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# **Winmostar™ User Manual**

***Release 10.1.0***

**X-Ability Co., Ltd.**

**Apr 02, 2020**

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This manual describes the operation method of each function of Winmostar (TM). The latest version of this document is available from [Official site](#). If you are using Winmostar (TM) for the first time, please refer to [Quick Manual](#). If there is an uncertain point or it does not move as expected, please confirm [Frequently asked questions · Troubleshooting](#) which is updated from time to time. For specific operational procedures for each purpose, such as chemical reaction analysis and calculation of specific physical properties, see [various tutorials](#).

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). For molecular modeling function it has been confirmed to operate up to 100,000 atoms. The function of MD calculation has been confirmed in a larger system.

### 1.1 About quotation

When announcing data created using Winmostar (TM) in academic presentations, articles, etc., please describe the Winmostar (TM) main body as follows, for example.

*Winmostar V10, X-Ability Co. Ltd., Tokyo, Japan, 2020.*

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:\winmos10\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.

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**Note:** Indicates supplementary matter.

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**Warning:** Indicates notes.

## 1.3 The libraries used

Winmostar uses the following libraries and softwares for some processings.

### OpenCubeGen

```
OpenCubegen
  Cube Generation for Gaussian, Gamess, and MOPAC packages
Author
  Mitsuo Shoji
  mitsuo.shoji@apchem.nagoya-u.ac.jp
  Home page: http://www.geocities.jp/dr_mitsuos/index.html
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### FermiSurfer

