list of jobs registered in the job scheduler. The same operation is possible with the button with the same command name in the window.

Show Information of Each Queue

Get the list of queues managed by the job scheduler. The same operation is possible with the button with the same command name in the window.

Show Usage of Each Queue

Get usage status of each queue. The same operation is possible with the button with the same command name in the window.

Show Information of All Nodes

Get information on all machines managed by Job Scheduler. The same operation is possible with the button with the same command name in the window.

Other menu

The same command as the item name is executed on the remote server.

Options Menu

Hide Other Users Info

Specifies whether to display information about other users when qstat -a is run.

Enable Admin Mode

Used to access the remote server with root privilege

7.5 Alias string available for remote job function

Arguments of shell scripts and submit commands used when executing jobs may change dynamically depending on calculation conditions, so you can use alias strings to deal with such situations. A list of available alias strings is shown below.

%WM_USER_ID%	Local user ID for remote directory creation
%WM_SOLVER%	Type of solver
%WM_INPUT%	Input file name
%WM_PREFIX%	Input file name minus extension
%WM_EXT%	Input file name extension
%% WM_NUM_PROC	Number of MPI processes
%WM_NUM_THREAD%	Number of threads per MPI process (or total threads if MPI is not used)
%WM_NUM_PARALLEL%	Product of% WM_NUM_PROC% and% WM_NUM_THREAD%

7.6 Remote job configuration file

Profile settings are saved in `UserPref\winmos_profile.ini` in Winmostar installation folder. When reading, in order to maintain compatibility with old versions of V8 or earlier, it is read in the following order of priority. `UserPref\winmos_profile.ini` > `UserPref\winmos_server.ini` > `wm_system\RemoteJobdefault_profile.ini`

7.7 How to use Windows server

A Windows PC are available as a remote server. The following preparations are required to use it.

- Install an OpenSSH server on the remote server so that clients can connect with SSH.
- Install Winmostar on the remote server and always start Winmostar Job Manager.

Set as follows.

- In the Profile edit window, select JM (Windows) for Queue.
- Set Winmostar Path installed on the remote server to Winmostar Path.
- Since the default shell script cannot be used, select *Use Template* to create a template file. The contents of the batch file that runs on Windows.

There are operational differences from other job schedulers as follows.

- It also checks whether the job manager is running when the *Test Connection* button is pressed.
- The information displayed by the *List Jobs* button is the same as Job Manager, from the left: number, status, priority, number of cores, job name, start date/time, end date/time, and batch file.
- If you want to cancel the job with the *Delete Job* button, enter the job name.

7.8 How to connect via HTTP proxy

To connect to a remote server via SSH through an HTTP proxy server, follow the steps below.

- *Tools* → *Cygwin* to start Cygwin.
- Enter the command as shown below. Where REMOTE_SERVER, PROXY_HOST_NAME, PROXY_PORT, and USER_NAME should be replaced by the remote server name, proxy server name, proxy port number, and user name, respectively.

ssh -L1234:REMOTE_SERVER:22 -o “ProxyCommand connect-proxy -H PROXY_HOST_NAME:PROXY_PORT %h %p” USER_NAME@REMOTE_SERVER

- With the above connection, set Host Name to localhost and Port to 1234 in the Edit Profile screen.

7.9 SSH public/private key authentication

Winmostar's remote job feature also supports connection methods using SSH public/private key authentication. Some versions of Winmostar only supports connections in PEM format. When generating keys in the terminal, run `$ ssh-keygen -m pem -f (filename of the private key)` to ensure they are generated in PEM format. (OpenSSH requires `-m pem` because the default key format may be RFC4716). To convert an already generated key to PEM format, run `$ ssh-keygen -p -N "" -m pem -f (private key filename)`. In some cases, it is necessary to change the permissions of the private key file before conversion, in which case you can run `$ chmod 600 (private key filename)` in advance. To convert a PuTTY Private Key (ppk) format file to PEM format, first launch PuTTYgen, which is included with PuTTY. Next, click "Load" under "Actions" and open the ppk file. If a passphrase has been set, enter the passphrase in the "Key passphrase" and "Confirm passphrase" fields. Then, from the Conversions menu, click Export OpenSSH key and enter the file name of the newly created private key in PEM format.

7.10 Test Connection

The Test Connection function is available in the Job Settings window, Remote Server Profile window, Control Remote Job/Server window, and Submit Remote Job window to test the status of remote jobs. The Test Connection function is available in the Job Settings window, Remote Server Profile window, Control Remote Job/Server window and Submit Remote Job window. If the test fails, you can open the file used for the test. test_connection.log contains detailed information about the test and is useful for reviewing the configuration. In *SSH connection only*, test the SSH connection by sftp-sending a file named send_file.txt to the server and then receive. If this test fails, review the various settings for Host Name, Port, User Name, Password, SSH Private Key, and Port Forward. The *SSH connection and job scheduler* tests the job scheduler by actually submitting a simple shell script, remote_test.sh, to the job scheduler and checking that the shell script returns the expected output, in addition to the *SSH connection only* test. The job scheduler is tested by actually submitting a simple shell script called remote_test.sh to the job scheduler and checking whether the shell script returns the expected output. This test will fail unless the job scheduler is actually free and the submitted job runs immediately. If this test fails even though there is room in the job scheduler, please review the various settings in Queue, Options, and Prefix for Queueing Commands. submit_stdout.txt will output the standard output of the submitted command. remotejob_stdout.txt will output the standard output of the job that was executed. In *SSH connection and job scheduler and (solver name)*, in addition to testing the *SSH connection and job scheduler*, you can test the various solvers by actually submitting a simple job to the job scheduler and checking whether the job returns the expected output. Solver testing is performed by actually submitting a simple job to the job scheduler and checking that the job returns the expected output. This test will fail unless the job scheduler is actually free and the submitted job executes immediately. If this test fails even though there is room in the job scheduler, review the various settings in the template script. submit_stdout.txt will output the standard output of the submitted command. remotejob_stdout.txt and remotejob_stderr.txt will output the standard output of the executed job and standard error. winmos_script.txt is the submitted shell script.

CHAPTER

EIGHT

ADD-ON

8.1 Frangment ER

Calculate relative binding free energy between protein and ligand using Fragment ER method. Purchase of add-on is necessary for using. We use NAMD for molecular dynamics solver.

8.1.1 Fragment ER window

File menu

New Project
Initialize the project.

Open Project
Open the project.

Save Project
Overwrite and save the project.

Save Project As
Save the project with a name.

Close
Close the Fragment ER window.

MD menu

NAMD Keywords Setup
Open *NAMD Configure window*.

Run NAMD
Run NAMD locally.

Run NAMD On Remote Server
Open Remote Job Submission window for NAMD execution on remote server.

Edit .log File
Open the log file at NAMD execution with a text editor.

Energy Plot
Draw graph of energy change from log file at NAMD execution.

Import NAMD Trajectory
Open the MD trajectory.

Clear NAMD Output Files

Delete the output file made by NAMD execution. Delete RunNAMD.bat, RunNAMD.log, various dcd, log, coor, namd, vel, xsc, xst files etc ..

Analysis menu

Calculate Free Energy

Calculate free energy.

Edit .log File

Open the log file at free energy calculation with a text editor.

Import Result

Import the free energy calculation result and display it in *Result display window*.

Clear Analysis Output Files

Delete the output file made by free energy calculation. Delete FreeEnergy.sh, FreeEnergy.log, calc_PdP_kai2.out, parameters_fe file, refs, soln folder etc.

Tools menu

Preferences

Preferences window is displayed.

Solution

Specify PDB file of solution type by clicking … button. If more than one ligand molecule is present, designate the ligand molecule. Ligand molecules are displayed in the view.

Set Core

By clicking on the atom of the fragment part from the initial ligand and clicking the *Set Core* button, the remaining part is set as the mother nucleus.

Add

After selecting a new fragment with a combo box, click the *Add* button to add the ligand with the new fragment added to the mother nucleus to the final ligand list.

Configure

Fragment ER setting window is displayed.

Check

It checks whether atom types of mother nuclear parts of various ligands match. At the same time it generates force field of ligand.

Setup

Generate input file (PDB, PSF file) of NAMD.

Close

Close the Fragment ER window.

8.1.2 Fragment ER setting window

Set up Fragment ER calculation. The setting contents are recorded in the project file.

Solvation

Drop water and solvate for In-protein

Set whether water molecules should be rearranged by calculation of In-protein system. If you do not do this, water molecules of the solution system you read will be used as a solvent. If this is not done, periodic boundary cells must be set.

Drop water and solvate for In-aqua
Set whether water molecules are rearranged by calculation of In-aqua system. If you do not do this, water molecules of the solution system you read will be used as a solvent. If this is not done, periodic boundary cells must be set.

Distance from solute to cell boundary
Specify the distance from the solute to the periodic border cell.

Forcefield for Ligands
Select the type of force field to use for the ligand.

N-terminal modification
Specify N-terminal modification of protein.

C-terminal modification
Specify the C-terminal modification of the protein.

Import trajectory Interval
Specify how often to thin out when trajectory is imported.

ERmod

# of bins for binding energy
Specify the division number of binding energy.

# of insersions for solute (maxins)
ermod Specify maxins at runtime.

# of division of the simulation (engdiv)
ermod Specify engdiv at run time.

# of OpenMP threads (for local run)
ermod Specifies the number of OpenMP threads on local execution.

# of MPI processes (for remote run)
ermod Specifies the number of MPI processes at remote execution.

OK
Save the settings and close the window.

Cancel
Close the window without saving the setting.

8.1.3 NAMD Configure window

Set up MD calculation by NAMD. The setting contents are recorded in the project file. Select the system to be calculated with the check box.

Conf
Set the input file for NAMD calculation of each system.

numdcd
Specify the output interval of the trajectory.

numlog
Specify the output interval of the log file.

temperature
Specify the temperature. In the equilibrium calculation of In-protein, it is the temperature at the first stage of the stage temperature rise.

timestep
Specify the time step of 1 step of MD.

numstep
Specify the number of MD steps.

Number of Therad
Specify the number of threads when NAMD is executed.

Generate Conf Files
Output the input file (namd file).

Run
Output the input file and execute NAMD locally.

Close
Close the NAMD Configure window.

Load Default
Load default setting condition.

Save Default
Save the current setting condition as the default setting.

Reset Default
The default setting condition is reset to the initial state.

8.1.4 Result display window

A summary of the results is displayed in Summary. A graph of the energy distribution function is displayed. You can select which system to display.

log
Open the log file with a text editor.

Excel
Save the data displayed in the graph as a CSV file and open it with the application.

Close
Close the result display window.

8.1.5 Preferences window

NAMD Path
Set the path of the NAMD executable file.

Protein Topology Path
Specify the protein topology file.

Protein parameter Path
Specify the protein parameter file.

8.2 DCDFTBMD

It is a menu related to the divide and conquer type density functional the strongly bound molecular dynamics method. Purchase of add-on is necessary for using. How to install DCDFTBMD is described in *Installing Winmostar and solvers*.

8.2.1 Configure

After setting, press the *OK* button. The *Reset* button returns to the default state. *Save* button to save the settings. *Load* button loads settings saved with *Save*.

Continue Simulation
Run a continuation job. The keyword RESTART = TRUE is set, and the calculation restarts from the `restart` information. See *Run* for details.

# of Threads
Specify the OpenMP parallel number.

Use MPI
Use MPI. Specify the MPI parallel number in the horizontal column.

Basic

Charge
Specify the charge of the entire system.

Multiplicity
Specify the spin multiplicity of the entire system.

Parameter Set
Select the type of parameter to use. The names of folders placed in the `DFTBParam` folder under the Winmostar installation folder (by default `C:\winmos10\`) are listed.The folder placed under the `DFTBParam` folder must contain parameter files such as skf. For example, a hierarchical structure of `C:\winmos11\DFTBParam\mio-1-1\C-C.skf` is assumed.

Open Directory for Parameter Set
Open the aforementioned `DFTBParam` folder.

Reload Parameter Set
Reload the aforementioned `DFTBParam` folder and update the list of *Parameter Set*.

Executable
Specifies the binary of DCDFTBMD used for the calculation. When using MPI, it is necessary to specify an MPI compatible binary such as `dftb_mpiomp_mpich.00.x`. The binary specified here must be passed through PATH on the remote server.

Advanced

Method
Select SCC or NCC.

THIRDFULL
Use third-order correction for SCC Hamiltonian.

DAMPXH
Use short-range damping of SCC interactions for X-H pairs.

MAXITER
Specifies the maximum number of SCC cycles.

ECONV

Specify the convergence condition of energy change. (atomic unit)

DCONV

Specify the convergence condition of the gradient change. (atomic unit)

DISP

Use empirical dispersion force correction.

DISPTYPE

Specifies the type of empirical dispersion force correction.

DC

Use divide and conquer method.

SUBTYPE

Specify how to create a subsystem.

BUFRAD

Specifies the radius of the spherical buffer area. (angstrom)

DELTAR

Grid when dividing system into cubic space with SUBTYPE = AUTO (angstrom)

OPT/FREQ

OPT

Perform structural optimization calculations.

MAXITER

Specify the maximum number of structural optimization cycles.

DCONV

Specify the convergence condition of the gradient change. (atomic unit)

FREQ

Perform harmonic vibration analysis

MO

Perform molecular dynamics calculations

NSTEP

Specify the number of steps. When *Continue Simulation* is checked, it is necessary to enter the sum of the number of steps of the job before continuing and the number of steps of the job to be run.

DELTAT

Specify time step (second)

BATHTEMP

Specify the heat bath temperature when using NVT and NPT ensembles. (Kelvin)

Ensemble

Specify the type of ensemble.

NVTTYPE

Specify the settings for the hot bath.

INITTEMP

Specify the initial temperature (Kelvin)

PRINT

Specify the output frequency to the file such as coordinates during simulation.

CALCPRESSURE
Calculate the pressure. Care should be taken when performing a continuous job, as it cannot be changed from the settings of the job before takeover.

Properties

PRINT

MO
Output molecular orbital coefficient (only when the number of subsystems is 1)

ATOME
Outputs the contribution from each atom to the total energy.

HS
Outputs zero-order Hamiltonian and overlap matrix (only when the number of subsystems is 1)

FORCE
Calculate energy and force.

STRESS
Calculate stress tensor and lattice vector

Options

Restore Working Folder
Click to return the working Folder to its pre-execution status, such as when a continued job ends abnormally.

8.2.2 Run

To run DCDFTBMD, open *Remote job*. See *Remote job* for detailed instructions. The execution method depends on the situation.

- **(Default) If *Continue Simulation* is unchecked**
  Save the input file (extension dci) with the name specified by the user at the time of execution, and execute the calculation using it.
- **When *Continue Simulation* is checked**
  Create a backup of the existing working directory associated with the input file opened in the main window, save the input file as `dftb.inp` in the newly created working folder, and use it to perform calculations .

The following files are generated with execution. As an example, the file/folder name when the input file is `water.dci` is also shown.

Type	Explanation
dco file `water.dco`	DCDFTMD standard output file. A copy of `dftb.out` in your working folder.
Shell script `water.sh`	To perform DCDFTBMD and its pre/post processing shell script.
conf file `water_conf.sh`	Contains variables used in the above shell script file.
Working folder `water_dc_data\`	working folder.

The following files are generated in the working folder. Only the main files are shown here.

Type	Explanation
`dftb.inp`	Input file actually passed to DCDFTMD
`dftb.out`	Standard output file
`dftb.dat`	Detailed output file
`traject`	Trajectory file in MD calculation
`restart`	Restart file

Hint: ** Working folder **

- A working folder is a folder with the suffix of the name of the file opened in the main window.

  - ** The suffix depends on the type of solver. **
  - For example, for Gromacs, if the file opened in the main window is `aaa.gro` and the suffix is `_gmx_tmp`, the name of the working folder is `aaa_gmx_tmp`.
- It must be on the same level as the file opened in the main window.
- Although processing continues in the working folder with the same name for continued jobs, by default, a backup of the previous job's working folder is created immediately before the continued job is executed.
  - The name of the backup will be the one with the lowest number in the range where there are no duplicate names. For example, if your working folder is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
  - ** Unnumbered directories are always up to date. **

8.2.3 Open Log File (dco)

Open the dco (standard output) file with a text editor.

8.2.4 Open Detailed Data File (dat)

Open the detailed output file in a text editor.

8.2.5 Animation

OPT (dco)

Select a dco file and animate optimization calculation trajectory. See *Animation operation area* for animation display operations. From the animation operation area, you can calculate radial distribution function, self-diffusion coefficient, mean square displacement, displacement of each atom, etc.

MD (traject)

Select dci and traject files and animate MD calculation trajectory. The main window file name does not change. See *Animation operation area* for animation display operations. From the animation operation area, you can calculate radial distribution function, self-diffusion coefficient, mean square displacement, displacement of each atom, etc.

8.2.6 Energy Plot

Select a log file and display graphs of various thermodynamic quantities such as energy and temperature. See *Energy Plot window* for how to operate subwindows.

8.3 Towhee

Menu about Towhee.

8.3.1 Assigning force fields

If you are performing a Gibbs Ensemble Monte Carlo (GEMC) or Grand Canonical Monte Carlo calculation, the main window must be in animated view at this point and the number of frames in the animation must be 2.For GEMC, the first phase must have been created on the first frame and the second phase on the second frame.In the case of GCMC, the system to be calculated must be created in the first frame and the molecules not included in the first frame must be created in the second frame. Sets the force field. The options change depending on the type of solver. After assigning a forcefield, use *Get Info* to check the assigned forcefield. In the case of LAMMPS, if a gro file with velocities is open in the main window at the time this feature is used, it will generate a data file with velocities.Similarly, in the case of Gromacs, if a data file containing velocity is open, a gro file containing velocity is generated.This is useful when you want to take over Gromacs and LAMMPS computed data with velocities. Once you assign a force field and run the MD calculation, the bond order is automatically determined from the equilibrium length of the force field parameters.Depending on the type of force field, the bond order determined at that time may be different from the bond order before the force field assignment.Some force fields are affected by the bond order. Use *Overwrite Bonds from File* if you want to return to the bond order before force field assignment.

Assign parameters automatically

Assign new force field parameters. Structures connected to each other by bonds in the molecule display area will be recognized as a single molecule.

(General)

Specifies the force field for molecules other than proteins and water molecules. Internally, **`acpype`** is used for GAFF, GAFF2, OPLS/AA-L+GAFF, an in-house program for Dreiding, a proprietary extension of OpenBabel for UFF, and mktop for OPLS-AA. The configuration for Dreiding is described in `polymer/dreiding.lib.txt`. Check *Universal Force Field* for details on UFF.

Exception

Assigns a user-specified LJ parameter to a specific molecule, instead of using the force field selected in (General). Check the molecules for which you want to assign LJ parameters in the left column of the sub-window and enter the LJ parameters in the right column.

Note: This is used, for example, when you want to assign LJ parameters to atoms in the solid phase in a solid-liquid interface system.

(Protein)

Specify the force field of the protein. Here, the atom to which the name of the amino acid residue is assigned in the PDB or gro format is recognized as a protein. Internally, **`gmx pdb2gmx`** is used.

Warning: This function is not available if the molecular structure is read from a file that does not contain residue names.

(Water)

Specifies the force field of water molecules. You must specify the water model selected in *Solvate/Build Cell*. Internally, the parameters are taken from the library of Gromacs topologies installed in Cygwin.

[position_restraints] added for proteins

If the protein is present, write information (in the `[position_restraints]` section) to the topology file to constrain the position with *-POSRES* in the *Advanced* tab. If the protein is not present, it is ignored.

[position_restraints] added for selected atoms

Writes information (in the `[position_restraints]` section) to the topology file for a user-specified molecule to constrain its position with *-POSRES* on the *Advanced* tab. This is used, for example, to constrain the solid phase in a solid-liquid interface system.

[distance/angle/dihedral_restraints] added for selected atoms

Writes information to the topology file to constrain the distance, angle, and dihedral angle with *-POSRES* on the *Advanced* tab for the molecule specified by the user.

Dump Now

Generate a file with force fields assigned based on the current settings.

Note:

- If you want to customize the forcefield information by editing it with a text editor or similar, first save the file containing the forcefield information using *Dump Now* and edit the top for Gromacs or the data file for LAMMPS with a text editor or similar. Please use a text editor or similar to edit the data file.
- Next, for Gromacs, import the gro file at *File → Import File* (select *Discard and Load*), then at *Assign Force Field* select :guilabel:` Select *Use parameters written in topology file* and click the *OK* button. You will then be asked for the location of the top file, so open the top file you just saved and edited.
- For LAMMPS, import the data file by *File → Import File* (select *Discard and Import*), select *Use parameters written in file in main window* for *Assign Force Field Use the parameters written in the file in the :guilabel:`main window* and click on the *Next* > button.If the data file does not contain force field information, you will be prompted to *Select the type of force field*, select the type of generic force field you want to use and click the *OK* button.
- Charges are taken from the structure displayed in the main window. If more than one type of charge is set in the main window (for example, if you open a GAMESS log file and set a Mulliken charge and a Lowdin charge), the (high priority) User charge > NBO charge > Lowdin charge > ESP charge > Mulliken charge (low priority) Priority is used in that order.

Using parameter files (for inorganic, ReaxFF, and DPD)

(for LAMMPS) Select if you want to use the potential for inorganic materials, ReaxFF or DPD. After pressing the *Next* > button, specify the type of force field you actually want to use. pair_style and Potential file must be set in [Tools]-[Preferences]-[Calculations] to allow the user to enter them freely.

Use parameters written in topology file

(For Gromacs) Select this option if you want to run MD calculations using a top file that already exists. The corresponding gro file must be opened or imported in the main window. If you edit the structure after opening or importing it, the correspondence with the top file will be broken and the calculation will not be possible. If you want to use this function after editing the structure after opening or importing it to the extent that it does not affect the force field information (for example, editing only the coordinates without changing the bonds), export the structure in gro format after editing it and open or import that file before using this function.

Use parameters written in file in main window

(For LAMMPS) Select this option if you want to run the MD calculation using a data file that already exists. The main window must have the data file you want to use open or imported. If you edit the structure after opening or importing the file, the correspondence with the top file will be broken and the calculation will not be possible. After pressing the *Next* > button, specify the type of force field to use.

8.3.2 Workflow Configuration

Set up and run Towhee's calculation flow in project mode.

Preset
Recalls and saves a preset of settings.

# of Jobs
Specifies the number of jobs.

Enable parameter/structure scan
This feature requires the purchase of an add-on. It allows you to run multiple calculations where only certain parameters differ (parameter scan) or to run calculations with the same parameters for multiple structures (structure scan). Click *Config* to open the configuration window for the scan calculation.For parameter scans, select %WM_SCAN1% for the *Target Variable* and enter the parameters you wish to set for %WM_SCAN1% in each row of the *Values*.Then, enter %WM_SCAN1% in the parameters you want to set in the Workflow Settings window or Keyword Settings window.For structure scan, select %WM_STRUCT% for *Target Variable* when the animation appears in the molecule display area (e.g., by opening an SDF file). After the scan calculation is finished, use *File → Project → Scan Results Viewer* to tabulate the calculation results.

Import
Load the settings output by Export. Click the arrow to the right of the button to recall settings used in the past on the same project or Winmostar.

Export
Output settings to file.

OK
Run a calculation or generate a file with your settings. See *For project mode* for details.

Details
Set detailed calculation conditions. The *Keyword Settings* will be launched.

Ensemble
Specifies the type of ensemble.

	Configuration
NVT	ensemble=nvt Ratio(Vol)=0 Ratio(Insert)=0
NPT	ensemble=npt Ratio(Vol)=0.001 Ratio(Insert)=0
uVT	ensemble=uvt Ratio(Vol)=0 Ratio(Insert)=0.001
GEMC-NVT	ensemble=nvt Ratio(Vol)=0.001 Ratio(Insert)=0.001
GEMC-NPT	ensemble=npt Ratio(Vol)=0.001 Ratio(Insert)=0.001

Temperature
Specify temperature.

Pressure
Specify pressure.

# of steps
Specifies the number of steps to execute.

# of snapshots
Specifies the number of steps to execute.

Chemical Potential
Specify chemical potential.

For equilibration
This is used for equilibration calculations, not for this calculation. It uses an algorithm that has no statistical validity but allows the system to relax quickly.

	Configuration
True	rmin=0.01 Specify nstep/maxdispfreq=False
False	rmin=1.0 Specify nstep/maxdispfreq=True

Calc as Rigid

Forces the CBMC probability to be zero and computes the numerator as a rigid body. This improves calculation speed because the computation of internal degrees of freedom is omitted.

Precision

Set calculation precision.

	Configuration
Low	rcut=8 ewald_prec=1d-4
Medium	rcut=10 ewald_prec=1d-5
High	rcut=12 ewald_prec=1d-6

8.3.3 Keyword Settings

Set the Towhee calculation conditions. After setting, press the *Run* button to run the calculation immediately, or press the *OK* button to return to the main window once more. :guilabel:See *Run Towhee* for behavior when *Run* is clicked. If there are molecules with no charge assigned, *Assign Charges Automatically* will automatically start up. If no forcefield is assigned, *Assigning force fields* will automatically raise. *Reset* button to return to the default state. The *Save* button saves your settings except for the Force Field. The *Load* button loads the settings saved at *Save*.

Continue Simulation

Running continuation job. See *Run Towhee* for details.

Preset

Specify presets for calculation conditions. Each preset changes the following keywords:

	NVT Equil	NVT Prod	NPT Equil	NPT Prod
ensemble	nvt	nvt	npt	npt
Ratio(Vol)	0	0	0.001	0.001
Ratio(Insert)	0	0	0	0
rmin	0.01	1.0	0.01	1.0
Specify nstep/maxdispfreq	False	True	False	True

	uVT Equil	uVT Prod
ensemble	uvt	uvt
Ratio(Vol)	0	0
Ratio(Insert)	0.001	0.001
rmin	0.01	1.0
Specify nstep/maxdispfreq	False	True

	GEMC-NVT Equil	GEMC-NVT Prod	GEMC-NPT Equil	GEMC-NPT Prod
ensemble	nvt	nvt	npt	npt
Ratio(Vol)	0.001	0.001	0.001	0.001
Ratio(Insert)	0.001	0.001	0.001	0.001
rmin	0.01	1.0	0.01	1.0
Specify nstep/maxdispfreq	False	True	False	True

Basic

nstep

Specify the number of steps.

ensemble

Specify ensemble.

temperature

Specify temperature.

pressure

Specify pressure.

chempot
Specify chemical potential.

random_seed
Specifies the seed of the random number.

random_allow_restart
In continuation jobs, inherit the state of random number generation in the previous job.

Specify ratio instead of cumulative probabilities
If checked, specifies the probability of each operation (translation, rotation, CBMC, volume, insertion). If unchecked, specifies the integration probability; CBMC is an update operation for intramolecular degrees of freedom.

Disable CBMC
Forces CBMC probability to 0. All molecules are treated as rigid.

Fix 1st component
Freeze the coordinates of the first molecular species that appears in the system (or the first molecular species that appears through the first or second system in the case of GEMC).

Specify nstep/maxdispfreq
Give trmaxdispfreq and volmaxdispfreq as a ratio to nstep.

trmaxdispfreq
Specify how often to automatically update the maximum displacement for translational and rotational operations.

volmaxdispfreq
Specify how often to automatically update the maximum displacement for volume operations.

Advanced (1)

pmtracm
Specifies the cumulative probabilities of translational operations; if Specify ratio instead of cumulative probabilities is checked, you cannot enter the value directly and the automatically calculated value will be displayed.

pmtcmt
Specifies the cumulative probability for each molecular species of a translational operation; if there are more than two molecular species, enter them separated by spaces.

rmtrac
Specifies the maximum displacement for translational operations.

tatrac
Specify the target adoption rate to update with trmaxdispfreq.

pmrotate
Specify cumulative probabilities for rotational operations.If Specify ratio instead of cumulative probabilities is checked, you cannot enter the value directly and the automatically calculated value will be displayed.

pmromt
Specifies the cumulative probability for each molecular species of the rotation operation.If there are more than two types of molecules, enter them separated by spaces.

rmrot
Specifies the maximum displacement for rotational operations.

tarot
Specify the target adoption rate to update with trmaxdispfreq.

pmcb
Specify cumulative probabilities for CBMC operations; CBMC is an intramolecular degree of freedom update operation.If Specify ratio instead of cumulative probabilities is checked, you cannot enter it directly and the value will be calculated automatically.

pmcbmt
Specifies the cumulative probability for each molecular species in a CBMC operation.If there are more than two types of molecules, enter them separated by spaces.

pmall
Specify the probability for each molecular species that the entire molecule will be regenerated in a molecular regenerating operation.If there are more than two types of molecules, enter them separated by spaces.

pmvol
Specify cumulative probabilities for volume operations.If Specify ratio instead of cumulative probabilities is checked, you cannot enter the value directly and the automatically calculated value will be displayed.

pmvlpr
Enter the total probability of volume operation for each phase, separated by spaces if there are more than two phases.

rmvol
Specifies the maximum displacement for volume operations.

tavol
Specifies the target adoption rate to update with volmaxdispfreq.

Advanced (2)

pmuvtcbswap
Specify cumulative probabilities for insert and delete operations in GCMC. If Specify ratio instead of cumulative probabilities is checked, you cannot enter the value directly and the automatically calculated value will be displayed.

pmuvtcbmt
Specify the cumulative probability for each molecular species for insert and delete operations in GCMC. If there are more than two types of molecules, enter them separated by spaces.

pm2boxrbswap
Specify the cumulative probabilities of rigid insertion operations in GEMC. If Specify ratio instead of cumulative probabilities is checked, you cannot enter the value directly and the automatically calculated value will be displayed.

pm2rbswmt
Specifies the cumulative probability for each molecular species of a rigid insertion operation in GEMC. If there are more than two types of molecules, enter them separated by spaces.

pm2rbswpr
Specifies the integration probability for each interphase of a rigid insertion operation in GEMC. If there are more than three phases of molecules, enter them separated by spaces.

pm2boxcbswap
Specify cumulative probabilities for flexible insertion operations in GEMC

pm2cbswmt
Specifies the cumulative probability for each molecular species of a flexible insertion operation in GEMC

pm2cbswpr
Specifies the integration probability for each interphase of a flexible insertion operation in GEMC. If there are more than three phases of molecules, enter them separated by spaces.

Output

printfreq
Specify how often statistics should be output on standard output.

moviefreq
Specify how often to output trajectory files.

blocksize
Specifies the size of the block when block averaging.

backupfreq
Specify how often to output the restart file.

restartfreq
Specify how often to output a restart file with the number of steps in the name.

pdb_output_freq
Specify how often to output PDB files.

pressure_virial_freq
Specify how often to calculate virial pressure.

chempotperstep
Specifies the number of times per MC step of additional insertion operations for chemical potential calculations.

loutchempotdata
Specify whether chemical potentials should be output to another file.

Interaction

rcut
Specifies the cutoff radius of the vdw(LJ) potential.

rmin
Specify a hard inner cutoff where no more atoms can approach. A reasonable value will speed up the calculation.

rcutin
Specifies the inner cutoff used by CBMC.

ltailc
Specifies whether the cutoff correction term for the vdw potential is present.

electrostatic_form
Specify whether electrostatic potential calculations are performed.

coulombstyle
Specifies how the electrostatic potential is calculated.

kmax
Specifies the maximum wavenumber in the Ewald method.

kalp
Specify the product of the alpha parameter of the Ewald method and the short side of the cell.

rcelect
Specifies the real space cutoff radius for the Ewald method.

ewald_prec
Specifies the relative precision of the Ewald method.

Options

Restore Working Folder
Click to restore the working folder to its pre-execution state, for example, when a continuation job terminates abnormally.

Reset
Reset settings.

Import
Loading configuration file.

Export
Output configuration file.

8.3.4 Run Towhee

Runs Towhee. The method of execution depends on the situation.

- **(Default)** ***Continue Simulation*** **is unchecked**
  Generate a new wmm file before starting the job.
- ***Continue Simulation*** **is checked**
  Start a job using `towhee_final` in the working folder associated with the wmm file open in the main window.

The following files will be generated upon execution. As an example, the file/folder name of the input file is `water.wmm`. Note that the `wmm` file is Winmostar's proprietary molecular structure file and is not directly read by Towhee.

Type	Description.
bat file `water.bat`	This is a a batch file for running Towhee and its pre- and post-processing.
Workign folder `water_twh_tmp\`	Working folder

The following files are generated in the working folder. Only the major files are shown here.

Type	Description.
`towhee_input`	This is the main input file with some of the calculation conditions and force field information.
`towhee_ff`	This file contains force field parameters and other information.
`towhee_coords`	File with initial coordinates.
`towhee_initial`	This is the `towhee_final` of the previous job at the time of the continuation job.
`lammps_data`	Coordinates and force field files for LAMMPS used to generate `towhee_coords` , `towhee_ff` , `towhee_input`.
`gromacs.top`	`lammps_data` and topology file for Gromacs with equivalent conditions. Can be used for result analysis.
`towhee.log`	Towhee's standard output (log file).
`towhee_movie`	Trajectory file generated by Towhee calculations.
`towhee_final`	This file contains the final state at the end of the calculation (coordinates, various parameters of the Monte Carlo method, etc.).

Hint: **Working Folder**

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.

  - **Suffixes vary depending on the type of solver. **
  - For example, in Gromacs, if the file open in the main window is `aaa.gro` with the suffix `_gmx_tmp`, the working folder is named `aaa_gmx_tmp`.
- Must be placed in the same level as the file that is open in the main window.
- Processing flows in the working folder of the same name even for continuation jobs, but by default, a backup of the working folder of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the lowest numbered to the extent that there are no duplicate names. For example, if your working folder is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
  - **Unnumbered directories are always up-to-date. **

Job will be run with *Winmostar Job Manager*.

8.3.5 Show log

Open the Towhee log file (`towhee.log`) in a text editor.

8.3.6 Displays excerpts of key information from the log file.

Displays excerpts of key information from the log file.

8.3.7 Animation

`towhee_input` and `towhee_movie` to animate the trajectory of the MC calculation. See *Animation operation area* for animation display controls.

8.3.8 Energy Change

Select `towhee.log` to display graphs of various thermodynamic quantities such as energy, temperature, and pressure. See *Energy Plot window* for subwindow operation.

CHAPTER

NINE

HOW TO ADJUST THE ATOMIC AND MOLECULAR STRUCTURE DISPLAY

9.1 How to display a specific molecule in the presence of many molecules such as MD

1. First load the entire system you want to display as usual. The same goes for animations.
2. Select a group of molecules to display. See *Select menu* for how to select a group.
3. *view* → *Transparency*, click *make all atoms transparent*, then click *make group selected atoms opaque* and adjust *transparency* as needed. Adjust *transparency* accordingly.

9.2 How to show/hide atoms just above the simulation cell at both ends of the cell in crystals

Display → *Display Presets* If you want more fine-tuning, adjust the settings for *Tools* → *Preferences* → *Display* → *Display Items* → *Atoms on cell boundaries duplicated at both ends*.

9.3 How to make a drawing (in two shades of black and white) for a patent application document

Tools → *Preferences*, click the *Display* tab, check the *Display for patent applications* checkbox and click *OK* If the outlines are too coarse, zoom the camera in.

CHAPTER

TEN

INTEGRATION WITH OTHER SOFTWARE

10.1 Integration with ChemDraw and Chem3D

Obtain and install ChemDraw or Chem3D at your own risk. Molecules created by drawing structural formulas in ChemDraw can be loaded into Winmostar via the following *SMILES format* or *mol format*.When importing 3D structures created by Chem3D, please use *Gaussian input format* from Chem3D to Winmostar, because the 3D structure and hydrogen atom information will be missing via SMILES or mol format.

10.1.1 Reading from ChemDraw in SMILES format

The operating procedure is as follows.

1. After modeling the molecule in ChemDraw, click *Edit* → *Copy As* → *SMILES*.
2. In Winmostar, click on *file* → *import* → *SMILES* and paste the string into the *Enter SMILES* field.
3. Click the *Import* button to model the molecule in the main window.

10.1.2 Reading from ChemDraw in mol format

The operating procedure is as follows.

1. After modeling the molecule in ChemDraw, click on *File* → *Save As* and select the MDL MolFile format to save the file.
2. Winmostar will automatically adjust the bond length and add hydrogen to the mol file because the mol file in ChemDraw does not contain hydrogen and the bond length is not appropriate.

10.1.3 Reading from Chem3D in Gaussian input file format

The operating procedure is as follows.

1. After modeling the molecule in ChemDraw, click on *File* → *Save As* and select the MDL MolFile format to save the file.
2. Open the file you just saved in Winmostar and the molecules will be displayed in the main window. After that, set up your calculations from Configure of the solver you want to use.

10.2 Working with VMDs

VMDs are obtained and installed by the user at his/her own risk.

10.2.1 For animation

1. With the animation displayed, click *Options* → *Export* → *Animated GRO File…* to save the gro file.
2. Start VMD, then click *File* → *New Molecule…* and open the gro file saved in 1.

10.2.2 If not animated

1. *File* → *Export File* and save it in gro or pdb format.
2. Start VMD, click *File* → *New Molecule…* and open the file saved in 1.

10.3 Working with VESTA

Obtain and install VESTA at your own risk.

1. *Tools* → *Preferences*, on the *Basic* tab, check *Use external viewer to view Cube files*, on the *Program path* tab *Cube Viewer* and specify the VESTA executable file (`VESTA.exe`).
2. When you open a cube file in Winmostar, a *Cube Plot* window will open, click the *Draw* button and VESTA will open.

CHAPTER

ELEVEN

OTHER TOPICS

11.1 How to launch from the command prompt

It is possible to start by specifying various options from the command prompt.
Specify the input file name and processing contents in the option.
The processing contents that can be specified are as follows.

Recognize input files as SMILES and build molecules (using Balloon) (Professional Edition Premium Elite Only)	smilesballoon
Recognize input files as SMILES and build molecules (using OpenBabel) (Professional Edition Premium Elite Only)	smilesbabel
Execution of MOPAC	-mopac1, -mopac2, -mopac3 These correspond to the three MOPAC binaries selected in *Tools → Preferences menu → Program Path*.
Molecular Surface Area & Volume	-molsv
Aspect Ratio	-aspect
Radius of Gyration	-radgyr
Adjust All Bond Lengths	-adjust
To all atoms	-hadd
Delete All Hydrogens	-hdel
Quick Optimization	-clean
Use RESP charges (only for one molecule)	-resp (charge value, 0 for neutral molecules)
Use AM1-BCC/Gasteiger charges (only for AM1-BCC one molecule) (Professional Edition Premium Elite Only)	-am1bcc (charge value, 0 for neutral molecules) (Professional Edition Premium Only)
Solvate/Build Cell (the first argument is ignored)	-pack (file name of 1st molecule type):(number of 1st molecule type):(file name of 2nd molecule type):(number of 2nd molecule type) … (density [g/cm^3])
Insert Molecules (Professional Edition Elite Only)	-insertmol (file name of 1st molecule type):(number of 1st molecule type):(file name of 2nd molecule type):(number of 2nd molecule type) … (enumerated similarly thereafter)
Calculation of LAMMPS (Local Job) (The lmpset file can be obtained from the Save button in the LAMMPS Preference window.) (lmpset files are specified by relative path from the first argument)	-lammps (type of forcefield) (preset name or lmpset file name of the 1st job):(preset name or setting file name of the 2nd job) … (parralel number)
Output LAMMPS coordinate file (see *Assign Force Field* for force field type) (Professional Edition Premium Elite Only) Specify UFF or Dreiding as “GAFF(1=UFF)” etc. for a partial species in the force field for general molecules.	-lammpsfile (type of force field for general molecules) (type of force field for water molecules) (name of data file to output)
Output Gromacs coordinate and force field files (see *Assign Force Field* for force field types)	-gromacsfile (type of force field for general molecules) (type of force field for water molecules) (name of output gro file) (name of output top file)

Use case:

```
\"C:\\winmos11\\winmostar.exe\" COO -s -smilesballoon -outfile ethanol.mol2
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\dbt.dat\" -s -mopac1
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\dbt.dat\" -s -molsv 1 2.0␣
↪0.02
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\dbt.dat\" -s -o pdb
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\dbt.dat\" -s -adjust -hadd␣
↪-clean -o gjf
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\ch4.mol2\" -s -pack ch4.
↪mol2:100:ethanol_am1.mol2:2 0.6 -outfile ch4_100_etoh_2.mol2
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\ch4_100_etoh_2.mol2\" -s -
↪lammps "Dreiding" "Minimize (fast):NVT (fast):NPT (fast)" 2
\"C:\\winmos11\\winmostar.exe\" \"C:\\winmos11\\samples\\ch4_100_etoh_2.mol2\" -s -
↪lammpsfile GAFF SPC/E ch4_100_ethoh_2_auto.data
```

Specify input file at first argument.

When -s is specified, Winmostar ends automatically after processing, so you can write DOS BAT file and run MOPAC etc. continuously. See Sampleswmjobs.bat for reference.

Commands starting with "-" except "-s" are executed in the order specified.

If you want to run Gaussian and GAMESS sequentially, use *Tools* → *Batch Queue* instead.

11.2 CygwinWM

CygwinWM is Cygwin for Winmostar. It is called internally by Winmostar in the processing described in this manual as follows.

Warning: To use this function, *CygwinWM setup* is required.

Installation method is described in *CygwinWM setup*.

Warning:

- Some security countermeasure software may automatically delete or interfere with normal module in CygwinWM due to malfunction.
- If you download and install the CygwinWM installer from the Winmostar official HP, you can easily check for missing files in CygwinWM by using *Help* → *Check CygwinWM* function. (Only the existence of the file is checked.)
- If trouble occurs with the function that uses CygwinWM, please also check the activity report of security countermeasure software.

If you select *Tools* → *Cygwin*, you can start the console of CygwinWM directly.

11.3 Force Field

11.3.1 Universal Force Field

The Universal Force Field (UFF) available in Winmostar's molecular dynamics calculations (Gromacs, LAMMPS) is implemented as follows. First, use OpenBabel's UFF parameter assignment function to assign parameters to the molecule of interest. Then, for atoms that do not correspond to the atom type described in the original UFF paper [Rappe1992], the Coordination is automatically changed and a closer atom type is assigned. See the OpenBabel source code for more information. The functional form of UFF cannot be completely reproduced by the functions available in Gromacs and LAMMPS, so the coefficients are converted for the functions available in Gromacs and LAMMPS using the method of OBGMX [Garberoglio2012]. For the Improper torsion, the same harmonic function (improper_style harmonic) is used instead of the LAMMPS improper_style fourier. Improper torsion is calculated using the same harmonic function (improper_style harmonic) as in Gromacs, instead of using the improper_style fourier in LAMMPS. In addition, fourth-order function is used in Winmostar because the Angle potential in the square planar and octahedral structures does not give a proper stable structure due to the fact that there is only one minuscule point int OBGMX method. The coefficients of the quadratic function were determined by the following policy.