```
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**libssh2 1.8.0**

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**openssl 1.0.2m**

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### Delphi/Pascal Wrapper around the library "libssh2"

```

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### 2.1 Software requirements

Winmostar supports the followings operating systems.

- Windows 10
- Windows 8
- Windows 7

In the case of Windows Server, please obtain the FREE edition or trial and use it after verifying the operation. For macOS and Linux, please use Winmostar after installing Windows OS on virtual machine such as VirtualBox. A version that works natively in these environments will be developed in the future. If you run the job on a machine other than the terminal where Winmostar is installed ( *remote server*), *setup method* introduces the procedure for CentOS. Basically, any OS such as Ubuntu can be used as long as it has the function.

- You can connect to that machine using scp or ssh.
- *Job scheduler* supported by Winmostar works.
- The solvers called from Winmostar can be installed or have already been set up on that machine.

### 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
- HDD: 4 GB or more free space

It can be used with general office work, PC surfing, etc. 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 Installing Winmostar and solvers

If you encounter an unexpected situation during installation, check [Frequently asked questions · Troubleshooting](#).

1. Download the installer `winmostar0_setup_X.X.XXexe` (where X.X.X indicates the version) from [Download](#), and execute it
2. Specify installation folder (the default location is `C:\winmos10`), and start installation, then a shortcut is created on the Start menu and on the desktop.

**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.
- When text or other items are enlarged or reduced in display setting, some display may be distorted.

---

**Note:**

- 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.
- If you want to inherit other Winmostar settings already installed, please copy the file under the `UserPref` folder in the installation folder.

- 
3. If you do not have a license code, please review the version to be used in [Features](#) and register or purchase the license code from the link below.
    - [FREE](#) edition
    - [STUDENT](#) edition
    - [PROFESSIONAL](#) edition
    - [PROFESSIONAL](#) edition (trial)
  4. In the case of a new installation, start Winmostar and set the license code in the dialog that appears at the first boot.
  5. Install the solver to be used on the Windows PC (local machine) on which Winmostar is installed by the following link destination procedure.
    - [GAMESS installation manual for Windows](#)
    - [NWChem installation manual for Windows](#)
    - [LAMMPS installation manual for Windows](#)
    - [NAMD installation manual for Windows \(only Japanese\)](#)
    - [Quantum ESPRESSO installation manual for Windows](#)
    - [FDMNES installation manual for Windows \(only Japanese\)](#)

---

**Note:**

- Gromacs, Amber, MODYLAS, OpenMX will be included in the `cygwin_wm` to be installed in the next step.

6. To use the MD, Solid Packages, and some other functions, build a Cygwin environment for Winmostar (called *cygwin\_wm*) by one of the following procedures.
  - (Recommended) [Installing pre-built cygwin\\_wm](#)
  - (for advanced users) [Building cygwin\\_wm from scratch](#)
  - [When using Windows Subsystem for Linux instead of Cygwin \(beta version\)](#).
7. If necessary, exclude the installation folder of Winmostar and *cygwin\_wm* from the monitoring target in the setting of the anti-virus software being used.
8. When you submit a job to a remote server (called *remote job*), check whether *the job scheduling software* is installed on that server. If it is not installed, install TORQUE by the following procedure.
  - [Installation guide for Linux](#)
9. When you submit a remote job, install the solver to be used for the server by the following procedure
  - [Installation guide for Linux](#)
  - GAMESS installation manual for Linux (only Japanese)
  - Gromacs installation manual for Linux (only Japanese)
  - LAMMPS installation 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)
10. Now, you are ready to use Winmostar. Please refer to [Tutorials](#) if necessary

Although not required, it is recommended to change the setting to display the extension of each file on Explorer.

**For Windows 7:**

- Open Explorer.
- Press **Alt** key.
- Open the *View* tab of the *Tools* → *File Explore Options* menu.
- Make sure that *Hide extensions for known file types* is unchecked.

**For Windows 8, 10:**

- Open Explorer.
- Open the tab *View*.
- Make sure *File name extension* is checked.

## 2.4 Update

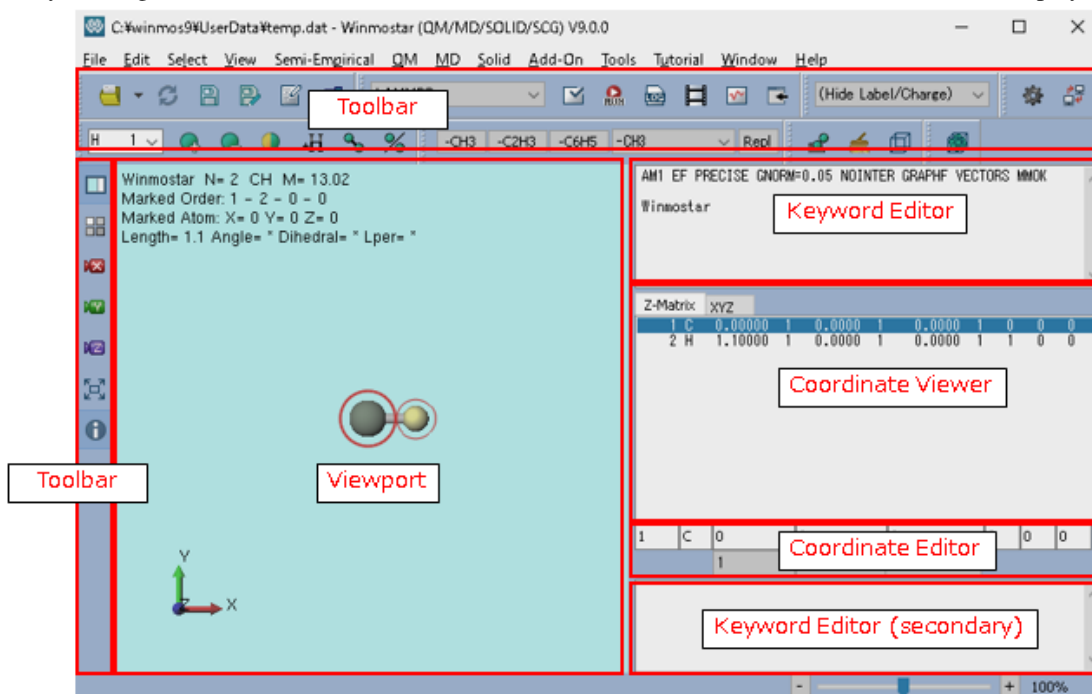
Updates and version upgrades are possible in the same way as installation. When installing by overwriting, close Winmostar before overwriting before installing.

## 2.5 Uninstalling Winmostar

You can uninstall by deleting Winmostar installation folder and shortcut.

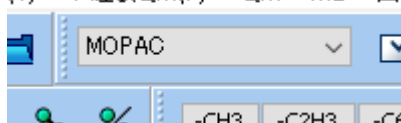
### 3.1 Role of each part

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.