- Reproducing the position (angle, energy) of two potential minimum points
- Reproducing the energy of a maximum point between two potential minima
- In the case of LAMMPS, however, the coefficient of zero order cannot be set, so only the energy is shifted by a constant amount (the force, which is a derivative of the energy, is the same for Gromacs and LAMMPS, so there is no practical effect).

Because of the above policy, the resulting equilibrium structure and distribution is expected to remain largely unchanged from the case using the UFF original potential. Note that the widely used OpenBabel also adds its own penalty function to the Angle potential, which strictly deviates from the UFF original potential. In Winmostar, the coefficients of Angle for square planer and octahedral are as follows. $C_{i,\mathrm{gro}}$ is the coefficient of Gromacs' fourth-order function, $k_{a,\mathrm{uff}}$ is the coefficient of UFF; in LAMMPS, only $C_{2,\mathrm{gro}}$ and $C_{4,\mathrm{gro}}$ are used.

$$\begin{aligned}
C_{0,\mathrm{gro}} &= \frac{1}{4}(2-\sqrt{2})k_{a,\mathrm{uff}} \\
C_{1,\mathrm{gro}} &= 0 \\
C_{2,\mathrm{gro}} &= -\frac{8}{\pi^2}(2-\sqrt{2})k_{a,\mathrm{uff}} \\
C_{3,\mathrm{gro}} &= 0 \\
C_{4,\mathrm{gro}} &= \frac{64}{\pi^4}(2-\sqrt{2})k_{a,\mathrm{uff}} \\
\theta_{0,\mathrm{gro}} &= \frac{3}{4}\pi
\end{aligned}$$

Also, the calculation of Improper torsion angle in Gromacs depends on the order of particle indices (jkl) (LAMMPS does not). Therefore, Winmostar automatically adjusts the index order so that the results in Gromacs and LAMMPS are consistent. (For details, see *Gromacs to LAMMPS force field file conversion*)

11.3.2 Dreiding

Dreiding, which is available in Winmostar's molecular dynamics calculations (Gromacs, LAMMPS), is implemented as follows. As for Improper torsion, Gromacs does not implement the function for dreiding, so I use harmonic (funct=2) in Gromacs and improper_style umbrella in LAMMPS to calculate it. In Winmostar, the coefficients are converted as follows. $k_{\xi,\mathrm{gro}}$ are the coefficients of Gromacs and K_{lmp} are the coefficients of LAMMPS. We adopt the form of the Taylor expansion at the potential minima, ignoring after the fourth-order terms.

$$K_{\mathrm{lmp}} = \frac{1}{2} k_{\xi,\mathrm{gro}}$$

11.4 Editing an SDF file

SDF files are widely used in material informatics and machine learning.

11.4.1 Visualization of SDF file

If you select a SDF file from *Open File* and open it, *Animation operation area* will be displayed and you can check each structure in the SDF file in turn.

11.4.2 Editing an SDF file

1. After opening the SDF as described above, you can choose *Options* → *Export All Frames Separately* in *Animation operation area* to output each structure as a separate file in the selected folder.
    - If you want to adjust bond lengths, add hydrogen, or do quick optimization for each structure in a SDF file, click *Automation* → *Check All* of *Animation operation area*, then do *Options* → *Export All Frames Separately* or *File* → *Export Run the `SDF File*.
    - If you want to output a Gaussian input file (gjf file), do *Configure* before executing *Options* → *Export All Frames Separately*.
2. Then drag and drop a file corresponding to each structure into *Open File* or Winmostar to open it, edit it, and save it from *Save* to overwrite it.
3. If you select the folder you just output from *Aggregate multiple files into SDF format*, you can create the SDF file again.

11.5 Functional verification of Winmostar

Winmostar maintains its high quality by calling on open source software used by researchers around the world. On the other hand, there are some features that strongly depend on Winmostar's own implementation, and here we show the validation results of such features. The verifications shown here have been performed prior to release.

11.5.1 Gromacs to LAMMPS force field file conversion

Winmostar generates a data file for LAMMPS using a generic force field by converting the top file for Gromacs. Here are the results of calculating the energy for the same system using Gromacs and LAMMPS with this conversion mechanism.

Table 1: Relative energy difference between Gromacs and LAMMPS for each energy component

Force Field	Bond	Angle	Dihedral	Improper	Coulomb	Vdw	Total
UFF	2.57E-8	6.965E-9	1.17E-8	2.11E-8	7.21E-8	3.71E-8	7.55E-9
Dreiding	6.32E-9	4.25E-8	7.20E-9	5.37E-8	7.21E-8	3.62E-8	2.47E-8
GAFF	2.82E-8	3.06E-8	1.10E-8	2.97E-9	7.61E-8	9.51E-10	3.62E-9
OPLS-AA/L+GAFF	2.82E-8	3.06E-8	1.10E-8	2.97E-9	7.22E-8	1.67E-8	6.31E-8
OPLS-AA	1.64E-9	2.60E-8	1.10E-8	2.97E-9	7.22E-8	1.67E-8	5.93E-9

The detailed calculation conditions are as follows

- One molecule of benzene, calculated with AM1-BCC charge
- Free boundary condition, cutoff radius 20 Å, no constraints on bond length or angle
- Gromacs uses the 5.0.7 double precision version, LAMMPS uses the March 9, 2016 version
- Coulomb, Vdw includes 1-4 interactions
- Dreiding's Improper is calculated with Improper Harmonic because Gromacs does not have a function equivalent to LAMMPS' Improper_style umbrella.
- Since the 1-4 interaction scaling coefficients in Gromacs are processed internally in single precision, the single precision equivalent coefficients are also set in LAMMPS.
- The files generated by mktop is used for OPLS-AA

From the above table, we can see that the energies of Gromacs and LAMMPS are in agreement by 8-10 orders of magnitude for all components. It is difficult to get an exact match due to minor implementation differences between Gromacs and LAMMPS (e.g., approximate calculations of various functions, parallel calculations, etc.). Similar tests have also been conducted on systems focusing on each component of energy, multi-molecular systems, etc.

11.6 Regarding various parameters

11.6.1 Physical constants

The physical constants used in Winmostar are the 2018 CODATA recommended values [2018CODATA].

11.6.2 Atomic data

The following are references for atomic data used in Winmostar.

Covalent radius (single bond)	[Cordero2008]
Covalent Radius (Multiple Coupling)	[Pyykko2008]
van der Waals radius (typical elements)	[Mantina2009]
van der Waals radius (transition metal elements)	[Rahm2016]
Atomic mass	[NIST966]

Note that you can set the display radius of each element to any value by editing the third column of `atoms1.wmx` in *Help → Open Preferences Folder*.

11.6.3 Combining Criteria

single bond decision

If the distance between two atoms is shorter than the sum of the covalent bond radii (single bond) of each atom multiplied by the *bonding coefficient*, then it is determined to be a single bond. As an exception, H-H, O-O, and F-F bonds are determined by multiplying the values in the following table (unit: Å) by the *bond coefficient*. The H_2, HOOH, and F_2, respectively, were calculated using structural optimization calculations in B3LYP/6-31G*.

H-H	0.74
O-O	1.45
F-F	1.40

Multiple join determination

For some two-atom combinations, if the distance between the two atoms is shorter than the sum of the covalent bond radii (multiple bonds) of the respective atoms times 1.03, it is determined to be a double or triple bond. If it is shorter than 1.03 times the sum of the averages of the single and double bonds, it is determined to be a 1.5-fold bond (aromatic bond). As an exception, N=N, O=O, and P=O double bonds are determined by multiplying the values in the following table (unit: Å) by 1.03. HNNH, O_2, H_3PO_4, respectively, were calculated using structural optimization calculations in B3LYP/6-31G*.

N=N	1.246
O=O	1.215
P=O	1.473

The following table shows the types of bonds that are being judged.

Binding type	1.5 double bond	double bond	triple bond
C-C	✓	✓	✓
C-N	✓	✓	✓
C-O		✓	
C-S	✓	✓	
N-N	✓	✓	✓
N-O	✓	✓	
O-O		✓	
P-O		✓	
P-S		✓	
S-O		✓	

CHAPTER

TWELVE

KNOWN PROBLEMS

- *If you start Winmostar with administrator privileges, you can not open files with drag-and-drop.*
- *Some software will not work if the Windows option "Use Unicode UTF-8 for worldwide language support" is enabled.*
- *Opening some subwindows such as Animation, Submit Job and so on, it will not appear even if you try to open again after closing.*
- *Graph display at the bottom of animation operation area is corrupted. Other UI displays are corrupted.*
- *If you select a range of text in the console window where the job of the local machine is flowing, the job is recognized as terminating on Job Manager.*
- *Gromacs freezes while running Gromacs on local machine.*
- *When using the RISM compatible version of Quantum ESPRESSO, it may be displayed that the main window keyword has been changed even though it has not been changed.*
- *MOL files that could be processed successfully with the ESM-RISM version of QE based on Quantum ESPRESSO 6 cannot be read properly when using QE 7.1.*
- *The units of Isothermal Compressibility and Adiabatic Bulk Modulus output by Gromacs are wrong.*
- *Molecules that should be connected to each other are displayed separately in the structure or the final structure after loading the Gromacs trajectory.*
- *When loading SMILES strings using [File]-[Import]-[SMILES], but the structure is not loaded as intended.*
- *Winmostar freezes when deleting the working directory or working folder directly on Windows (Explorer) while Winmostar is processing.*
- *Cannot open large size cube file in Winmostar Viewer.*
- *Winmostar toolbar and tool buttons are displayed incorrectly when Windows display magnification is other than 100%.*
- *Under some conditions, LAMMPS fails to recognize elements in the structure file after the calculation is completed when using a potential file.*
- *Cannot exit a job from the Stop menu from Job Manager in Windows 11.*
- *Molecules with the same composition and different binding modes are recognized by the same molecular species in the force field assignment function.*
- *The crystal symmetry detection process fails when the security software McAfee is running.*

12.1 If you start Winmostar with administrator privileges, you can not open files with drag-and-drop.

In the current Winmostar (Winmostar V.8), if you start Winmostar with administrator privileges, you can not open the file by dragging and dropping. It is due to be fixed in the future, but the working time is unknown. (Reported on May 24, 2018)

12.2 Some software will not work if the Windows option "Use Unicode UTF-8 for worldwide language support" is enabled.

In Windows 10, if [Control Panel] - [Clock and Region] - [Change Date, Time, and Numeric Format] - [Manage] - [Change System Locale] - [Use Unicode UTF-8 for World Wide Language Support] is checked, various remote job executions, LAMMPS execution, and FDMNES execution failed when the "Use Unicode UTF-8 for World Wide Language Support" checkbox is checked. The problem is due to files being output with a BOM. We are working to address Winmostar sequentially at the time the problem occurred, but please let us know if you experience similar problems with other functions. (Reported May 25, 2018)

12.3 Opening some subwindows such as Animation, Submit Job and so on, it will not appear even if you try to open again after closing.

It has been confirmed in only a few environments. If it does not appear, a menu such as [Return to original size] [Move] [Size change] … will appear when you press Alt + Space key, so when selecting [Move] and dragging it, the window reappears I will. Alternatively, it can be resolved by restarting Winmostar. We are currently considering better countermeasures. (Reported on 14th June 2018)

12.4 Graph display at the bottom of animation operation area is corrupted. Other UI displays are corrupted.

If you change the size of desktop text or other items from the default value (100%), the display will collapse. For Windows 8, set [Control Panel] - [Customize Desktop] - [Display] - [Change the size of all items] to Small -100% (prescribed). For Windows 10, set [Windows setting] - [system] - [display] - [custom scaling] to [100]. (Reported on June 26, 2018)

12.5 If you select a range of text in the console window where the job of the local machine is flowing, the job is recognized as terminating on Job Manager.

In the Windows 10 console window, selecting the range of the log text of the job being executed will recognize that the job has ended. If this causes a problem, open the log file to be output directly with a text editor, and select and copy the range of the text there. If processing is interrupted after selecting the range, processing will resume by pressing the Enter key. It occurs in Windows 10 or later. (Reported on July 20, 2018)

12.6 Gromacs freezes while running Gromacs on local machine.

On some machines, Gromacs freezes while running Gromacs on the local machine. It occurs during MD calculation and the contents of standard output do not change. There is no reproducibility in the place where it freezes. In such cases, you can avoid by setting "# of Threads" of Gromacs Configure to 1. As a matter of course, processing becomes slower, please use remote job submission function using remote server if you want to run full-scale calculation. LAMMPS can be used with Winmostar in a similar way to Gromacs, so you can also choose to use LAMMPS. (Reported on December 4, 2020)

12.7 When using the RISM compatible version of Quantum ESPRESSO, it may be displayed that the main window keyword has been changed even though it has not been changed.

During constant-mu calculation (lfcpopt = .True.), it is erroneously determined that the value of fcp_mu has been updated. Since the value is not actually changed, it can be used as is. (Reported on June 2, 2019)

12.8 MOL files that could be processed successfully with the ESM-RISM version of QE based on Quantum ESPRESSO 6 cannot be read properly when using QE 7.1.

This problem occurs when a string in a tag such as MOL_INFO contains an & (ampersand) (e.g., H2O.tip5p.MOL, which is provided with the program). Removing the ampersand will allow normal processing. (Reported on January 29, 2025)

12.9 The units of Isothermal Compressibility and Adiabatic Bulk Modulus output by Gromacs are wrong.

In the gmx energy log, the units for Isothermal Compressibility is "J/m^3", but the correct unit is "m^3/J". Similarly, the Adiabatic Bulk Modulus unit is correctly "J/m^3". (Reported on June 29, 2020)

12.10 Molecules that should be connected to each other are displayed separately in the structure or the final structure after loading the Gromacs trajectory.

This is due to a bug in Gromacs itself. The longer the calculation time, the more likely it is to occur. However, there is no problem with the MD calculation itself, since the atomic configuration is correct when periodic boundaries are taken into account. The problem occurs especially when two systems are joined by an interface builder. There are two ways to put a disjointed molecule back together. The first method is to select [MD]-[Gromacs]-[Assign Force Field], then [Use Parameters Written in Topology File] and select the top file of the target data. In the second method, first, in [Edit]-[Rearrange atoms based on periodic boundary conditions], click [Rearrange atoms inside cells atom by atom] → click [Apply] → click [Revert rearranged structure atom by atom] → click [Apply] → click [OK]. However, since this operation must be performed in the same cell as when the calculation was performed, please perform it before using the interface builder, etc. (Reported on December 25, 2020)

12.11 When loading SMILES strings using [File]-[Import]-[SMILES], but the structure is not loaded as intended.

There are several programs in the world that load SMILES, and each of them has a slightly different implementation that can change the molecules generated. Winmostar uses either OpenBabel or Balloon to import SMILES, and you can choose which one to use in the Import SMILES window. For example, in OpenBabel, “C[C@@H]1CCCC[C@@@H]1C” (originally cis-1,2-Dimethylcyclohexane) was recognized as trans-1,2-Dimethylcyclohexane. (Reported on January 29, 2020)

12.12 Winmostar freezes when deleting the working directory or working folder directly on Windows (Explorer) while Winmostar is processing.

Delete when the process is finished or when Winmostar is closed. (Reported on December 24, 2021)

Hint: **working folder**

- A working folder is a folder whose name is the name of the file opened in the main window plus a suffix.
  - **The suffix varies depending on the type of solver.**
  - For example, in Gromacs, if the file opened in the main window is `aaa.gro` and the suffix is `_gmx_tmp`, the working folder will be named `aaa_gmx_tmp`.
- It must be placed in the same directory as the file opened in the main window.
- The process runs in a working folder of the same name during a continuation job, but by default, a backup of the working folder of the previous job is created just before the continuation job is executed.
  - The name of the backup will be the one with the lowest number, as long as there are no duplicate names. For example, if your working folder is `aaa_gmx_tmp`, then it will be `aaa_gmx_tmp1`.
  - **Un-numbered directories are always up-to-date.**

12.13 Cannot open large size cube file in Winmostar Viewer.

Please use other cube file visualization software such as VESTA or VMD. You can directly launch them instead of Winmostar Viewer by checking [Tools]-[Preferences]-[Basic]-[Use external viewer to display cube files] in Winmostar and specifying the cube file visualization software in [Program path]-[Cube Viewer]. You can directly start those software instead of Winmostar Viewer. (Reported October 21, 2022).

12.14 Winmostar toolbar and tool buttons are displayed incorrectly when Windows display magnification is other than 100%.

In Windows 10, this can be changed by going to Settings→System→Display→Scaling and Layout. If the display is too small to read the text, reduce the screen resolution. (Note that this feature in Windows is also a problem for various applications other than Winmostar.) (Reported on October 28, 2022)

12.15 Under some conditions, LAMMPS fails to recognize elements in the structure file after the calculation is completed when using a potential file.

For example, if you use the MEAM potential available in the NIST repository to calculate the mass of a Sn crystal, the file output by the write_restart command will show a mass of "118" instead of "118.7107". Winmostar recognizes elements based on their mass values, and if it cannot recognize an element, it judges it as a coarse-grained atom such as CGA. This is a bug in LAMMPS (at least confirmed in the 20160309 version), so please correct the masses in the Masses section of the final structure data file using a text editor, etc. (Reported on December 8, 2022)

12.16 Cannot exit a job from the Stop menu from Job Manager in Windows 11.

Please close the calculation window or terminate the process using Task Manager or similar. In the case of NWChem, some users have reported that the CPU usage of the Job Manager becomes so high that it cannot even be terminated. (Reported on May 20, 2023)

12.17 Molecules with the same composition and different binding modes are recognized by the same molecular species in the force field assignment function.

This has been fixed in Winmostar V11.2.0. Users of Winmostar V10 or earlier should upgrade to Winmostar V11.

12.18 The crystal symmetry detection process fails when the security software McAfee is running.

When the security software McAfree is running, the symmetry detection process that is executed when starting the slab creation function or the workflow setup and keyword setup functions of Quantum ESPRESSO, OpenMX, VASP, AkaiKKR, etc. may fail. This may be caused by the automatic removal of an internal module called findprim_spglib.exe. In this case, stopping (or pausing) McAfee will allow the process to run successfully. (Reported on February 27, 2025)

CHAPTER
THIRTEEN

FREQUENTLY ASKED QUESTIONS · TROUBLESHOOTING

- *Purchase*
  - *Q. Please tell me how to pay the price.*
  - *Q. Please tell me the types of documents issued by the company.*
  - *Q. How do I place an order other than an end user, such as an agency?*
  - *Q. Is it possible to split the price of Winmostar and maintenance? Is it possible to sell maintenance only?*
  - *Q. Is there a warranty for the product?*
  - *Q. Is there any discount for personal use? Do you have a license for individuals?*
  - *Q. I am both an educational and research institution. Can I use my institution's budget to purchase a license for an educational institution?*
  - *Q. What is the process of signing a site license agreement when purchasing a site license from a distributor?*
  - *Q. Can I purchase on a daily or monthly basis?*
  - *Why is Winmostar more cost-effective than similar GUI software products from other companies?*
- *License Code*
  - *Q. Is it possible to change the registered user of a specific user license?*
  - *Q. If I move from the institution where I purchased my educational license to another institution, can I continue to use that license?*
  - *Q. Do I need to reinstall the software when I change editions, such as from a free edition to a student edition, or from a free trial to a professional edition?*
  - *Q. Can I install different editions of Winmostar, such as the free version and the professional version?*
  - *How do I change an already entered license code?*
  - *Q. Please tell me how to display the MAC address.*
  - *Q. Does Winmostar license fee include Gaussian and/or VASP license fee, and is there a Winmostar lineup with Gaussian and/or VASP license?*
  - *Q. What will happen to my Winmostar when the license expires?*
  - *Q. Can I purchase a license for an educational institution for my personal learning purposes?*
  - *Q. What is the procedure for renewing my license?*

  - *Q.. What if a teacher wants to pre-evaluate the student edition that the supervising student is going to use?*
  - *Q. What happens when the Professional Edition (Trial) expires? Will I have to pay a fee?*
- *Support and Maintenance*
  - *Q. What does maintenance include?*
  - *Q. If I have a question, can I email the person in charge directly?*
  - *Q. What is the difference between paid e-mail support (support on how to operate via e-mail) and free inquiry form questions?*
  - *Q. Can I get support for bugs or patches?*
  - *Q. How long do you plan to support and maintain the previous version?*
  - *Q. Who is the developer (manufacturer) of Winmostar? Where is it manufactured?*
  - *Q. Can I get in touch with the developer (manufacturer) directly?*
  - *Q. Is it possible to update/upgrade version of the Winmostar I am using?*
  - *Q. Are there any precautions when asking a question?*
  - *Q. Do you sell maintenance only?*
  - *Q. Do you sell maintenance only?*
  - *Q. What happens when the annual maintenance on a perpetual licence expires?*
  - *Q. Do you offer technical support for your various solvers? How can I get technical support for various solvers?*
  - *Q. Do you provide support via telephone or online meetings?*
- *Functions and use of the software*
  - *How to pronounce Winmostar.*
  - *Q. Does Winmostar connect to internal and external servers or the cloud, or can it be used without a LAN connection?*
  - *Q. Please tell me the minimum and recommended specifications of PC for Winmostar.*
  - *Q. Is it possible to use the data generated by Winmostar for conference presentations and papers? How should I quote at conference presentations and paper submissions?*
  - *Q. Is it possible to upload videos or images of the Winmostar screen to YouTube or other web sites?*
  - *Q. Do you have any calculation software installed on Winmostar itself?*
  - *Q. Do you let Winmostar run calculations in the cloud?*
  - *Q. Does Winmostar support GPU computation?*
  - *Q. Which CPU is more suitable for operation, Intel or AMD? Which one would you recommend?*
  - *Q. Is it possible to do parallel computation using Winmostar?*
  - *Q. Is there an upper limit to the number of cores that can be used for parallel computing using Winmostar? Does the cost vary depending on the number of cores available?*
  - *Q. Does Winmostar work on macOS and Linux?*
  - *Q. How can I install Gaussian?*

  - *Q. How can I install VASP?*
  - *Q. Windows or Explorer freezes when I start the CygwinWM installer. What should I do?*
  - *Q. How many atoms or molecules can I calculate with Winmostar? Is there an upper limit to the number of atoms or molecules that can be handled?*
  - *Q. Can I use Winmostar to calculate coarse-grained models?*
  - *Q. What is the difference between the latest stable version and the latest development version? Which do you recommend?*
  - *Q. Who owns the rights to the calculation results and output files obtained using Winmostar?*
- *Software operations*
  - *Q. I can not create a model as I expected. It can not calculate. It does not work.*
  - *Q. "ERROR: I/O error 32" is displayed and the processing fails.*
  - *Q. Process using Cygwin will end abnormally. /* Help → Check CygwinWM *function will display* … ERROR …. */ Cygwin's black window shows* child_info_fork :: abort: … Loaded to different address: parent … ! = Child ….
  - *Q.* Help → Check CygwinWM *function displays* No reference file (… filelist_cygwinwm.txt) was found….
  - *Q.* Help → Check CygwinWM *function will display* WARNING … some files are missing.
  - *Q.* Tools → Diagnose CygwinWM *function shows* ERROR … Failed to generate a current file list.
  - *Q.* Tools → Diagnose CygwinWM *function displays* ERROR: Getting SMILES …. *OpenBabel process terminates abnormally.*
  - *Q. The job registered in Job Manager is not executed.*
  - *Q. When executing a job, an alert saying "Unable to execute (Access denied.)" appears and the job will not start.*
  - *Q. In the functions where a black console window appears, such as various functions of Winmostar or the execution of the solver, the processing of the black console window does not end and does not proceed.*
  - *Q. When I open a file or model a molecule, the bonds no longer appear or a lot of extra bonds have come to appear.*
  - *Q. How do I view the extension in Windows Explorer?*
  - *Q. Markers (red circles) and group selections (blue circles) are not displayed. Atoms can no longer be selected.*
  - *Q. The toolbar and tool buttons are not displaying properly. Can I fix it?*
  - *Q. What is an optimization flag?*
  - *Q. Can I have Winmostar not run calculations directly from Winmostar and just save the file, or can I edit the file that Winmostar generates and then run the job?*
  - *Q. Is it possible to use the latest version of each solver or a version not listed in Winmostar's operating environment?*
- *File I/O*
  - *Q. I cannot open files created by other than Winmostar with Winmostar. When I edit the file generated by Winmostar and try to open it with Winmostar, it cannot be opened.*

  - *Q. When opening a file in MOL or SDF format, the bond length becomes unnatural. Hydrogen does not appear.*
  - *Q. When I load SMILES, it does not generate the intended structure. Why is this? What should I do?*
- *On the modeling of molecules and creation of systems*
  - *Q. How do I change the type of chemical bond (single, double etc.)?*
  - *Q.* MD → Solvate/Build Cell *function will display* Error: Failed to solvate. *and processing will fail.*
  - *Q. When I run some functions, I get* \357\273\277 *etc. and the process fails.*
- *MPI on local machine, parallel execution*
  - *Q. Why does the parallel computation that flows by itself terminate abnormally? The parallel test in the installation test succeeds. Serial calculations also terminate normally.*
  - *Q. MPICH ends during computation.*
  - *Q. When executing parallel MPI of LAMMPS or Quantum ESPRESSO, warning is displayed as* Unable to open the HKEY_LOCAL_MACHINE\SOFTWARE\MPICH\SMPD\process\???? registry key, error 5 , Access denied.
  - *Q. The installation of .NET Framework 3.5 using dotNetFx35setup.exe fails. What should I do?*
  - *Q. I cannot find the number of parallels I want to set when I pull down the Number of Parallels combo box. How can I set the number of parallels I want?*
- *Remote Jobs*
  - *Q. Please tell me how to submit a job to a supercomputer or a linux server in my company or my campus.*
  - *Q. I cannot connect from Winmostar to a server that allows SSH connections with various terminal software.*
  - *Q. SSH connection with public key method fails, when I specify the same private key file with other software such as TeraTerm or Cygwin, the connection succeeds. Is there a solution?*
  - *Q. The connection test with* Test Connection *succeeds, but the job submission fails.*
  - *Q. Connection test with* Test Connection *succeeds, but Putty's WARNING is displayed and various operations fail.*
  - *Q. What type of MPI (MPICH, OpenMPI, etc.) can I use on the remote server?*
  - *Q. Why are some environment variables (e.g. PATH) that should be set on the remote server by filling in bashrc, etc., not set when running from Winmostar? What should I do in such cases?*
  - *Q. Is there any difference in behavior between the Windows version of the solver and the Linux version of the solver?*
  - *Q. Can I run calculations simultaneously for remote jobs that run on different servers?*
  - *Q. Where are passwords entered in the remote job profile stored? Is the password information stored in the project folder?*
  - *Q. Why can I SSH to an Ubuntu machine, including WSL2 use, but cannot successfully execute a remote job?*
- *Simulation in general*
  - *Q. Is it possible to calculate the interaction between one substance and another substance with Winmostar?*
  - *Q. Can I calculate bond energies and bond divergence energies for a given bond in a molecule?*

- *MOPAC, CNDO/S, GAMESS, NWChem, Gaussian*
  - *Q. I get an error while running a quantum chemistry calculation, what should I do?*
  - *Q. The Hamiltonian calculation method (Hamiltonian) or basis function (Basis Set) that I want to use is not found in the Configure window or the Easy Setup window for MOPAC, GAMESS, Gaussian and NWChem. How do I set it up?*
  - *Q. How are bonds determined when opening an input/output file or when regenerating bonds?*
  - *Q. Unnecessary bonds are displayed while modeling the system or when reading the calculation results. Or the bonds are not displayed. How can I fix this?*
  - *Q. Is it possible to optimize substructures from Winmostar using quantum chemical calculations?*
  - *Q. Why does the Dipole moment value displayed at the bottom of the Winmostar molecule display area differ from the dipole moment value manually calculated from the charges assigned to each atom, such as Mulliken charges?*
  - *Q. How many atoms can be calculated with MOPAC?*
  - *Q. It will display abnormally with the message* ATOMS **, **, AND ** ARE WITHIN. **** ANGSTROMS OF A STRAIGHT LINE *displayed in the MOPAC log.*
  - *Q. When MOPAC is executed, “UNRECOGNIZED KEY - WORDS: (PM 6 (Hamiltonian name))” is output to the log and the calculation ends.*
  - *Q. How do I use the solvent effect (COSMO method) in the MOPAC attached with Winmostar?*
  - *Q. When I calculate with MOPAC other than Winmostar built-in (e.g. MOPAC2016), only some molecular orbitals are displayed.*
  - *Q. It can not be calculated when Method=INDO is used in CNDO/S.*
  - *Q. Is there a guideline for the maximum number of atoms (memory requirement) that can be calculated in GAMESS, Gaussian, and NWChem?*
  - *Q. Is it possible to speed up 3D display of ESP (electrostatic potential) of GAMESS, Gaussian, and NWChem?*
  - *Q. When running GAMESS, “* ERROR: MEMORY REQUEST EXCEEDS AVAILABLE MEMORY” etc. will be output to the log and the calculation will end abnormally.*
  - *Q. Immediately after installing GAMESS for Windows, I was able to use it without any problems, but at some point, all the calculations started to terminate abnormally in the middle. Is there a way to fix this?*
  - *Q. GAMESS outputs “WARNING. NUMBER OF INTERNAL COORDINATES IS GREATER THAN (3N - 6), BUT NO SYMMETRY COORDINATES ARE GIVEN.” in the calculation of only one atom and abnormally ends.*
  - *Q. The message* `**** ERROR **** PCM SPHERE (S) MUST HAVE A POSITIVE RADIUS` *is displayed in the log of GAMESS and abnormally ends.*
  - *Q. When GAMESS is executed, “ERROR: BAD DELOCALIZED COORDINATES GENERATED !!!” is output to the log and the calculation ends abnormally.*
  - *Q. When I try to run NMR calculation in GAMESS (using RUNTYP=NMR), I get an error.*
  - *Q. When I use Diffuse functions in GAMESS, the SCF calculation does not converge.*
  - *Q. For some molecules, after optimization of Firefly, when I check the Molecular Orbit UVvis. . . , I get the error '*******' is not valid floating point value”.*

  - *Q. How do I deal with the message "THE GEOMETRY SEARCH IS NOT CONVERGED!" when I run a structural optimization calculation with GAMESS?*
  - *Q. I cannot download the GAMESS installer. How can I do this?*
  - *Q. The DFT calculation in GAMESS does not converge after displaying "CONVERGED TO SWOFF, SO DFT CALCULATION IS NOW SWITCHED ON". Is there any way to deal with this?*
  - *Q. When parallel execution of NWChem, the calculation outputs "Please specify an authentication passphrase for smpd:" to the log and dows not run.*
  - *Q. When I run NWChem, I get the message "sym_geom_project: sym_center_map is inconsistent with requested accuracy" in the log and the calculation does not run.*
  - *Q. How can I put the solvent effect in NWChem?*
  - *Q. When executing NWChem, lines including "out of memory", "alloc failed", "ma_push failed", "nga_create failed", and "Global memory limit unreasonable" are printed in the log and calculations do not run.*
  - *Q. The Gaussian calculation may or may not work correctly.*
  - *Q. I read the Gaussian log file, but the orbital (eigen) energy etc. are not written.*
  - *Q. How do I calculate the chk file read in Gaussian?*
  - *Q. I get an error when I try to load a Gaussian fchk file that is several GB in size and display molecular orbitals.*
  - *Q. How can I perform vibration calculations in Gaussian that take isotope effects into account?*
- *LAMMPS, Gromacs*
  - *Q. I would like to run molecular dynamics calculations, but which should I use, LAMMPS or Gromacs?*
  - *Q. I get an error while running a molecular dynamics calculation, what should I do?*
  - *Q. How can we equilibrate the system in molecular dynamics calculation?*
  - *Q. I ran MD calculations from the same initial configuration but got different results. Why is this?*
  - *Q. The final density obtained from the NPT calculation is much lower than the density predicted from experimental values and other sources. What should I do?*
  - *Q. In the MD calculation, how does the constraints by the SHAKE method etc. affect the calculation result? How do I choose a constraint method ?*
  - *Q. Why do molecules sometimes come out of the cell when in the trajectory or the final structure afterMD calculation?*
  - *Q. When I create a cell by adding water molecules from a cell in the [Solvate/Build Cell] menu to a large molecule such as a protein, the molecules sometimes stick out of the cell.*
  - *Q. The [MD]-[Solvate/Build Cell] and [Insert Molecule] processes do not finish after many minutes. Is there a solution?*
  - *Q. In the [MD]-[Assign Charges Automaticcally] menu, the error message "Topology file not found" is displayed. Is there a solution?*
  - *Q. The process of assigning the force field takes a long time and never ends. Is there a solution?*
  - *Q. I get an error message when assigning a force field. Is there a solution?*
  - *Q. How do I assign a point charge to a polymer?*
  - *Q. Can I calculate dielectric constant from Gromacs or LAMMPS (Molecular Dynamics Calculation)?*

  - *Q. When I try to run an MD calculation from a structure created with the interface builder, the force field assignment fails or the MD calculation fails. Is there a solution?*
  - *Q. When pressure control (constant NPT or NPH) is used, the calculation fails in the middle of the process. Is there a solution?*
  - *Q. How do I decide interaction parameters between liquid (organic) and solid (inorganic) in LAMMPS and Gromacs?*
  - *Q. When I run Gromacs, I get the error "There is no domain decomposition for 49 ranks that is compatible with the given box and a minimum cell size of…". error. How should I deal with this?*
  - *Q. When I load the final structure or animation from Gromacs, or when I edit it in some way and then run the MD calculation again, the force field assignment fails or the MD calculation breaks down. Is there a solution?*
  - *Q. When loading the final structure or animation in Gromacs, the molecules are sometimes displayed in pieces.*
  - *Q. Even if Gromacs ER method result loading is executed, the result can not be displayed / an error will appear.*
  - *Q. The error message "Out of range atoms - cannot compute PPPM" appears in the LAMMPS log and the calculation terminates abnormally. Please let me know how to deal with this.*
  - *Q. How can I plot the trajectory of a specific atom?*
  - *Q. The dissipative particle dynamics (DPD) calculation gave me a different result than intuitive. Why is this?*
- *About Quantum ESPRESSO, OpenMX*
  - *Q. I installed the Quantum ESPRESSO pseudopotential file as per the instructions, but it is not recognized.*
  - *Q. I don't know how to find a pseudopotential file for Quantum ESPRESSO. How do I find them?*
  - *Q. Calculation using Quantum ESPRESSO fails. An error appears in displaying the calculation result.*
  - *Q. When executing Phonon calculation using Quantum ESPRESSO, "third order derivatives not implemented with GGA" is output in the ph.x output (ph.out), and the calculation result cannot be obtained.*
  - *Q. Quantum ESPRESSO, OpenMX SCF calculation or structure optimization calculation does not converge.*
  - *Q. I cannot visualize the three-dimensional distribution of electron density, spin density, and potential in Quantum ESPRESSO.*
  - *Q. The SCF calculation of Quantum ESPRESSO is displayed as "too few bands" in the output file (.pwout or .out) and abnormally ends. I do not know how to set nbnd.*
  - *Q. The SCF calculation of Quantum ESPRESSO terminates abnormally with "fixed occupations and lsda need tot_magnetization" displayed in the output file (.pwout or .out). How do I resolve this?*
  - *Q. Quantum ESPRESSO's structural optimization calculation (vc-relax) terminates abnormally with the output file (.pwout or .out) showing "smooth g-vectors missing ! in the output file (.pwout or .out) and terminates abnormally. How can I resolve this?*
  - *Q. The SCF calculation of Quantum ESPRESSO on metal is terminated abnormally with "charge is wrong" displayed in the output file (.pwout or .out). How do I resolve this?*
  - *Q. When calculating the dielectric function using Quantum ESPRESSO, "bad band number" is displayed in the epsilon.x output (eps.out) and it is not possible to acquire the dielectric function.*

  - *Q. When calculating the dielectric function using Quantum ESPRESSO, "USPP are not implemented" is displayed in the epsilon.x output (eps.out) and it is not possible to acquire the dielectric function.*
  - *Q. My Phonon calculation using Quantum ESPRESSO failed and I cannot get the results.*
  - *Q. I cannot find a norm-preserving, LDA functional pseudopotential file for Quantum ESPRESSO for the element I want to calculate in the pseudopotential files installed by default. How can I find it?*
  - *Q. When I try to output the Fermi surface, they do not appear.*
  - *Q. Can I calculate the dielectric constant from Quantum ESPRESSO (band calculation)?*
  - *Q. How do you set up the type of functionalities in Quantum ESPRESSO?*
  - *Q. Why does the cell size structure optimization in Quantum ESPRESSO result in discontinuous changes or energy increases in the final structure energy?*
  - *Q. Quantum ESPRESSO terminates normally for systems with a small number of atoms, but for large systems it terminates abnormally with an error such as "cannot allocate …". for large systems. What can I do about this?*
  - *Q. Why do the values for Total DOS appearing in Projected DOS (PDOS) and DOS appearing in Density of States (DOS) differ in Quantum ESPRESSO?*
  - *Q. When I set Hubbard U in Quantum ESPRESSO for structural optimization, it terminates abnormally with the error message "NR-step length unreasonably short". What can I do about this?*
  - *Q. Why does the number of cycles required for convergence of SCF calculations before and after Quantum ESPRESSO 6.6 change so much?*
  - *Q. When I use hybrid functional (e.g. HSE) in Quantum ESPRESSO, the band structure collapses. Is there a way to deal with this?*
  - *Q. Unnecessary bonds are displayed while modeling the system or when reading the calculation results. Or the bonds are not displayed. How can I fix this?*
  - *Q. When setting up workflow and keywords in Quantum ESPRESSO, even if the cell is not converted to a primitive cell, it is converted to a primitive cell when the calculation is executed.*
  - *Q. When I run a calculation on a local machine with MPI enabled in OpenMX, I get the error tcp_peer_send_blocking: send() to socket 12 failed: Transport endpoint is not connected.*
  - *Q. After running a structural optimisation calculation with a change in cell size in OpenMX, if I run a continuation job with SCF.Restart=On, the standard output shows Failed (3) in reading the restart files, <Restart> Could not find restart files.*
- *Addons*
  - *Q. When calculating the Hansen solubility parameter of a polymer using the solubility parameter calculation module, the output value changes depending on how the repeating structure (monomer) of the polymer is taken.*
  - *Q. The value of the Hansen solubility parameter obtained using the solubility parameter calculation module is significantly different from the literature value.*

13.1 Purchase

13.1.1 Q. Please tell me how to pay the price.

A.
[For corporations]
It becomes postpay under the following conditions.

Payment method: Cash transfer to our designated bank account
Payment due date: End of the next month of the purchase date

[For individuals]
Pay with credit card at PayPal.

13.1.2 Q. Please tell me the types of documents issued by the company.

A.
An invoice, a delivery note and a quotation will be issued.
In the case of PayPal, please obtain a receipt from PayPal.
Please consult us when you wish other documents. However, please understand that it may be refused depending on the matter.

13.1.3 Q. How do I place an order other than an end user, such as an agency?

A.
Please see Price and Purchase for more information.

13.1.4 Q. Is it possible to split the price of Winmostar and maintenance? Is it possible to sell maintenance only?

A.
Cannot be split. But only for the educational lineup after V11, you can only purchase maintenance if the maintenance has expired after purchasing the V11 unit.

13.1.5 Q. Is there a warranty for the product?

A.
There is no warranty document, but the Terms of Use and Support Service Terms, which you agree to when you purchase the product, contain the text equivalent to the contents of the warranty for maintenance, etc. Please use the Terms of Use and Support Service Terms as a substitute for the warranty.

13.1.6 Q. Is there any discount for personal use? Do you have a license for individuals?

A.

None in particular. The free version can be used by individuals. For the Professional Edition, please purchase a license for educational institutions if you belong to an educational institution and intend to use it for your own purposes, or for private companies and government offices if you do not belong to an educational institution.

13.1.7 Q. I am both an educational and research institution. Can I use my institution's budget to purchase a license for an educational institution?

A.

Not available. If the purchasing organization is a research institute, it is necessary to purchase a license for private companies or government agencies.

13.1.8 Q. What is the process of signing a site license agreement when purchasing a site license from a distributor?

A.

As with direct sales, we will conclude a site license agreement between our company and the customer (end user).

13.1.9 Q. Can I purchase on a daily or monthly basis?

A.

This is only possible for the first year of a site license. If you need a specific user license or a node-locked license that operates only until the end of the fiscal year due to budget constraints, for example, we can issue a license that operates only until the desired date within one year from the license start date, without discount.

13.1.10 Why is Winmostar more cost-effective than similar GUI software products from other companies?

A.

There are several reasons.

First of all, we do not develop the programs (solvers) that run the simulations themselves in-house, but use open source software that is well proven throughout the world. However, the Winmostar support team is familiar with each solver at the source code and algorithm level, so we can provide sufficient support. We can also improve and modify the solvers as needed, so you can be assured of the quality of the software.

Another advantage is that Winmostar is a purely domestic software. Winmostar is available in Japan without any exchange rate effects.

However, Winmostar has been developed and supported for more than 20 years and its experience is reflected in its products and services, so its functions, quantity and quality of documentation (manuals), defect countermeasures and quality control, and support for beginners are as good as those of higher priced products.

13.2 License Code

13.2.1 Q. Is it possible to change the registered user of a specific user license?

A. This is not possible in the case of private companies and public offices. For educational institutions, it is possible to change if more than one year has passed since the last user change (or purchase if it is the first time). Please understand that the specific user license is set at a low price instead of being available only to a specific individual.

13.2.2 Q. If I move from the institution where I purchased my educational license to another institution, can I continue to use that license?

A. If you are no longer affiliated with the institution at the time of purchase, you will not be able to use the software, even if it is a perpetual license. This is because the license for educational institutions is specially priced for students, researchers, and faculty who belong to the educational institution and use the software only for the educational institution's business.

13.2.3 Q. Do I need to reinstall the software when I change editions, such as from a free edition to a student edition, or from a free trial to a professional edition?

A. Not required. Enter the licence code you want to use from now on in the *Tools → Preferences* menu under *Licence code*. All settings except the licence code will be taken over.

13.2.4 Q. Can I install different editions of Winmostar, such as the free version and the professional version?

A. Yes, it is possible. In this case, please specify a separate installation location for each edition in the Winmostar installer.

13.2.5 How do I change an already entered license code?

Enter the license code you want to use from now on into *license code* in *Tools → Preferences* menu.
If you are a student and want to switch from the free version to the student version, check the student version on the License registration page and register the license again.
In that case, the settings other than the licence code will be taken over.