**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*.

**Keyword Editor** The contents set in the configuration window of each solver are displayed. By default MOPAC settings are displayed.

**Coordinate Viewer** The coordinates of each atom of the molecular structure displayed in Viewport are displayed. You can switch the display format and output format on the upper tab. By default *Z-Matrix* is selected. In a state where no group is selected, the line selected in Coordinate Viewer matches the atom with the marker (red circle). Group selection (blue circle) can be done by selecting multiple lines by `Ctrl+left click` or `Shift+left click`.

**Coordinate Editor** You can enter the coordinates (Z-Matrix or XYZ format) of the atom with the marker (red circle) and the optimization flags.

**Keyword Editor (secondary)** It is basically the same as *Keyword Editor*, but the contents entered here will appear after the coordinates in the input file of the solver. It is used only for some solvers such as GAMESS and Quantum ESPRESSO.

## 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	Replace with fragment	Zoom in/out
Shift	Select molecule or unselect	Pan camera	Delete atom	
Ctrl	Select each atoms or unselect	Select atoms in rectangle area		

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

### 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

---

 Basic Operation Flow
 

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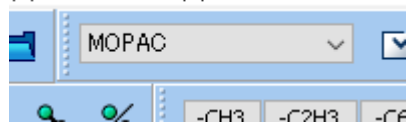
Here, we introduce the basic operation flow of quantum chemical calculation, molecular dynamics calculation, or first principles calculation using Winmostar.

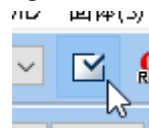
## (1) Create initial structure

Follow the procedure described at *Structure Building* to create the system you want to calculate.

## (2) Configure simulation conditions

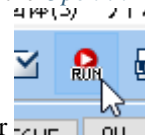
Select the solver you want to use at *Sovlver* pull-down menu

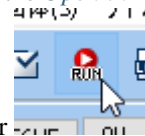


, and click *Configure* button . For some solvers, if you put a pointer over the keyword column, the meaning of that keyword will appear.

## (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 .

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 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*



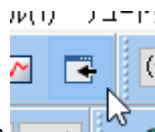
button on the tool bar to set up connection to the server. After that, press the *Send & Submit* button on the *Submit Remote Job* window to save and transfer (send) the input file and register the job at the remote server (submit) at once. Registered jobs are executed in order on the remote server. 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. For details, see *Submitting remote job*.

#### (4) Confirm log



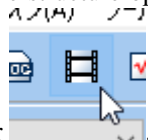
Press the *Open Log File* button on the toolbar. You are asked which file to open. If the input file of the calculation you want to check log is displayed in the main window, open the file selected by default. The log file is displayed with a text editor, then check whether the job has ended normally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

#### (5) Display and analyze physical quantities



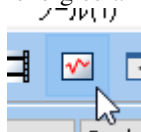
If the job has ended normally, press the *Analysis* button on the toolbar and select the menu of physical quantities you want to display. You will be asked which file to open, so choose as appropriate. As with log checking, the one associated with the file displayed in the main window is selected by 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 *Extending Simulation* in the configure window.
- For Quantum ESPRESSO, set *Continue to Output Directory* 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.

## 5.1 Modelling a single molecule

Select one of the following methods.

- Open a various format file at *Open* or drag and drop to the main window.
- Read SMILES format string from *File* → *Import* → *SMILES*.
- Build molecular structure from scratch on the main window.

Select the appropriate operations from *Edit menu*.

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.
- For polymers, the entire molecule can be modeled directly, but it is more efficient to use *MD* → *Polymer Menu*.

- To create the crystal structure, slab model or cluster model, execute *Crystal Builder*, *Cleave Plane*, *Insert Vacuum* or *Build Cluster Model*.

## 5.2 Assigning point charges

For MD simulation of organic compounds, point charge must be set by the following methods. When using the default AM1/BCC charge, it is not necessary to explicitly set charge. Also, for water molecules, the charge value of the selected water model is automatically applied. When using charges other than AM1/BCC, create one molecule by the procedures in *Modelling a single molecule*, assign electric charge in the following way, and then check *Use user-defined charge* at *Force Field* tab of configure window. The assigned charge can be displayed and confirmed by changing *View* → *Label/Charge*.

- Assign Gasteiger charge.
  - Go to *MD* → *Assign Charges* → *By Acptype*. For ions, enter the charge into *Total charge [e]*. The AM1/BCC charge is also explicitly assigned in a similar procedure.
- Assign RESP charge.
  1. Go to *QM* → *GAMESS* → *Configure* → *Easy Setup*, check *ESP/RESP* and the other settings. In the case of ions, enter the charge into *ICHARG*.