13.2.6 Q. Please tell me how to display the MAC address.

A. For Winmostar V11, the MAC addresses of the machine is displayed when it is started with an unregistered license.

Winmostar V10 or lower and Windows 10, first click *Start Menu → Windows System Tools → Command Prompt* to launch the command prompt. Next, in the Command Prompt window, type **`ipconfig /all`** and press Enter. Various information will be output, look for the "physical address" line in the output. Its contents are the MAC address. If there is more than one "physical address" line, basically any "physical address" can be used as the MAC address for Winmostar's node-locked license purchase.

13.2.7 Q. Does Winmostar license fee include Gaussian and/or VASP license fee, and is there a Winmostar lineup with Gaussian and/or VASP license?

A. Winmostar license fee does not include Gaussian and/or VASP license fee. There is no Winmostar lineup with Gaussian license. Please purchase it separately from Gaussianand/or VASP distributor.

13.2.8 Q. What will happen to my Winmostar when the license expires?

A. When you start Winmostar after the license expiration date, a window for entering the license code will open and the various functions that were previously available will no longer be available. If you update your Winmostar license and enter it again, you will be able to use the software as it was before the license expired.

13.2.9 Q. Can I purchase a license for an educational institution for my personal learning purposes?

A.

At this time, you cannot purchase a license for an educational institution unless you belong to an educational institution and use it for your own purposes. For individual use, see *Q. Is there any discount for personal use? Do you have a license for individuals?*.

13.2.10 Q. What is the procedure for renewing my license?

A.

If you have purchased the Professional Edition, please inform us of your renewal request from the email source at the time of delivery or via the contact form. If you are a free or student version, please check to see if the terms of use apply to you before registering again.

If you have purchased the Professional Edition, please inform us of your renewal request from the email source at the time of delivery or via the contact form. After informing us of your renewal request, we will send you a quotation for the renewal. The licence code for the renewal will then be delivered within three working days after the order has been formally placed with us. In the case of free or student editions, please check whether the terms and conditions of use apply to you before registering again.

13.2.11 Q.. What if a teacher wants to pre-evaluate the student edition that the supervising student is going to use?

A.

Please obtain and evaluate the student version through your current student affiliation. In this case, use for purposes other than evaluation is prohibited. If teachers wish to use the software to further their own research, please purchase the Professional Edition. If you do not currently have any students affiliated with you, please contact us individually via the Contact Form.

13.2.12 Q. What happens when the Professional Edition (Trial) expires? Will I have to pay a fee?

A.
After the expiration date, Winmostar cannot be activated. There is no automatic charge for this service. If you wish to continue using the software, please request a quote. Data generated during the trial period will be available for viewing after purchase.

13.3 Support and Maintenance

13.3.1 Q. What does maintenance include?

It is written in the contents of the Terms of Use. Here it is (Winmostar Terms of Use).

13.3.2 Q. If I have a question, can I email the person in charge directly?

A. If you have a question, please do not email the person in charge directly, but first contact us via the Contact Form. The reason for this is that it is easier for the user to get the desired answer in a shorter period of time if you ask your question via the form. If the information required for a response is not included in the e-mail, we will need to ask you for it again, which will cause unnecessary back-and-forth. Also, if you do not use the form, it will take time for us to assign a person in our company who can respond to your questions accordingly.

13.3.3 Q. What is the difference between paid e-mail support (support on how to operate via e-mail) and free inquiry form questions?

A. The clear definition of paid e-mail support (support for operating instructions by e-mail) is described in the Support Service Terms and Conditions). Otherwise, you can use the free Contact Us Form to ask questions.

In practice, questions, inquiries, and bug reports related to Winmostar-specific functions are free of charge, while all other inquiries will be supported by e-mail for a fee. Winmostar Specific Function refers to the operation of Winmostar GUI itself, and does not include open source or other modules (including solvers) developed by third parties that Winmostar runs in the background.

Specifically, for free inquiries, we will focus on the documentation (tutorials and user manuals). If you would like an answer to a question that is covered in the documentation but is more tailored to your research problem, you can ask a question for a fee.

If you are in doubt, please first use the free contact form to ask your question. We will let you know if we will be able to help you for a fee.

13.3.4 Q. Can I get support for bugs or patches?

This will be done in accordance with the terms of use. The latest terms of use are here (Winmostar V11 Terms of Use).

13.3.5 Q. How long do you plan to support and maintain the previous version?

A. Based on the terms of use in effect for your version of Winmostar. In addition, simple instructions on how to operate the system will be provided to the extent possible.

13.3.6 Q. Who is the developer (manufacturer) of Winmostar? Where is it manufactured?

A. X-Ability Co. Ltd.. Place of manufacture is Japan.

13.3.7 Q. Can I get in touch with the developer (manufacturer) directly?

A. You can contact us through the contact form, but our availability is subject to our terms and conditions. The latest terms of use are here (Winmostar V11 Terms of Use).

13.3.8 Q. Is it possible to update/upgrade version of the Winmostar I am using?

A. Minor version (and revision) updates can be done as many times as you like during the availability period. Renewal of a major version requires renewal of the license for a permanent license, and is enforceable for an annual license.

As an example, for "V8.039", "8" refers to the major version and "039" to the minor version. For V9.1.0, "9" refers to the major version, "1" to the minor version, and "0" to the revision.

For example, a perpetual licensee of Winmostar V9 can update from V9.1.0 to V9.1.5 or V9.4.4, but it is not possible to update to V10.0.0.

13.3.9 Q. Are there any precautions when asking a question?

A. If you have a question that the calculation does not work properly, please send us an input or output file that reproduces the situation in principle.

13.3.10 Q. Do you sell maintenance only?

A.

Please check *Q. Is it possible to split the price of Winmostar and maintenance? Is it possible to sell maintenance only?*.

13.3.11 Q. Do you sell maintenance only?

A.

Please check *Q. Is it possible to split the price of Winmostar and maintenance? Is it possible to sell maintenance only?*.

13.3.12 Q. What happens when the annual maintenance on a perpetual licence expires?

A.

You can continue to use the software in the version that was available before the maintenance expired. Renewing maintenance allows you to update to the version released after the renewal. However, if you wish to upgrade across different major versions, you must purchase a new licence.

13.3.13 Q. Do you offer technical support for your various solvers? How can I get technical support for various solvers?

A.

We provide technical support for various solvers, but we do not provide stand-alone technical support for various solvers, except in special cases such as organizational unit partnerships and collaborations.

We provide technical support for various solvers as part of Winmostar ancillary support.

Please purchase Winmostar first and ask email questions within the scope of support that comes with the product itself.

If you have used up the support included with the product, please purchase additional support as needed.

For questions that require the support team to spend some man-hours to answer, we will prepare a separate estimate at that time.

In the case of other vendors, we have seen a form of open source solver technical support that is set at a fixed price regardless of the content, and on the surface unlimited support.

However, in practice, there are often no guarantees as to how much support will be provided for that amount of money, and we believe that such a format is not fair to both the vendor and the user, as there are many variations in the level of difficulty of the support provided. We provide support in the above format.

13.3.14 Q. Do you provide support via telephone or online meetings?

A. With the exception of payment inquiries, we do not provide telephone or online meeting support. Consultations about product content prior to purchase and questions about features and support are handled via our contact form or email. There are two reasons for this. The first is that Winmostar covers a wide range of methods, and some questions/supports require a support team of multiple people, which is not efficient if we have to call or set up meetings at specific times. Second, our goal is to continue to provide our high-quality products and support at a low price, and to reduce inefficient support as much as possible.On the other hand, we will hold meetings for the paid individual follow-up and individual planning as many times as you request, so if you absolutely need a meeting for support, please request that.

13.4 Functions and use of the software

13.4.1 How to pronounce Winmostar.

A. win·mo·str

13.4.2 Q. Does Winmostar connect to internal and external servers or the cloud, or can it be used without a LAN connection?

A. Yes, it is possible. Download the software described in *Installing Winmostar and solvers* and copy it to a PC not connected to the network. Then, follow the procedure in *Installing Winmostar and solvers* to install the software.

13.4.3 Q. Please tell me the minimum and recommended specifications of PC for Winmostar.

A. See *Hardware requirements* for Winmostar itself.

If you do not know the recommended specs, including the execution of the solver and not Winmostar itself, please do the following

This question is for those who do not have much experience with calculations and do not have a clear picture of the specific calculation conditions and calculation load.

Basically, when you start up an atomic-scale simulation business, it is rare to keep it running 24/7 as a routine work like CAE (structural and fluid calculations), and in most cases, especially when you start learning it, it is likely to be used as a research tool on a spot basis.

In such cases, it is not advisable to worry too much about the specifications of the calculator from the beginning, since most of the time is spent in planning and discussing the calculation rather than in computing time.

Therefore, it is more important to first develop an understanding of the calculations than the capabilities of the calculator, so we recommend installing Bronze Support or higher support.

Improper planning of calculations can result in calculations that are dozens of times more wasteful than would be the case if they were appropriate.

Next, we recommend the use of a PC (workstation) with as many cores as possible costing 500,000 to 1,000,000 yen if possible, but it is not required.

If the computing power of the PC at hand is not sufficient for your immediate research project, you can use a cloud service such as FOCUS supercomputer or HPC Systems Science Cloud and other cloud services can be used to temporarily secure a large amount of computing power.

After 1-2 years, you will know the amount of calculations required for your business, and it would be a good idea to select a PC to keep on hand on that basis.

GPUs do not need to be considered because Winmostar does not allow them to be used for calculations on local jobs. Even for remote jobs, we recommend that you do not consider GPUs for the time being, since the benefits of installing GPUs are limited to cases where the cost and effort of installing GPUs outweigh the benefits.

13.4.4 Q. Is it possible to use the data generated by Winmostar for conference presentations and papers? How should I quote at conference presentations and paper submissions?

A. No problem with using it. When presenting it please quote as *About quotation*.

13.4.5 Q. Is it possible to upload videos or images of the Winmostar screen to YouTube or other web sites?

A. Yes, you can. When uploading, please cite the URL of Winmostar's website and state that you are using Winmostar and the version of Winmostar you are using. It is strictly prohibited to upload the preferences window where the license key is displayed.

13.4.6 Q. Do you have any calculation software installed on Winmostar itself?

A. Only MOPAC and CNDO/S are installed in Winmostar. Other software is not bundled with Winmostar due to licensing issues and must be installed separately. Many software can be installed for free, and the instructions are described in *Installing Winmostar and solvers*.

13.4.7 Q. Do you let Winmostar run calculations in the cloud?

A. It is possible to have it calculated in the cloud, or not. By default, we don't use the cloud, but let you run the calculations on a Windows PC with Winmostar installed.

13.4.8 Q. Does Winmostar support GPU computation?

A. GPU calculations are supported, but the default setting is to not use the GPU. Some solvers are GPU-enabled, but you will have to pay for the work to verify that they work, build them, and configure them. If you have already built a solver with a GPU configuration and have already verified that it works without Winmostar, you can use GPU calculations from Winmostar with only Winmostar configuration. Due to reasons on the solver side, not on the Winmostar side, depending on the combination of OS, machine configuration (including GPU), and solver type/version, it may not be possible to build with a configuration that uses GPU (rather, most cases fall into this category), so before installing a GPU, please contact a vendor that provides hardware for simulation. We recommend that you consult with the vendor that provides the hardware for your simulation.

13.4.9 Q. Which CPU is more suitable for operation, Intel or AMD? Which one would you recommend?

A. In general, there is no such thing as a better simulation.

13.4.10 Q. Is it possible to do parallel computation using Winmostar?

A. It is possible. Details can be set in the Keyword Settings window for each solver in file mode, or in the Job Settings window in project mode.

13.4.11 Q. Is there an upper limit to the number of cores that can be used for parallel computing using Winmostar? Does the cost vary depending on the number of cores available?

A. You can specify an unlimited number of parallels within the range of user-provided hardware. Winmostar's price does not change depending on the number of parallels. In the case of a local job, change the maximum number of cores because the job will not run if it exceeds the maximum number of cores set by *Winmostar Job Manager*.

13.4.12 Q. Does Winmostar work on macOS and Linux?

A. Winmostar only supports Windows OS. You can check the supported Windows operating systems at System Requirements. If you want to run the Winmostar application on macOS or Linux, please install Windows OS in a virtual environment such as VirtualBox.
Linux and macOS can be used as the computer to run the remote job.

13.4.13 Q. How can I install Gaussian?

A. For instructions on installing Gaussian, get them from your Gaussian distributor. After installing Gaussian, In the *Tools* → *Preference* → *Program Path*, select the Gaussian program path(g03.exe, g09.exe, g16.exe etc.).

13.4.14 Q. How can I install VASP?

A. Installation instructions for VASP can be obtained from your VASP distributor. VASP is only available for remote jobs; after installing VASP, edit the template script and specify the directory where you placed the VASP binary and pseudopotential files.

13.4.15 Q. Windows or Explorer freezes when I start the CygwinWM installer. What should I do?

A. It is very likely that your security software is interfering with the CygwinWM installer, please specify the CygwinWM installer as an exception to be monitored by your security software. This can happen in a variety of cases. This was actually reported on June 9, 2025 when cygwin_wm_20250413.exe was launched in a Windows 11 environment running Trend Micro Apex One.

13.4.16 Q. How many atoms or molecules can I calculate with Winmostar? Is there an upper limit to the number of atoms or molecules that can be handled?

A. Assuming that the operating speed is not considered, we have confirmed the operation of up to about 1 million atoms. Since the operating speed strongly depends on the execution environment, please check it with the free trial before purchasing. We are planning to increase the speed of Winmostar in future versions.

13.4.17 Q. Can I use Winmostar to calculate coarse-grained models?

A. As coarse-grained models in the sense that they are not pure quantum chemical, ab initio, or classical molecular dynamics calculations, dissipative particle dynamics (DPD) calculations using LAMMPS and the Kremer-Greset model are supported (please inquire separately for Kremer-Greset). The United atom model and its derived coarse-grained models will be supported in the future. For other models, please contact us separately. The reason for this is that we recognize that most research using coarse-grained models cannot be meaningfully accomplished by simply using the software, but requires careful consulting. Winmostar's support case study shows the simulation results of a well validated coarse-grained model.

13.4.18 Q. What is the difference between the latest stable version and the latest development version? Which do you recommend?

A. The latest development version is the latest revision of the latest minor version, and the latest stable version is the latest revision of the previous minor version. (For example, in the case of V11.10.3, 11 is the major version, 10 is the minor version, and 3 is the revision.) When a minor version is updated, new features are added or relatively large specification changes are made. When a revision is updated, defects are fixed and relatively small specification changes are made.

If you do not need to use new features that are only available in the latest development version, we recommend using the latest stable version.

13.4.19 Q. Who owns the rights to the calculation results and output files obtained using Winmostar?

A. Belongs to the user. The user is free to use it.

13.5 Software operations

13.5.1 Q. I can not create a model as I expected. It can not calculate. It does not work.

A. First, please perform the following basic checks.

- Check the *Installation precautions*.
- Check whether Winmostar in use is a free version, a student version, a professional version, or a professional version (trial), and whether the function causing the problem is available in that version with function table.
- Check the activity record of the security software in use and check whether there is any record in which the activities of the application under Winmostar, CygwinWM and each solver's installation folder are disturbed.
- Update Winmostar to the latest version (it is possible to coexist with the version you are using), check if there is a situation similar to *Known problems* and *Frequently asked questions · Troubleshooting*.
- If the names of files to be saved and directories containing them (including all upper layers) contain multibyte characters such as Japanese and special symbols including sapces, some solvers may cause problems. Therefore, use only single-byte alphanumeric characters.
- Check the working folder to see if the log is being output by the executed process and check the contents of the log.

- If calculation is started but the calculation result is wrong, click "Open Log File" etc from the solver menu used in the main menu and check the contents of the log.
- For the calculation failure, check that the version of the solver is the same as the version recommended in the Winmostar installation guide. (Especially Gromacs, LAMMPS, or Quantum ESPRESSO)
- Disable the "Use Unicode UTF-8 for worldwide language support" option on Windows if it is enabled. (See *Some software will not work if the Windows option "Use Unicode UTF-8 for worldwide language support" is enabled.* for details)
- If a project or file is saved and used on a network drive and unexpected behaviour is observed, save and use it on a non-network drive (e.g. C drive).

Next, please make it possible to record subsequent work with Notepad etc. If you find out how to reproduce the problem, you may be able to fix it in a relatively short time if you report along with the record of work.
Please trace the basics tutorial of the solver you want to use in tutorials.
If you fail to trace the basics tutorial, try the following.

- Ensure that the calculations are carried out using exactly the same substances and conditions as in the basic version. (This is not limited to Winmostar, but in all cases where the substances and conditions are different, the calculations may not always end successfully using the methods described in the tutorial).
- Trace again to confirm that it is not a misoperation.
- If parallel execution is performed, switch to serial execution (parallel number 1).
- Restart Winmostar.
- Restart the OS.
- With security software, Exclude Winmostar, installation folder of CygwinWM, and solvers including MPI from monitoring.
- If you are using CygwinWM, run *Help* → *Check CygwinWM* and perform a simple diagnosis of CygwinWM.
- Reinstall Winmostar, CygwinWM and the solver you are using.
- Try with another PC.

Next, trace the tutorial which seems to be as close as possible to what you want to calculate finally. If it succeeds, please change the calculation condition such as Number of atoms, size of super cell, degree of polymerization, type of element, number of phases, etc. so that it finally gets to calculate what you want to calculate and try to identify where the problem occurs.

- Please check for similar cases in *Frequently asked questions · Troubleshooting*.
- If the problem is occured in the part where Winmostar calls external software, Please check also information of the software.
- If there is a problem with processing using Cygwin, please confirm *Cygwin general problem*.

13.5.2 Q. "ERROR: I/O error 32" is displayed and the processing fails.

A. The file related to processing may be opened by an application or process other than Winmostar, locked, or it may have been deleted.
Restart OS and try again in the situation other applications are not open.

13.5.3 Q. Process using Cygwin will end abnormally. / *Help* → *Check CygwinWM* function will display *... ERROR ....* / Cygwin's black window shows *child_info_fork :: abort: ... Loaded to different address: parent ...! = Child ....*

A. Please do the following procedure one by one from the top, and re-do the process where the error occurred each time.

1) Perform general *dealing with common problems*.
2) Restart your PC
3) Open Windows Security and go to *App & browser control* and click *Exploit protection*. Then change the value of *Force randomization for images* to *Off by default* or *Use default (Off)*.
4) If the value of *force image randomization* is reset after restarting Windows, start PowerShell with administrator privileges and execute the following command.

```
cd C:\cygwin_wm
Get-ChildItem -Recurse -File -Include *.exe | %{ Set-ProcessMitigation -
↪Name $_.Name -Disable ForceRelocateImages }
```

Then double-click `make_symlink.cmd` under `C:\cygwin_wm`.

5) Check the operation with other applications closed. (In rare cases, there may be conflicts with other applications.)
6) Search and delete anything other than `cygwin1.dll` and restart the machine

Warning:

- This operation is necessary in some cases if `cygwin1.dll` exists in addition to CygwinWM on the same machine.
- `cygwin1.dll` may be included in various freeware etc even if you do not install Cygwin in other location.

7) With all Cygwins on the machine being used terminated, at the [Run] of Windows `C:\cygwin_wm\bin\ash.exe` (when CygwinWM is installed in `C:\cygwin_wm`), execute the **`/bin/rebaseall -v`**, and restart the machine.
8) Temporarily disable security software.
9) Disable software that tends to cause problems described in Cygwin FAQ .
10) In addition, try the method described in Cygwin FAQ fork() related failures.
11) Install a new version of Cygwin from the Cygwin official site and check if you can start a terminal.

13.5.4 Q. *Help* → *Check CygwinWM* function displays *No reference file (... filelist_cygwinwm.txt) was found....*

A. The first thing the CygwinWM diagnostic function does is to look for a file named filelist_cygwinwm.txt directly under the folder where CygwinWM was installed, and the error message is that this file is missing. Please look for filelist_cygwinwm.txt in the location where CygwinWM was installed (by default `C:\cygwin_wm`) and specify the folder directly above it in [Tools]-[Preferences]-[Program Path]. Find filelist_cygwinwm.txt in the location where CygwinWM was installed (by default `C:\cygwin_wm`) and specify the folder directly above it in [Tools]-[Preferences]-[Program Path]. If you cannot find filelist_cygwinwm.txt, the installation of CygwinWM may have failed, so please review the settings of your security software and reinstall CygwinWM.

13.5.5 Q. *Help* → *Check CygwinWM* function will display *WARNING ... some files are missing*.

A. Please reinstall CygwinWM.

If it is displayed even after the reinstallation, temporarily disable the security software, or exclude installation destination and installer from monitoring.

13.5.6 Q. *Tools* → *Diagnose CygwinWM* function shows *ERROR ... Failed to generate a current file list*.

A. Your Cygwin environment may be corrupted. Please check *Cygwin common bugs*.

13.5.7 Q. *Tools* → *Diagnose CygwinWM* function displays *ERROR: Getting SMILES ....* OpenBabel process terminates abnormally.

A. If OpenBabel for Windows is installed separately from CygwinWM, Winmostar's internal processing may use OpenBabel for Windows when it should use OpanBabel for CygwinWM, causing a problem. Uninstall the Windows version of OpenBabel or delete the Windows OpenBabel installation folder from the PATH environment variable.

13.5.8 Q. The job registered in Job Manager is not executed.

If the specified parallel number of MPI is larger than the MaxCore setting of Job Manager, the job will not be executed.

The default value of MaxCore should be set to the number of cores of the running PC, but make sure that it has not been changed or that the number of parallel MPIs has not been set higher.

If you want to run without using Job Manager, uncheck "Run MOPAC using Job Manager" or "Run the other solvers using Job Manager" in *Calculation* tab of the *Tools* → *Preferences* window.

13.5.9 Q. When executing a job, an alert saying "Unable to execute (Access denied.)" appears and the job will not start.

A. Please try *general errors*. In particular, remove the installed Winmostar and Solver folders from the monitoring of your security software.

13.5.10 Q. In the functions where a black console window appears, such as various functions of Winmostar or the execution of the solver, the processing of the black console window does not end and does not proceed.

A. If you happen to click on the black console window, the process will be suspended from there due to the Windows specification.
The processing will resume when ESC key is pressed while the console window is active.

13.5.11 Q. When I open a file or model a molecule, the bonds no longer appear or a lot of extra bonds have come to appear.

A. First of all, in quantum chemical calculations and first-principles calculations (solid-state physics calculations), bond information does not affect the calculation results in any way, so please assume that the presence or absence of bonds is only a display issue.If the bond generation behavior has changed since you installed Winmostar, the *bonding factor* value in *Tools* → *Preferences* → *Edit* may not be appropriate. Either reset it to the default value or set it to a value around 1.15. If the default value does not give you the desired result, use *edit* → *Add/Change Bond* or *Edit* → *Delete Bond* to create or delete bonds.

13.5.12 Q. How do I view the extension in Windows Explorer?

In the case of Windows 7:

- Open Explorer
- Press the `Alt` key.
- Open *View* tab in *Tools* → *Folder Options* menu
- uncheck *hide extensions for known files type*

For Windows 8, 10

- Open Explorer
- Open *View* tab
- Check *File name extensions*

13.5.13 Q. Markers (red circles) and group selections (blue circles) are not displayed. Atoms can no longer be selected.

A. Check the *display* → *display items* → *selective atom markers* checkbox.

13.5.14 Q. The toolbar and tool buttons are not displaying properly. Can I fix it?

A. First, close Winmostar, make a backup of the UserPref folder, then delete the contents of the UserPref folder and restart Winmostar. If that doesn't make a difference, try the *Winmostar toolbar and tool buttons are displayed incorrectly when Windows display magnification is other than 100%.* workaround.

13.5.15 Q. What is an optimization flag?

A. See *Optimization Flags*.

13.5.16 Q. Can I have Winmostar not run calculations directly from Winmostar and just save the file, or can I edit the file that Winmostar generates and then run the job?

A. Yes. Follow the instructions in *Basic Operation Flow* if you do not want to run the calculation directly from Winmostar and only want to save the file.

13.5.17 Q. Is it possible to use the latest version of each solver or a version not listed in Winmostar's operating environment?

A. It depends on the type of functionality you want to use with that solver. While we expect most basic functionality to work, we do not guarantee it, so if you want to use a version that is not listed in Winmostar's Checking, we recommend you check it out in a trial before you buy it. The versions listed in the Confirmation of Operation are the versions used in Winmostar's pre-shipment testing. For some solvers (LAMMPS, Quantum ESPRESSO, etc.), you can use *Tools* → *Preferences menu* to switch the version of the solver that Winmostar outputs.

Winmostar plans to update the supported solver versions as they become available. If there is no specific timeline for updating supported versions and you need immediate support, please consider using paid customization.

13.6 File I/O

13.6.1 Q. I cannot open files created by other than Winmostar with Winmostar. When I edit the file generated by Winmostar and try to open it with Winmostar, it cannot be opened.

A. Please check if the line break code or encoding has been changed. If you still cannot open the file, please attach the file and contact us using the contact form.

13.6.2 Q. When opening a file in MOL or SDF format, the bond length becomes unnatural. Hydrogen does not appear.

Follow the steps below to modify the molecular structure. (1) *Adjust All Bond Lengths* (2) *Regenerate Z-Matrix* (3) *To marked atoms (Auto)* In the case of SDF files, refer to *Editing an SDF file* procedure.

13.6.3 Q. When I load SMILES, it does not generate the intended structure. Why is this? What should I do?

A. The characteristics of the external program that reads SMILES may not generate the intended structure; switching the external program that reads SMILES may solve this problem. In File -> Import -> SMILES, select either *Use OpenBabel* or *Use Balloon*.

13.7 On the modeling of molecules and creation of systems

13.7.1 Q. How do I change the type of chemical bond (single, double etc.)?

A. You can change it by the following method, for example.
1) *Edit → Automatically Adjust Atoms/Bonds → Add/Change Bond* or by pressing the *Add/Change Bond* button at the top of the main window multiple times.
2) *Edit → Automatically Adjust Atoms/Bonds → Regenerate All Bonds* is selected, the type of chemical bond is automatically changed by the bond degree determined from the interatomic distance. If you optimize the structure with *Edit → Automatically Adjust Atoms/Bonds → Quick Optimization* in advance, it may be changed automatically more reasonably.
3) If only one small molecule is displayed, execution of MOPAC calculation will automatically change the coupling order using the population analysis result.

13.7.2 Q. *MD → Solvate/Build Cell* function will display *Error: Failed to solvate.* and processing will fail.

——— Question details ——— When executing *MD → Solvate/Build Cell*, the following is output to `generate.log` and processing does not end normally.

```
gmx insert-molecules -try 100 -f gmx_tmp_water.gro -o gmx_tmp_water_tmp.gro -ci mol0.gro␣
↪-nmol 64
...
set +v
Error : Failed to solvate.
```

A. Try *general errors* and *Cygwin general errors* and execute after reducing the number of molecules or reducing the density.

13.7.3 Q. When I run some functions, I get *\357\273\277* etc. and the process fails.

——— Question details ——— When I run *MD* → *Solvate/Build Cell*, the following output appears in `packmol.log` and the process does not end normally. ::: *packmol.log*.

```
/cygdrive/C/winmos11/UserData/builder_tmp/packmol.sh: line 1: $'\357\273\277packmol':␣
↪command not found
```

A. \357\273\277 is a code contained in a UTF format text file called BOM and is not supported by programs in Cygwin and Linux environments. If you have checked [Beta: Use Unicode UTF-8 with worldwide language support] in [Clock and Region] - [Change Date, Time, and Numeric Format] - [Administration] tab - [Change System Locale] in the Control Panel, please uncheck the box if you do not mind.

13.8 MPI on local machine, parallel execution

13.8.1 Q. Why does the parallel computation that flows by itself terminate abnormally? The parallel test in the installation test succeeds. Serial calculations also terminate normally.

A. Gradually increase the number of parallels to 2, 4, 6. . . . and observe the behavior. If the number of parallelisms is too large for the problem size, the program may terminate abnormally. Also, if you are using a generation Intel Core series CPU with a high-performance core (P-core) and a high-efficiency core (E-core), make sure that the number of parallels does not exceed the number of cores in the P-core.

13.8.2 Q. MPICH ends during computation.

——— Question details ———

While executing MPICH, the following error may be displayed and the calculation may be ended prematurely.

op_read error on left context: Error = -1

op_read error on parent context: Error = -1

unable to read the cmd header on the left context, Error = -1

unable to read the cmd header on the parent context, Error = -1

Error posting readv, An existing connection was forcibly closed by the remote host.(10054)

connection to my parent broken, aborting.

state machine failed.

A.

This error is because MPICH uses the network adapter even if it is localonly and the network adapter is disconnected in the middle.

However, if the network adapter has disconnected from the beginning, this error will not occur because MPICH does not use the network adapter.

When computing for a long time using MPICH, please disable the network adapter and start the calculation.

13.8.3 Q. When executing parallel MPI of LAMMPS or Quantum ESPRESSO, warning is displayed as *Unable to open the HKEY_LOCAL_MACHINE\SOFTWARE\MPICH\SMPD\process\???? registry key, error 5 , Access denied.*

A. MPICH tries to rewrite the registry but it failed because there is no administrator authority.

If you start Winmostar with administrator privileges, you will not get a message. Even when a message is displayed, the calculation itself is executed normally, so it can be ignored.

13.8.4 Q. The installation of .NET Framework 3.5 using dotNetFx35setup.exe fails. What should I do?

A. You may be able to avoid this problem by installing from Windows PowerShell. Start Windows PowerShell with administrator privileges and enter the following command.

```
Set-ItemProperty -Path 'HKLM:\Software\Policies\Microsoft\Windows\WindowsUpdate\AU' -
↪Name 'UseWUServer' -Value 0;
restart-service wuauserv;
dism /online /Enable-Feature /FeatureName:NetFx3;
Set-ItemProperty -Path 'HKLM:\Software\Policies\Microsoft\Windows\WindowsUpdate\AU' -
↪Name 'UseWUServer' -Value 1;
```

13.8.5 Q. I cannot find the number of parallels I want to set when I pull down the Number of Parallels combo box. How can I set the number of parallels I want?

A. Enter a value in the Number of Parallels field using the keyboard instead of selecting it by pull-down. You can enter any value in the Number of Parallels field using the keyboard.

13.9 Remote Jobs

13.9.1 Q. Please tell me how to submit a job to a supercomputer or a linux server in my company or my campus.

A. If you need environment settings specific to the computer to which you are connecting, you can do it by creating a template script for remote jobs.

See *Remote job* for more information.

13.9.2 Q. I cannot connect from Winmostar to a server that allows SSH connections with various terminal software.

A. First check the steps described in *Remote job*. If this does not solve the problem, you may be able to connect by changing the version of libssh, the library used by Winmostar for SSH connections. Check [Tools] - [Preferences] - [Compute] - [Use older version of libssh2 (1.8.2) for SSH connections].

13.9.3 Q. SSH connection with public key method fails, when I specify the same private key file with other software such as TeraTerm or Cygwin, the connection succeeds. Is there a solution?

A. The key format may not be supported by Winmostar. See *SSH public/private key authentication*.

13.9.4 Q. The connection test with *Test Connection* succeeds, but the job submission fails.

A. There are various reasons. Here are some examples

1. If there is a limit on the number of SSH connections such as TSUBAME3.0, please consult us to avoid it without executing SSH connection every time.
2. In some cases, this can be avoided by activating password authentication as well as secret key authentication on the server side.
3. If there are multiple login server entities and they are automatically selected in the background, you may be able to avoid this by using only a specific login server or connecting until all servers are registered in the cache .
4. Even if Winmostar submits a job submission command (such as **`qsub`**) from the local machine, the command may not be found on the remote server. This can be avoided by filling *Profile –> Edit Profile…' in the :guilabel:`Submit Remote Job* window with the path of an executable such as **`qsub`**. To avoid this problem, add the path of an executable such as **`qsub`** to *Prefix for queueing commands* of *Profile –> Edit Profile…* in the *Edit Profile. For example, if the full path of :command:`qsub* is **`/usr/local/bin/qsub`**, type “/usr/local/bin/” in *Prefix for queueing commands*.

13.9.5 Q. Connection test with *Test Connection* succeeds, but Putty's WARNING is displayed and various operations fail.

——— Question details ———
Even though the result of TestConnection is OK, various commands can not be executed.
And the following dialog is displayed at the time of launching remote job submission window or TestConnection etc.
WARNING: Putty default host name was found in registry.
(\SOFTWARE\SimonTatham\PuTTY\Sessions\Default%20Settings\HostName)
This may cause errors while job submission.
Clear this setting.

A.
Reason:
This WARNING occurs when Putty's HostName is set.
Since Putty's settings are saved in the Windows registry, even if the Putty is other than Winmostar bundled version, this problem will occur when some sort of character string is saved in HostName.
Solution:

Launch Putty from *Connection* → *Open Putty* Remote Job Submit window. Check a character string is set in the HostName field of Default Settings.

You can solve this problem by deleting this string and saving it with Default Settings selected.

(The input contents in the Port column are not particularly affected.)

13.9.6 Q. What type of MPI (MPICH, OpenMPI, etc.) can I use on the remote server?

A. Basically any type of MPI is available. We have experience with MPICH, OpenMPI and MVAPICH.

By editing the template script, you can freely execute commands such as source, module, and export, and set up the environment for executing any MPI.

The solver used must be compiled with the MPI (mpicc, mpif90) used.

13.9.7 Q. Why are some environment variables (e.g. PATH) that should be set on the remote server by filling in bashrc, etc., not set when running from Winmostar? What should I do in such cases?

A. This is because the processing flow on the remote server may differ between interactive shell operations in the terminal and direct command execution with ssh command arguments. bash command arguments may do the same. As a workaround, please create a template script and explicitly fill in the environment variable settings, etc. separately in the script.

If you have an Ubuntu machine including WSL2 as a remote server, please also refer to *here*

13.9.8 Q. Is there any difference in behavior between the Windows version of the solver and the Linux version of the solver?

A. There is essentially no difference in functionality except for calculation speed. Performance varies depending on compiler, MPI, and compilation settings.

13.9.9 Q. Can I run calculations simultaneously for remote jobs that run on different servers?

A. Yes. However, in project mode, each job is tied to the runtime profile information, so create a different profile for each server.

13.9.10 Q. Where are passwords entered in the remote job profile stored? Is the password information stored in the project folder?

A. Passwords are stored encrypted in winmos_profile.ini under the user settings folder (UserPref in the Winmostar installation folder). It is not stored anywhere else, so there is no password information stored in the project folder. For example, when you send us your project folder for support, we will not send you the password information.

13.9.11 Q. Why can I SSH to an Ubuntu machine, including WSL2 use, but cannot successfully execute a remote job?

A. On Ubuntu machines, because of the following part written at the beginning of the .bashrc file, remote job execution does not reflect the PATH and other settings that are set after this.

```
# If not running interactively, don't do anything
case $- in
    *i*) ;;
        *) return;;
esac
```

Delete or comment out these lines.

Also, for WSL2 Ubuntu, since zip is not included by default, please also run the following command to install zip.

```
sudo apt-get install zip unzip
```

13.10 Simulation in general

13.10.1 Q. Is it possible to calculate the interaction between one substance and another substance with Winmostar?

A. This kind of question is very common, but the definition of the word "interaction" is broad, so it depends on the definition.

First of all, please check the manual of each solver beforehand, because Winmostar depends on what each solver (GAMESS, Gaussian, LAMMPS, Gromacs, Quantum ESPRESSO) can do, in terms of whether it can perform quantum chemistry, molecular dynamics, and ab initio calculations itself for the material you are focusing on.

Secondly, interactions in the sense of wanting to know the mechanism of some physical property or phenomenon that we are focusing on cannot be answered immediately, because it requires knowledge specific to that material system, and the investigation of whether it is computable requires sufficient investigation itself. We also offer a service to conduct investigations for a fee for private companies

If you want to quantitatively evaluate the bonding or association caused by the interaction, you can discuss the change of energy versus bonding distance for absolute zero, or the radial distribution function between binding materials or the autocorrelation function of the bonding time series data for the kinetic state.

Finally, if you know the specific analysis, such as Kitaura-Morokuma analysis or interaction energy analysis such as Coulomb-vdW interaction in MD, please ask about it.

13.10.2 Q. Can I calculate bond energies and bond divergence energies for a given bond in a molecule?

A. Perform quantum chemical calculations of the stable conformations of the bound and dissociated states and calculate from the energy difference between them. The two molecules in the dissociated state should be calculated separately, and the spin and charge should be set carefully.

13.11 MOPAC, CNDO/S, GAMESS, NWChem, Gaussian

13.11.1 Q. I get an error while running a quantum chemistry calculation, what should I do?

A. First trace the Winmostar tutorial. If that fails, you may have failed to build the environment, and for Gaussian, also check if the license allows parallel computation.

Next, if you did the calculation in project mode, check the error column in the working folder for the corresponding calculation. You can also hover the mouse pointer over the working folder to see the error. If the error message is in the FAQ, try the workaround described there. Especially for IR calculations of large molecules, the default amount of memory specified may not be enough and the calculation may stop.

If the energy (SCF) calculation does not converge, please check or try the following.

- Check for proper initial structure, charge, and spin multiplicity.

- Using large basis functions and diffuse functions makes convergence difficult. Consider using smaller basis functions.

- If the DFT calculation in GAMESS does not show “DFT CODE IS SWITCHING BACK TO THE FINE GRID” after displaying “CONVERGED TO SWOFF, SO DFT CALCULATION IS NOW SWITCHED ON” without approaching convergence please set the variables NRAD0 and NLEB0 in the DFT tab of the Keyword Setup window.

- In Gaussian, if the result of a small basis function is used as the initial trajectory, it is more likely to converge in the large basis function. In project mode, the energy calculation is first performed on the small basis function, and then a continuation job is performed on the large basis function. At that time, the continuation source should be specified as a small basis function calculation, and in addition, the guess=read checkbox should be checked in the Keyword Setup window.

13.11.2 Q. The Hamiltonian calculation method (Hamiltonian) or basis function (Basis Set) that I want to use is not found in the Configure window or the Easy Setup window for MOPAC, GAMESS, Gaussian and NWChem. How do I set it up?

A. If you can enter directly on the keyboard in the Calculation Method and Basis Function setting fields, you can do so directly. Please check the manual of the respective solver, as the description of how to specify polarization functions (represented by “*”, “p”, “d”, or “f”) may differ from solver to solver.

13.11.3 Q. How are bonds determined when opening an input/output file or when regenerating bonds?

A. *Combining Criteria*.

13.11.4 Q. Unnecessary bonds are displayed while modeling the system or when reading the calculation results. Or the bonds are not displayed. How can I fix this?

A. *See this FAQ* for more information.

13.11.5 Q. Is it possible to optimize substructures from Winmostar using quantum chemical calculations?

A. As of V11.3.1, the support is as follows
  MOPAC6: Only Z-Matrix is supported
  GAMESS: not supported
  Gaussian: only Z-Matrix supported (opt=z-matrix required)
  NWChem: only Z-Matrix supported

13.11.6 Q. Why does the Dipole moment value displayed at the bottom of the Winmostar molecule display area differ from the dipole moment value manually calculated from the charges assigned to each atom, such as Mulliken charges?

A. The Dipole moment value displayed at the bottom of the Winmostar molecule display area is the dipole moment for the entire molecular system directly output by MOPAC, GAMESS, Gaussian, and NWChem. This value is the exact dipole moment calculated by calculating the center of gravity of all negatively charged electrons and the center of gravity of all positively charged nuclei. In the calculation of this value, no operation to assign an electron to each atom is involved.

On the other hand, in atom-by-atom charge calculations such as Mulliken charge, the boundary between atoms cannot be uniquely determined and remains arbitrary. The formula for assigning a charge to each atom differs depending on the method of charge calculation, such as Mulliken or NBO charge. Therefore, the dipole moment values calculated from Mulliken charges, etc. are slightly different from the dipole moment values for the entire molecular system output by MOPAC, GAMESS, Gaussian, and NWChem, which are displayed at the bottom of the Winmostar molecular display area.

13.11.7 Q. How many atoms can be calculated with MOPAC?

A. 70 heavy atoms (other than hydrogen) and 90 light atoms (hydrogen).

You can also download the executable binary of MOPAC6 for large molecules (up to 420 atoms) from the *here <https://winmostar.com/jp/mop6wxxx.zip>*.

Winmostar has been confirmed to work with MOPAC2016.

MOPAC2016 will be available free of charge from 2021 with no limit on the number of atoms.

MOPAC main page

13.11.8 Q. It will display abnormally with the message *ATOMS **, **, AND ** ARE WITHIN. **** ANGSTROMS OF A STRAIGHT LINE* displayed in the MOPAC log.

——— Question details ———

It stops with an error saying that 3 atoms are linear as shown below.

```
CALCULATION ABANDONED AT THIS POINT

THREE ATOMS BEING USED TO DEFINE THE
COORDINATES OF A FOURTH ATOM, WHOSE BOND-ANGLE IS
NOT ZERO OR 180 DEGREEES, ARE IN AN ALMOST STRAIGHT
LINE. THERE IS A HIGH PROBABILITY THAT THE
COORDINATES OF THE ATOM WILL BE INCORRECT.
THE FAULTY ATOM IS ATOM NUMBER 69
```

Finally, comes

```
ATOMS 68, 57, AND 54 ARE WITHIN .0134 ANGSTROMS OF A STRAIGHT LINE
```

.

A.

It is displayed when an angle close to 180 degrees is included in Z-Matrix.

Change the connectivity of atoms by the coordinate editing function in the lower right of the main window so that there is no angle close to 180 degrees from Z-Matrix.

If you are new to Z-Matrix, you may be able to avoid this error by adding “XYZ” to the keyword as a different method.

Alternatively, by adding a dummy atom of the atomic type XX to a position out of the line where three atoms are aligned in a straight line and designating it as a connection destination on the Z-Matrix of the atoms arranged in the line,

Sometimes it is possible to avoid errors.

13.11.9 Q. When MOPAC is executed, “UNRECOGNIZED KEY - WORDS: (PM 6 (Hamiltonian name))” is output to the log and the calculation ends.

A. If you can avoid the error by changing Hamiltonian to AM1 with MOPAC Configure, the selected Hamiltonian is not supported by the MOPAC you are using.

Check *the list of Hamiltonians* supported by each version and select the appropriate Hamiltonian.

If it still does not work, please take action of *general errors* .

13.11.10 Q. How do I use the solvent effect (COSMO method) in the MOPAC attached with Winmostar?

A. MOPAC which is included in Winmostar does not support the solvent effect (COSMO method). Please consider using GAMESS which is more accurate than MOPAC, although it takes more time to calculate.

13.11.11 Q. When I calculate with MOPAC other than Winmostar built-in (e.g. MOPAC2016), only some molecular orbitals are displayed.

A. Check the ALLVECS checkbox in the MOPAC Setup window to create an input file and perform the calculation.

13.11.12 Q. It can not be calculated when Method=INDO is used in CNDO/S.

A. The elements after F are not supported by Method=INDO.

set Method=CNDO, or use a non-empirical solver such as GAMESS.

13.11.13 Q. Is there a guideline for the maximum number of atoms (memory requirement) that can be calculated in GAMESS, Gaussian, and NWChem?

A. There is no simple guideline for the amount of memory required, as it depends on the molecule size, basis functions, calculation contents, and number of parallels.

When a calculation is actually performed and stops due to insufficient memory, the log file will indicate how much is missing, so it is common to make a judgment based on that value.

13.11.14 Q. Is it possible to speed up 3D display of ESP (electrostatic potential) of GAMESS, Gaussian, and NWChem?

A. If you have installed the Windows version of Gaussian, check the Cubegen check box in the Cubegen window that appears when you open the Cube file, and the processing will be relatively fast using the Cubegen program included with Gaussian.

In the future, we plan to speed up the cube file processing program (OpenCubegen) included with Winmostar.

13.11.15 Q. When running GAMESS, "* ERROR: MEMORY REQUEST EXCEEDS AVAILABLE MEMORY" etc. will be output to the log and the calculation will end abnormally.

A. This means that the amount of memory specified in the input file is not enough.

Increase the value of MWORDS in the $SYSTEM column of the Advanced tab of the GAMESS Configure window. (MWORDS number) x 8MB is the maximum amount of memory used per CPU core. For example, if MWORDS is 200, the maximum amount of memory per CPU core is 200 x 8MB = 1600MB = 1.6GB. Please set MWORDS according to your computer and the number of parallels.

13.11.16 Q. Immediately after installing GAMESS for Windows, I was able to use it without any problems, but at some point, all the calculations started to terminate abnormally in the middle. Is there a way to fix this?

A. First of all, please take action of *general errors*. If this does not work, perform the following steps in order.

1. Launch the GAMESS installer -> Select Remove -> Uninstall GAMESS.
2. Go to Windows Settings -> Apps -> Apps and Features -> Select Microsoft MPI -> Uninstall Microsoft MPI
3. Reinstall GAMESS and MS-MPI according to the GAMESS installation manual for Windows in the Winmostar Installation Guide.

In particular, when it shows "mpiexec … server rejected credentials" etc. in the console window when running GAMESS, this method may be effective.

13.11.17 Q. GAMESS outputs "WARNING. NUMBER OF INTERNAL COORDINATES IS GREATER THAN (3N - 6), BUT NO SYMMETRY COORDINATES ARE GIVEN." in the calculation of only one atom and abnormally ends.

A. This is a message indicating a problem caused by using Z-Matrix in a system with only one atom.

In this case, Cartesian coordinates are used (COORD=UNIQUE) to solve it.

Set UNIQUE to COORD on Wimostar's GAMESS Configure window.

13.11.18 Q. The message `**** ERROR **** PCM SPHERE (S) MUST HAVE A POSITIVE RADIUS` is displayed in the log of GAMESS and abnormally ends.

A. GAMESS may not contain Cavity radius for some atoms.

To specify the Cavity radius, add the following statement just after the $PCM line.

$PCMCAV RIN(13)=1.55, RIN(15)=1.55 $END

In this example, Cavity radius is set to the 13th and 15th atoms.

13.11.19 Q. When GAMESS is executed, "ERROR: BAD DELOCALIZED COORDINATES GENERATED !!!" is output to the log and the calculation ends abnormally.

A. In the GAMESS Configure window of Wimostar, select the Z-Matrix tab and uncheck $ZMAT.

13.11.20 Q. When I try to run NMR calculation in GAMESS (using RUNTYP=NMR), I get an error.

A. GAMESS NMR calculations are only compatible with the closed-shell Hartree-Fock method, and other DFT methods cannot be used.

Also, the execution of NMR calculations in GAMESS can be slow, so we recommend using NWChem or Gaussian instead.

If you really want to calculate with GAMESS from Winmostar, uncheck the DIRSCF checkbox in the $SCF of the Advanced tab in the Setup window.

In addition, parallel computing is not supported, so please set the parallel number to 1.

You can find detailed instructions in the log file with an error, so please refer to that as well.

13.11.21 Q. When I use Diffuse functions in GAMESS, the SCF calculation does not converge.

A. Add ICUT=11 to the Others column in the $CONTRL box on the Basic tab of the GAMESS Setup to make the cutoff value for the two-electron integration smaller (stricter).

13.11.22 Q. For some molecules, after optimization of Firefly, when I check the Molecular Orbit UVvis…, I get the error '*******' is not valid floating point value".

A. The linear dependence of the basis is large because 6-31+G* has the diffuse functions.
Therefore, a part of the value of the molecular orbital coefficient becomes very large, and **** is output in the log.

The solutions are
1. Use 6-31G* basis set
2. If you use 6-31+G*, use GAMESS instead of Firefly
.

Because GAMESS has processing of linear dependency,
Firefly and GAMESS may have slightly different energy values.
execute a series of calculations with either Firefly or GAMESS.

13.11.23 Q. How do I deal with the message "THE GEOMETRY SEARCH IS NOT CONVERGED!" when I run a structural optimization calculation with GAMESS?

If the animation shows structural optimization information and the energy continues to drop, the calculation has been completed with insufficient number of structural optimization cycles. Please perform the structural optimization calculation again with the final structure.
For some larger molecules (roughly 100 atoms or more), structure optimization with DLC=.T. may result in a significant loss of structure. In that case, unchecking $MAT's Set DLC=.T.… unchecked and run, which may resolve the problem.

13.11.24 Q. I cannot download the GAMESS installer. How can I do this?

A. If an error occurs on the download site and the registration form does not appear, please try another browser. If you are using Microsoft Edge, try accessing the site again in Internet Explorer mode. Also, sometimes the download site system is down, in which case please wait up to a week.

13.11.25 Q. The DFT calculation in GAMESS does not converge after displaying "CONVERGED TO SWOFF, SO DFT CALCULATION IS NOW SWITCHED ON". Is there any way to deal with this?

A. GAMESS DFT energy calculations are typically performed in three steps to improve convergence and calculation efficiency. The first step is a Hartree-Fock calculation, followed by a DFT calculation on a rough grid, and finally a DFT calculation on the default or input-specified grid. When "CONVERGED TO SWOFF, SO DFT CALCULATION IS NOW SWITCHED ON" is displayed, the second step of DFT calculation with the rough grid starts, but for some molecules, the grid is too rough to converge and the "DFT CODE IS SWITCHING BACK TO THE FINE GRID" may not be displayed.

To increase the number of grid points in the second step, enter "NRAD0=99 NLEB0=302" in the Others field on the DFT tab of the GAMESS Keyword Setup window.

13.11.26 Q. When parallel execution of NWChem, the calculation outputs "Please specify an authentication passphrase for smpd:" to the log and dows not run.

A. If you omit the pass phrase (passphrase) when installing MPICH 2, such an error may occur.

There are several solutions, but after uninstalling MPICH2, reinstalling MPICH 2 may resolve it.

In that case, you need to stop smpd before uninstalling MPICH2 and install smpd after reinstalling MPICH2.

Also, if you are using 32-bit MPICH2 on 64-bit Windows, use the 64-bit version.

13.11.27 Q. When I run NWChem, I get the message "sym_geom_project: sym_center_map is inconsistent with requested accuracy" in the log and the calculation does not run.

A. If the structure deviates slightly from NWChem's molecular symmetry criterion, it will stop with an error. Select [Tools]-[Point Group Analysis] in the Winmostar main window and click [Analyze], then [Symmetrize] to make the structure with exact symmetry, or check noautosym in the Advanced tab of the Keyword Settings window, or move one atom slightly to make the structure with broken symmetry.

13.11.28 Q. How can I put the solvent effect in NWChem?

A. Please put the name of the solvent molecule in ***. Please see https://nwchemgit.github.io/COSMO-Solvation-Model.html#solvents-list-solvent-keyword for more information about supported solvent molecules.

13.11.29 Q. When executing NWChem, lines including "out of memory", "alloc failed", "ma_push failed", "nga_create failed", and "Global memory limit unreasonable" are printed in the log and calculations do not run.

A. None of the calculations are stopped because the amount of memory specified in the input is not sufficient. Please increase the value of Memory in the Basic tab of the NWChem Keyword Setup window.

13.11.30 Q. The Gaussian calculation may or may not work correctly.

A. In case of single core version of Gaussian, Gaussian will be terminated when you try to run more than two jobs. If you want to run two or more Gaussian local jobs sequentially on Winmostar using a single-core version of Gaussian, set the parallel number of each job (%nproc or %nprocshared) to 1, and set Max Cores of Winmostar JM to 1. Please set the Max Cores of Winmostar JM to 1.

13.11.31 Q. I read the Gaussian log file, but the orbital (eigen) energy etc. are not written.

A. It is not output if pop=full and gfprint is missing in the Gaussian input file.

When you open a Gaussian input or output file in Winmostar, not only the structure but also the calculation conditions will be loaded. If you open such a file and set the keywords, make sure that pop=full and gfprint are set.

13.11.32 Q. How do I calculate the chk file read in Gaussian?

A. For remote jobs, check [Advance] in the SubmitJob window and uncheck [Delete *.chk] to leave the chk file. And the chk file is loaded and the calculation runs when the same name was used.

> The method using *–Link1–* is simpler in setting itself, so please consider using it as well.

13.11.33 Q. I get an error when I try to load a Gaussian fchk file that is several GB in size and display molecular orbitals.

A. We can handle fchk files up to roughly 2 GB. The upper size depends on the molecule size and basis functions. We plan to eliminate the fchk file size limitation in the future.

13.11.34 Q. How can I perform vibration calculations in Gaussian that take isotope effects into account?

A. Set freq=readisotopes in the Freq column of the Gaussian Keyword Setup window and write the following items one line at a time in the Subsection column.

Temperature (K) Pressure (atm)

Mass of the first atom

Mass of the second atom

. . .

Mass of the n-th atom

13.12 LAMMPS, Gromacs

13.12.1 Q. I would like to run molecular dynamics calculations, but which should I use, LAMMPS or Gromacs?

A. If you are not sure, we recommend LAMMPS, which is slower than Gromacs, but it supports a wider range of force fields and allows for more flexible schemes for non-equilibrium calculations. Winmostar allows you to use LAMMPS and Gromacs with the same ease of use, making the transition to Gromacs relatively easy.

13.12.2 Q. I get an error while running a molecular dynamics calculation, what should I do?

A. First trace the Winmostar tutorial. If that fails, you may have failed to build the environment.

Next, check if the error is reproducible. If it is not reproducible, it is often an environmental (either or both hardware and software) problem or a random number derived problem.

Next, calculate one molecule of each component, without charge. If you still get an error, change the type of force field as well.

If no error occurs with one molecule of each component and no charge, set the charge or increase the number of molecules and observe the behavior.

Next, if you get errors with long calculations, increase the equilibration time.

If you get an error during the equilibration process, try the following.

- Check for conservation of conserved quantities (total energy, extended Hamiltonian) and reduce the time increments.(1 fs→0.5 fs→0.2 fs→0.1 fs, and so on, gradually decreasing the time increments to find the value at which stable operation is achieved.)

- If parallel computation is not performed or it is impractical to set the number of parallels to 1 due to computation time issues, the number of parallels should be reduced gradually.

- If parallel computation is not performed or it is impractical to set the number of parallels to 1 due to computation time issues, the number of parallels should be reduced gradually.

- Use Berendsen and velocity scaling methods for temperature and pressure control.

- Use double precision (for Gromacs)

- Do not use constraints (such as the SHAKE method). Instead, use time increments of about 0.1 fs.

- If the cell size is less than twice the cutoff radius, the calculation fails due to the implementation of the solver, so the number of numerators is increased to increase the cell size and the calculation is performed again.

- Separate the calculation by a short number of steps and repeat the continuation. (Especially useful when initial and final densities differ significantly during pressure control).

- Change the initial density (decrease or increase).

Change the random number seed for initial speed generation.

Change the random number seed for initial structure generation.

If it finishes successfully up to the NVT calculation but fails in the NPT calculation, see *Q. When pressure control (constant NPT or NPH) is used, the calculation fails in the middle of the process. Is there a solution?*.

13.12.3 Q. How can we equilibrate the system in molecular dynamics calculation?

A. First of all, describing the case where the calculation of the aggregation system (liquid and solid, not gas) of the equilibrium state of low molecular is target.

When aligning molecules in the initial state, please set the density as close as possible to the final density.

However, when it is not possible to arrange it unless it is considerably low density, it does not matter.

After that, please carry out energy minimization, constant temperature calculation, constant temperature pressure calculation until the change of the potential energy, temperature and density converge.

If the initial density is too low, compress it with a pressure higher than the target pressure (for example, about 100 times) by constant temperature pressure calculation.

Finally, if you are interested in the ensemble average physical quantity and reaching the target temperature and pressure after equilibration, the difference in the fine equilibration procedure is less likely to have a significant influence on the calculation result.

In the case of polymers and glasses, in most cases it is impossible to obtain an equilibrium state in a real sense, because realistic computation time is almost impossible, so the convergence of energy, temperature and density, the influence on the physical quantity to be observed is affected Equilibrium calculation is carried out for a time to the extent that the correlation of physical quantities considered to be large reaches zero.

Since pressure control is unstable in the case of gas, equilibrium state is obtained only by energy minimization and constant temperature calculation.

Also, it may be difficult to reach equilibrium density for tonic or bulky molecules, see *Q. The final density obtained from the NPT calculation is much lower than the density predicted from experimental values and other sources. What should I do?* in that case.

13.12.4 Q. I ran MD calculations from the same initial configuration but got different results. Why is this?

A. The floating-point arithmetic used inside MD programs has the characteristic that the result changes when the order of addition and subtraction is changed (the digits near the end of significant digits change), and in normal parallel computation, the order of addition and subtraction changes depending on the accidental timing of communication, i.e., the result during parallel computation In other words, there is no reproducibility in the results of parallel calculations. In addition, because many-body problems such as those calculated with MD have the property that very small differences in values expand exponentially over time (chaotic nature), changes in values during parallel calculations can change the trajectory of each atom in many ways. The reason why different calculation results are obtained is due to this change. This change in results is reasonable because the distribution of results is expected to converge to a similar distribution if the MD calculation is performed for a sufficient amount of time and sampling is sufficient.

13.12.5 Q. The final density obtained from the NPT calculation is much lower than the density predicted from experimental values and other sources. What should I do?

First, check to see if it has equilibrated sufficiently, and if it is the last case where the temperature, potential energy, pressure, and density are still changing significantly, calculate for a longer simulation time.

Second, if the molecule is a solid or bulky molecule with multiple aromatic rings, it may take a very long simulation time to converge to the equilibrium density at the desired temperature and pressure. This is especially true for liquid crystals and large monomeric polymers. This is due to the fact that the molecules (monomers) are hard or large, and once they aggregate, it is difficult to get another configuration. In such cases, density equilibration can be greatly accelerated by interspersing equilibration at a higher temperature than the target temperature (e.g. 600 K when 300 K is the target temperature) as appropriate. In the LAMMPS, Gromacs workflow setup, such equilibration can be easily set up by using Preset=12-Step Compression or 21-Step Compression-Decompression.

13.12.6 Q. In the MD calculation, how does the constraints by the SHAKE method etc. affect the calculation result? How do I choose a constraint method ?

A. The SHAKE, RATTLE, LINCS, and SETTLE methods are applied between atoms that are covalently bonded to restrict the bond length, so that the time step can be increased and even longer computations can be performed more stably with the same amount of computation. “Stable” is in terms of Hamiltonian (total energy) conservation.

Functions that express covalent bonds when not constrained also do not accurately represent actual phenomena. Therefore, assuming that stable calculations are being performed, there are deviations from the actual phenomena due to the respective circumstances both in the case of restraining and in the case of not restricting, in terms of the effect on various calculated physical properties.

Unless the vibrational motion in the molecule itself has the purpose of calculation, it is basically recommended to select the condition that the Hamiltonian preserves for a long time in each case.

However, if the bonds of the hydrogen atoms are not constrained, the atoms will move at high speed significantly in the system, which may cause the drift of the Hamiltonian. Therefore, in many cases, the bonds of the hydrogen atoms are constrained.

13.12.7 Q. Why do molecules sometimes come out of the cell when in the trajectory or the final structure afterMD calculation?

A. Using periodic boundaries, the entity of the molecule should be inside the cells of the periodic boundaries.

But, solvers such as Gromacs and LAMMPS record trajectories with translational values as they are without folding coordinates even when molecules cross over cell boundaries to calculate mean square displacement, etc.

Either way, the result will be properly considered and the same result will be output during the result analysis, so there is no effect on the result analysis.

If the appearance of molecules jumping out of the cell is not good, adjust the settings of *View - Wrap Around Cell Boundary*.

13.12.8 Q. When I create a cell by adding water molecules from a cell in the [Solvate/Build Cell] menu to a large molecule such as a protein, the molecules sometimes stick out of the cell.

A. Select [View]-[Wrap/Unwrap Around Cell Boundary]-[Wrap for each atoms] and if there is no interference between protein and water molecules, then there is no problem in the calculation.

If you want to center the protein, which is a matter of appearance only, select the atoms near the center before adding the solvent and perform [Edit]-[Adjust Axes]-[Set Origin to Marked Atom] to move the molecule near the center.

13.12.9 Q. The [MD]-[Solvate/Build Cell] and [Insert Molecule] processes do not finish after many minutes. Is there a solution?

A. Reduce the density. When the molecules are relatively small (generally within 30-40 atoms), set the density at 50-75% of the expected density. If the molecules are large or depending on the shape of the molecules, it may be necessary to further reduce the density (several percent to 10%, etc.), so observe the behavior while gradually reducing the density. Even if the initial density is far from the original density, it is expected to eventually change to an appropriate density by running MD calculations with pressure control.

13.12.10 Q. In the [MD]-[Assign Charges Automaticcally] menu, the error message "Topology file not found" is displayed. Is there a solution?

It is very likely that the molecule you are trying to assign a charge to is not compatible with Acpype. Check the log file and sqm.out under the [filename]_charge_tmp folder. If there is an atom that is not supported, please assign a charge with MOPAC or QM, or enter it manually.

13.12.11 Q. The process of assigning the force field takes a long time and never ends. Is there a solution?

A. Especially when GAFF or OPLS-AA/L+GAFF is selected as the type of force field, it may take a long time to process. This is caused by the fact that acpype is used to allocate GAFF, OPLS-AA/L+GAFF, and acpype processing is slow. In the case of macromolecules with nearly 10,000 atoms per molecule, we have confirmed that the process can be completed normally after about 5-6 hours. Depending on the environment, it may be faster than this, or conversely, it may be slower. In the future, Winmostar will work on speeding up the process of allocating these force fields.

13.12.12 Q. I get an error message when assigning a force field. Is there a solution?

It is very likely that the molecule you are trying to assign force field to is not compatible with Acpype. Check the log file and sqm.out under the [filename]_charge_tmp folder. If there is an atom that is not supported, try a versatile force field such as UFF or Dreiding.

13.12.13 Q. How do I assign a point charge to a polymer?

A. Polymers have large molecular weights, and using the point charge assignment method commonly used for small molecules would require quantum chemical calculations for huge molecules, which would require extremely long calculation times and would be impractical. Also, polymers assume various conformations in vacuum, and the effect of these conformations would be significant when performing quantum chemical calculations for the entire molecule, but the model in the classical force field for polymers does not want extreme charge changes between repetition units. For this reason, polymers are usually assigned point charges in a different way than small molecules. Winmostar's Polymer Builder allows you to assign point charges in the state of the repeating unit, which are then used to automatically configure the polymer charge. Details can be found in *Homo Polymer builder* , *Block Polymer Builder* , *Random Polymer Builder*.

13.12.14 Q. Can I calculate dielectric constant from Gromacs or LAMMPS (Molecular Dynamics Calculation)?

A. Since the dielectric constant is a physical property dependent on the frequency of the external field, and the mechanism is different for each frequency band, we cannot answer them all.

The dielectric constant calculated from Winmostar's Gromacs and LAMMPS is a component derived from molecular orientation on the assumption that intramolecular polarization does not change with time.

And among them, it is the infinitely slow low frequency limit value calculated from the fluctuation of the dipole moment of the whole system within the simulation time of molecular dynamics calculation.

Be careful for substances with large molecular weights and slow relaxation, such as polymers, because only information within the range that can be observed within the simulation time is known.

The dielectric function calculated from Winmostar's Quantum ESPRESSO is the dielectric function of the high frequency component derived from the polarization of the electron with the atomic coordinates fixed.

It is necessary to plan the calculation considering how to obtain the experimental value of the dielectric constant to be compared, the properties of the material, and the research purpose.

In addition, it is possible to help with planning with our paid support.

13.12.15 Q. When I try to run an MD calculation from a structure created with the interface builder, the force field assignment fails or the MD calculation fails. Is there a solution?

A. If the distance between the layers is too short, the molecules of the two layers will collide, and unwanted covalent bonds will be created based on the interatomic distance, or a large force will be applied at the start of the MD calculation, causing the MD calculation to fail. The best way is to increase the value of [Direction]-[Interval] in the interface builder and take a long time to equilibrate

13.12.16 Q. When pressure control (constant NPT or NPH) is used, the calculation fails in the middle of the process. Is there a solution?

A. First of all, in a situation where the interaction between molecules is extremely weak, such as in the gas phase or when other phases are dispersed in the gas phase, the pressure control is not stable, so try a method without pressure control. Next, look at the change in density over time in the broken calculation to see what's going on. Also, the energy, temperature, and pressure must be sufficiently equilibrated at a constant density before pressure control can be performed. At the end of equilibration at constant density, the pressure (the mean value of) is preferably 0 or negative. If the pressure value is large at the end of equilibration at a constant density, the system size will change drastically immediately after starting pressure control. If you want to reduce the pressure at the end of equilibration at a constant density, reduce the initial density (Approximate 50% of final density, possibly larger or smaller). If this does not solve the problem, (1) change the pressure control to Berendsen method instead of Parrinello-Rahman (Nose-Hoover) method, (2) increase the time constant of the pressure control, and (3) divide the calculation with the pressure control into several short calculations.

13.12.17 Q. How do I decide interaction parameters between liquid (organic) and solid (inorganic) in LAMMPS and Gromacs?

A. First, collect as much information as possible what experimental facts are known and related research about the liquid-solid interface. In particular, it is desirable to know the atomic structure of the surface (e.g., Miller's index, functional groups, etc.) and the chemical properties of the surface (rough things such as wettability, hydrophobic or hydrophilic).

If the LJ parameter and charge values are listed in the appropriate relevant research literature, it is best to use those values. In Winmostar, Set values as follows.

- For the charges, save them once in mol2 format and rewrite the values of the charges to the values in the paper.
- For LJ parameters, use the [Assign Force Field] function to enter the values for each element from [Exception].

If the appropriate values were not listed in the literature, but some chemical properties are known, run simulations with several different charge and LJ parameters, compare the results of the calculations and adopt the parameters that seem reasonable.

If only the atomic structure of the surface is known, the parameters are determined with ab initio calculations (Quantum ESPRESSO).

In some cases, the Lowdin charge function of Quantum ESPRESSO can be used to determine the charge. However, when using lowdin charges, the total value of the charges does not equal zero, so adjustment of the values (e.g., shifting charges of all atoms) is necessary. It is also important to note that the polarization may be overestimated in Lowdin charges.

For LJ parameters, use known parameters (e.g., Dreiding, UFF, CLAYFF, etc.) or calculate them from ab initio calculations and algorithms such as Force Matching.

This complexity of the liquid (organic) - solid (inorganic) interaction parameters stems from the following facts.

1. The interaction parameters (epsilon, sigma, and charge) depend on the atomic position in classical MD, however, The approximation error is larger in the organic-inorganic interface system than in the organic-organic system.
2. Although the surface of inorganic materials in real devices is covered with oxide films, it is not easy to observe them experimentally and it is difficult to model accurately at atomic resolution.

13.12.18 Q. When I run Gromacs, I get the error “There is no domain decomposition for 49 ranks that is compatible with the given box and a minimum cell size of…”. error. How should I deal with this?

A. Most MD simulation software divides the simulation cell during parallel computation and assigns the divided region (subregion) to each process. Gromacs (and other major software) is designed in such a way that each edge of this subregion cannot fall below the cutoff radius of the uncoupled interaction (the near component of LJ or Coulomb). This error means that each edge of the subregion is below the cutoff radius. There are several ways to deal with this problem, but basically, the number of molecules (number of atoms) should be increased or the number of parallelism should be reduced to a level where the error does not occur. Although there may be requests to increase the number of parallels to the limit, in reality, if the small area becomes smaller than a certain level, the amount of communication increases in relation to the amount of calculation, and the parallel efficiency drops significantly.

13.12.19 Q. When I load the final structure or animation from Gromacs, or when I edit it in some way and then run the MD calculation again, the force field assignment fails or the MD calculation breaks down. Is there a solution?

A. There is a possibility that the molecules are separated due to a bug in Gromacs. To determine if a molecule is separated or not, go to [Select]-[Select by molecular species] and see if there are any unexpected components. If it is separated, please refer to *Molecules that should be connected to each other are displayed separately in the structure or the final structure after loading the Gromacs trajectory.*.

13.12.20 Q. When loading the final structure or animation in Gromacs, the molecules are sometimes displayed in pieces.

A. Please refer to *Molecules that should be connected to each other are displayed separately in the structure or the final structure after loading the Gromacs trajectory.*.

13.12.21 Q. Even if Gromacs ER method result loading is executed, the result can not be displayed / an error will appear.

A. Please check the contents of ermod.out generated in the output destination directory specified when executing the ER method.

If it says “The minimum of the energy coordinate is too large” in ermod.out, press the [Options] button on the ER method execution window and select [For Solution System] Please reduce the value of [minimum value of the solute-solvent energy (ecdmin)].

For details on how to set concrete values, please see ERmod wiki FAQ.

Similarly, check the contents of ermod.out and ERmod wiki FAQ and if you need to change the setting of ermod, set it in [Options] of ER method execution window.

13.12.22 Q. The error message “Out of range atoms - cannot compute PPPM” appears in the LAMMPS log and the calculation terminates abnormally. Please let me know how to deal with this.

A. That message is displayed when an MD calculation fails in a general sense. See *Q. I get an error while running a molecular dynamics calculation, what should I do?*.

13.12.23 Q. How can I plot the trajectory of a specific atom?

A. Please operate as follows

1) Display animation

2) Click the atom for which you want to draw a trajectory in the molecular display area.

3) Click [Custom Plot] in the animation operating window.

4) Check the second item under [X axis] and select “Atomic position (x)” (choose an appropriate direction as appropriate).

5) Click [Apply] under [X axis].

6) Check the second item under [Y axis] and select “Atomic position (y)” (choose an appropriate direction as appropriate).

7) Click [Add] under [Y axis].

8) Uncheck [Y axis] except for “Atomic position (y)”.

9) Uncheck [Autoscale] from [X Axis] and [Y Axis] below the graph and set [Min] and [Max] accordingly.

In addition, we are planning to develop a function that simplifies the above operations.

13.12.24 Q. The dissipative particle dynamics (DPD) calculation gave me a different result than intuitive. Why is this?

There is no single pathway to approximate actual molecular assemblies with a DPD model, and it is likely that this is where the model was inadequate. It is also likely that the interactions between DPD particles are modeled quite boldly, and that the system you want to represent is beyond the expressive power of DPD in the first place. The construction of coarse-grained MD models, including DPD models, is highly individualized, and in many cases, a coping strategy will not lead to a fundamental solution, so Winmostar's support basically consists of individual consulting, starting with asking about the original research objectives.

13.13 About Quantum ESPRESSO, OpenMX

13.13.1 Q. I installed the Quantum ESPRESSO pseudopotential file as per the instructions, but it is not recognized.

A. Copy the pseudopotential files with the .UPF extension (e.g. `O.pw-mt_fhi.UPF`, `Au.pbe-dn-rrkjus_psl.0.1.UPF`, etc.) to the pseudo folder under the Quantum ESPRESSO installation folder (By default, this is C:\Program Files\Quantum ESPRESSO 64-bit 5.2.1pseudo etc.) under the Quantum ESPRESSO installation folder. However, if you download and save the UPF file using a browser such as the old Internet Exproler, there have been reports of problems such as the extension being changed without your permission, so please also try a browser such as Edge or Chrome.

13.13.2 Q. I don't know how to find a pseudopotential file for Quantum ESPRESSO. How do I find them?

A. It is described in Quantum ESPRESSO for Windows Installation Manual.

13.13.3 Q. Calculation using Quantum ESPRESSO fails. An error appears in displaying the calculation result.

A. First of all, please take action of *general errors*.

Next, since Winmostar continuously executes each module of QE by batch processing, we look at the flow of processing described in Winmostar generated bat file (local execution) or sh file (remote execution) While checking the generated output file (pwout or out) file in order.

For example, check ph.x output log (ph.out) for phonon calculation.

Please take action on the place where error such as "Error in routine . . . " appears first, then execute the job again.

Errors related to specific keywords, please confirm the setting of that keyword *official site <https://www.quantum-espresso.org/Doc/INPUT_PW.html>*.

Typical QE error handling is described in *official site FAQ <http://www.quantum-espresso.org/resources/faq>*.

If you change to nosym=.True. and the calculation flows, you may be experiencing a bug that originates from the detection of symmetry in the atomic configuration.

Reducing the number of parallels may cause the calculation to flow normally; changing the diagonalization (david, cg, rmm-*, etc.) may solve this problem. Since this phenomenon varies depending on the type of compiler, MPI, or numerical library that built Quantum ESPRESSO, it is also useful to change these settings and rebuild Quantum ESPRESSO as necessary in the case of remote jobs. For remote jobs, changing the parallel distribution method (-nk, -nt, -nb, -nd) can also improve the results, so it is useful to adjust the pw.x arguments in the template script accordingly.

13.13.4 Q. When executing Phonon calculation using Quantum ESPRESSO, “third order derivatives not implemented with GGA” is output in the ph.x output (ph.out), and the calculation result cannot be obtained.

A. This can be solved by selecting a pseudopotential other than GGA.

13.13.5 Q. Quantum ESPRESSO, OpenMX SCF calculation or structure optimization calculation does not converge.

A. Please carry out the following countermeasures in order.
Always to try:
· First-principles calculations have many setting items, so do not change the calculation conditions appropriately, and stream a series of calculations while recording properly.
Take action for *general problem of QE*.
· Plot the Estimated accuracy against the number of SCF cycles for QE. It is still good if it is a log-log plot.
· Spin Polarization State · Determine whether electric charge is appropriate.
· Gives the order of up/down spins.
· If you shift K_POINTS in Hexagonal crystal, remove the shift.
· Constrain the magnetic moment of the whole system.
· Use a reasonable initial structure.
· Use structures obtained by experiments and other calculation methods.
· Check to see if the calculation converges with a simpler model, such as a surface model only for an interface (adsorption) model, a bulk model for a surface model, or a bulk model for a defect model.
· If there are atoms whose placement is arbitrary in the calculation (light elements invisible in X-rays, solid solutions, defects, non-integer compositions, slab surface end structures, etc.), try a different placement.
· For slabs, reconsider the cutout and modification of the termination structure.
· In cases where solid solution · defects are included, make the initial structure so that large dipole moment does not occur in the system.

Try next:
· Adjust mixing_mode and diagonalization.
· Make mixing_beta smaller.
· Increase nbnd.
· Change the type of pseudopotential file.
· Adjust the initial value of spin polarization. (Atomic unit or whole system)
· If the entire system may have a dipole moment, such as in a slab model, consider using a dipole correction or using the ESM method (bc=1) or changing the surface composition.
· If the U parameter is used, gradually increase it from U=0 to check the behavior.
· If relatively complicated conditions such as external electric field, defect, adsorption, etc. are set, try them under simpler conditions than eliminating them, and if the calculation converges, the final state of the calculation (atomic arrangement · wave function Etc.) as the initial state and starts the calculation.
· Calculation is started from halfway of computation that did not converge (SCF algorithm depends on history).

Try in balance with calculation time / calculation precision:
· Take a large cutoff energy.
· Take a lot of K points.

Try with balance with calculation accuracy:

· In the case of spin polarization calculations, first check for convergence without spin polarization.

· Adjust smearing (use/not use, type, width).

Loosen the convergence parameter of the SCF.

13.13.6 Q. I cannot visualize the three-dimensional distribution of electron density, spin density, and potential in Quantum ESPRESSO.

A. First trace the Quantum ESPRESSO Basics section of the Winmostar tutorial and see if you can display them on a small system size. If not, please refer to *Q. I can not create a model as I expected. It can not calculate. It does not work.* and rebuild your environment. If the tutorial works fine but does not, first check if a cube file has been generated in your working folder, if so, this may be due to a problem with Winmostar Viewer. If a cube file is generated, please refer to *Cannot open large size cube file in Winmostar Viewer.* to fix the problem.

13.13.7 Q. The SCF calculation of Quantum ESPRESSO is displayed as "too few bands" in the output file (.pwout or .out) and abnormally ends. I do not know how to set nbnd.

A. First of all, please check nbnd description of the QE official manual.

If you do not use nbnd when you do the calculation, QE automatically calculates nbnd by setting it automatically, so please uncheck "Use nbnd" on the keyword setting screen of Winmostar.

To increase nbnd, set nbnd to a value larger than the value of "number of Kohn-Sham states" that is output to the pwout or out file when executed without using nbnd.

Also please refer to the value of "# valence bands:" displayed at "Use nbnd" on Configure window of Winmostar (See *Solid → Quantum ESPRESSO menu* for detail).

13.13.8 Q. The SCF calculation of Quantum ESPRESSO terminates abnormally with "fixed occupations and lsda need tot_magnetization" displayed in the output file (.pwout or .out). How do I resolve this?

A. Select smearing in the occupations section, or use tot_magnetization instead of starting_magnetization.

13.13.9 Q. Quantum ESPRESSO's structural optimization calculation (vc-relax) terminates abnormally with the output file (.pwout or .out) showing "smooth g-vectors missing ! in the output file (.pwout or .out) and terminates abnormally. How can I resolve this?

A. Recalculate using the structure output at the end of the pwout or out file. on the Winmostar GUI, create a new job with the structure optimization animation displayed and the final structure.

13.13.10 Q. The SCF calculation of Quantum ESPRESSO on metal is terminated abnormally with "charge is wrong" displayed in the output file (.pwout or .out). How do I resolve this?

A. First try the *Q. Quantum ESPRESSO, OpenMX SCF calculation or structure optimization calculation does not converge.* procedure.

The "charge is wrong" is immediately preceded by "WARNING: integrated charge= … expected= …" in the log, the charge or spin polarization calculation settings may not be appropriate for the model. is wrong, the settings for charge or spin polarization calculation may not be appropriate for your model, so please set tot_charge, nspin, starting_magnetization or tot_magnetization accordingly. For example, if the number of electrons in the simulation cell is odd, such as in a defect or surface model, one might set nspin=2 and tot_magnetization=1.

If this does not solve the problem, make sure that occupations is set to smearing in the Quantum ESPRESSO Keyword Settings window, and if necessary, set ecutrho to a larger value (such as 400 Ry) and the number of k-point divisions to a larger value (gradually increasing) Set the k-point divisions as large (gradually increasing) as necessary.

13.13.11 Q. When calculating the dielectric function using Quantum ESPRESSO, "bad band number" is displayed in the epsilon.x output (eps.out) and it is not possible to acquire the dielectric function.

A. It is solved by increasing the number of bands (nbnd) by SCF calculation.

13.13.12 Q. When calculating the dielectric function using Quantum ESPRESSO, "USPP are not implemented" is displayed in the epsilon.x output (eps.out) and it is not possible to acquire the dielectric function.

A. Select a norm preserving pseudopotential in the SCF calculation.

13.13.13 Q. My Phonon calculation using Quantum ESPRESSO failed and I cannot get the results.

A. First, please do not run the Phonon calculation, but use the same pseudopotential file and other calculation conditions to make sure that the SCF calculation finishes successfully. Next, check the ph.out (the output file of the Phonon calculation module ph.x) in the working directory (the folder ending in _qe_data). If it says "The phonon code with US-PP and raman or elop not yet available" there, you can solve it by selecting a norm-preserving pseudopotential. Also refer to *Q. I cannot find a norm-preserving, LDA functional pseudopotential file for Quantum ESPRESSO for the element I want to calculate in the pseudopotential files installed by default. How can I find it?* when looking for pseudopotential files. Similarly, if you are using a PAW potential, Raman calculations, etc., are not supported, and you can solve this problem by choosing a norm-preserving pseudopotential. If you are experiencing symmetry-related errors, please run [Solids]-[Refine Lattice] before running the Phonon calculation.

13.13.14 Q. I cannot find a norm-preserving, LDA functional pseudopotential file for Quantum ESPRESSO for the element I want to calculate in the pseudopotential files installed by default. How can I find it?

A. This DB <https://pseudopotentials.quantum-espresso.org/legacy_tables/hartwigesen-goedecker-hutter-pp>`_ contains a relatively large number of norm-preserving and LDA-functional pseudopotential files. The pseudopotential file is not limited to this pseudopotential file. Please verify the cutoff energy and the number of k-points used in your calculations, not limited to this pseudopotential file.

13.13.15 Q. When I try to output the Fermi surface, they do not appear.

A. First, make sure that the target substance is a metal. Next, output the density of states, and confirm that the density of states is not 0 on Fermi energy.

13.13.16 Q. Can I calculate the dielectric constant from Quantum ESPRESSO (band calculation)?

A. See *Q. Can I calculate dielectric constant from Gromacs or LAMMPS (Molecular Dynamics Calculation)?*.

13.13.17 Q. How do you set up the type of functionalities in Quantum ESPRESSO?

A. In Quantum ESPRESSO, since a pseudopotential file is created for each function, the function is basically determined when the pseudopotential file is selected. Some functions (e.g., HSE, vdw functions) select the pseudopotential file created by the base function (e.g., PBE in the case of HSE) and then use the input_dft keyword to override the function's settings.

13.13.18 Q. Why does the cell size structure optimization in Quantum ESPRESSO result in discontinuous changes or energy increases in the final structure energy?

A. The reason for the slight discontinuity in the energy change at the end is that Quantum ESPRESSO is reworking the plane wave set to use only the last calculation to avoid problems caused by the Pulay pressure.

This energy jump can be reduced to some extent by increasing the cutoff energy.

If the final structure differs significantly from the initial structure, continue and run the structural optimization calculation again.

13.13.19 Q. Quantum ESPRESSO terminates normally for systems with a small number of atoms, but for large systems it terminates abnormally with an error such as "cannot allocate . . . ". for large systems. What can I do about this?

A. Please refer to the FAQ on memory usage in the official QE documentation.

13.13.20 Q. Why do the values for Total DOS appearing in Projected DOS (PDOS) and DOS appearing in Density of States (DOS) differ in Quantum ESPRESSO?

A. In Quantum ESPRESSO, PDOS is calculated by projecting the electronic states obtained in the plane-wave basis onto the atomic basis, but this projection is not perfect. This is a property of plane wave basis DFT codes in general, not just Quantum ESPRESSO.

13.13.21 Q. When I set Hubbard U in Quantum ESPRESSO for structural optimization, it terminates abnormally with the error message "NR-step length unreasonably short". What can I do about this?

A. If the version of Quantum ESPRESSO is 5 series, the force calculation for Hubbard U is not implemented and this error occurs. Therefore, upgrading to Quantum ESPRESSO version 6 or later will solve this problem.

13.13.22 Q. Why does the number of cycles required for convergence of SCF calculations before and after Quantum ESPRESSO 6.6 change so much?

A. One reason is that the default value of diago_david_ndim was changed from 4 to 2 in Quantum ESPRESSO 6.6 and later. Even after QE6.6, if diago_david_ndim is explicitly set to 4, the behavior is similar to earlier versions.

13.13.23 Q. When I use hybrid functional (e.g. HSE) in Quantum ESPRESSO, the band structure collapses. Is there a way to deal with this?

A. Unfortunately, as of version 7.1, Quantum ESPRESSO itself does not support band structure calculations with hybrid functionals (mixed functionals). It is possible to do so by post-processing using an external module (such as Wannier90), but Winmostar (as of V11.6.4) does not support such post-processing, so users must perform post-processing on Winmostar's output results themselves. The user must perform the post-processing on the Winmostar output.

13.13.24 Q. Unnecessary bonds are displayed while modeling the system or when reading the calculation results. Or the bonds are not displayed. How can I fix this?

A. *See this FAQ* for more information.

13.13.25 Q. When setting up workflow and keywords in Quantum ESPRESSO, even if the cell is not converted to a primitive cell, it is converted to a primitive cell when the calculation is executed.

A. Do not check "Use Bravais-lattice index" or "Set ibrav = N and celldm".

Q. Is there any scaling factor proposed for first-principles calculations (e.g. Quantum ESPRESSO) such that the vibrational spectra (IR, Raman) obtained from calculations such as quantum chemical calculations (e.g. GAMESS, Gaussian) are matched to experimental values?

A. It seems to be not proposed. The reason is that quantum chemical calculations (Gaussian basis) have only Hamiltonian (including functional) and basis functions as parameters, whereas ab initio calculations (plane-wave basis pseudopotential method) have many parameters, and it is difficult to propose a generic scaling factor that takes them into account. There is no guarantee that this will work, but if you are in a situation where you can compare experimental and calculated values, you may want to construct your own scaling factor for a particular combination of pseudopotential, k-point density, cutoff energy, and functional.

13.13.26 Q. When I run a calculation on a local machine with MPI enabled in OpenMX, I get the error tcp_peer_send_blocking: send() to socket 12 failed: Transport endpoint is not connected.

A. For issues specific to Cygwin's OpenMPI, go to Windows Settings - Network and Internet - Change Adapter Options and disable the network adapter you are not using. Also, OpenMX recommends that you use OpenMP on the local machine.

13.13.27 Q. After running a structural optimisation calculation with a change in cell size in OpenMX, if I run a continuation job with SCF.Restart=On, the standard output shows Failed (3) in reading the restart files, <Restart> Could not find restart files.

A. The error message indicates that the number of charge density meshes in the restart file is different from the number of meshes you are about to calculate. This can happen if the cell size changes significantly during the structural optimisation calculation. In such cases, a new SCF calculation must be performed after the structural optimisation calculation.

13.14 Addons

13.14.1 Q. When calculating the Hansen solubility parameter of a polymer using the solubility parameter calculation module, the output value changes depending on how the repeating structure (monomer) of the polymer is taken.

A. It is because of the group contribution algorithm implemented. When searching for an atomic group, the search is started from the largest atomic group. It is recommended that functional groups that seem to be important be included in the repeating unit.

13.14.2 Q. The value of the Hansen solubility parameter obtained using the solubility parameter calculation module is significantly different from the literature value.

A. The solubility parameter calculation module outputs Hansen solubility parameters using the group contribution method trained by the neural network using various literature values as learning data. Therefore, it does not return exactly the same value as the literature value. Please note that the unit of the solubility parameter differs depending on the literature.

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