  2. Close the *Easy Setup* window with the *Close* button and press the:guilabel:Run button in the configure window to execute the calculation.
  3. When GAMESS calculation is finished, obtain RESP charge with *QM* → *GAMESS* → *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 *Charges (arc)*.
  - For Quantum ESPRESSO, use *Solid* → *Quantum ESPRESSO* → *Lowdin Charge*.
  - Otherwise, open the log file in the main window.
- Enter values for each element.
  - Use *MD* → *Assign Charge* → *By Manual Entry*.
- 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*.
- In the case of polymers, it takes time to directly calculate the AM1/BCC or RESP charge of the whole molecule. So use *MD* → *Polymer Menu*.

## 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. At *Create/Edit Cell* set *Create* → *Distance* and press *Create* button. After fine-tuning the size of the cell, press *OK* button.

## 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 in mol2 format.
4. Procedures 1 to 3 are performed for all molecular species to be calculated.
5. Select *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 mol2 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 high, it may fail to create the system. Start with a slightly lower density and gradually compress to the desired density and pressure with constant pressure calculation.
  - Use *Modify Selected Group* → *Replicate Group*, *Create/Edit Cell* and *Append* when *cygwin\_wm* is not installed or it is difficult to arrange with *Solvate/Build Cell*.
- 

## 5.5 Creating polymer melt system

1. Create repeating units (called monomers here) of the polymer you want to calculate (See *Modelling a single molecule*).
2. In the case of MD simulation, assign point charges (See *Assigning point charges*).
3. In *Viewport*, left click on the two atoms to be connected with the next monomers and register it as a monomer at *Register Monomer*.
4. Depending on the structure of the polymer you want to create, execute *Homo Polymer builder*, *Block Polymer Builder* or *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 monomer at *Register Monomer* and execute *Homo Polymer builder*.
- 

5. Execute the operation of *Polymer Cell Builder* to create a simulation cell.
6. If the small molecules are dissolved in the polymer, set the density to a smaller value at procedure 5. Next, prepare a structure of the small molecule (see *Modelling a single molecule* and *Assigning point charges*) and save it in mol2 format. Then, execute *Insert Molecules* and select the mol2 file for the small molecule.

## 5.6 Creating gas-liquid interface

1. Create a liquid phase (see *Creating a small molecule liquid system*).
2. At *Create/Edit Cell*, set *Expand* → *Width* and *Axis* and press *Expand* button. The size to be expanded is equivalent to the size of the gas phase. Then press the *OK* button.

---

**Note:**

- When expanding the structure of liquid phase after relaxation by MD calculation, there are many atoms with coordinates outside the simulation cell. So select *Wrap Around Cell Boundary* before expanding. Select *Wrap for each molecules* or *Wrap for each atoms* for organic (molecular) or inorganic systems, respectively.
-

### 6.1 File menu

#### 6.1.1 New

It returns to the state immediately after startup.

---

**Hint:** The shortcut is `Ctrl+N`.

---

#### 6.1.2 Open

Read the molecular structure from file into the main window. It corresponds to the format of various software.

---

**Hint:** The shortcut is `Ctrl+O`.

---

#### 6.1.3 Open Recent File

Open a recently opened file.

#### Clear History

Empty the history of recently opened files.

### 6.1.4 Open Project

Open project file with wmpj extension.

---

**Hint:** The shortcut is `Ctrl+Alt+O`.

---

### 6.1.5 Open Recent Project

Open a recently opened project file.

#### Clear History

Empty the history of recently opened project files.

### 6.1.6 Reload

Load the file displayed in the title of the main window again.

### 6.1.7 Append

Add the molecular structure of the selected file to the molecular structure displayed in the main window.

### 6.1.8 Save

Overwrite and save the molecular structure displayed in the main window. For details, see *Save As*.

---

**Hint:** The shortcut is `Ctrl+S`.

---

### 6.1.9 Save As

Save the molecular structure displayed in the main window as a different name. 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.

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`

---



### 6.1.10 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 is also executed at the same time. A working folder named \*\_smiles\_tmp will be created as an intermediate file.

### 6.1.11 Export

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

#### SMILES

It outputs the molecular structure displayed in the main window as SMILES formatted character string. It can not be used when multiple molecules are displayed in the main window. I use OpenBabel on Cygwin.

**Warning:** To use this function, *cygwin\_wm 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, *cygwin\_wm setup* is required.

#### Image

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

#### VRML

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

#### CHARMM crd File

Outputs the contents displayed in the main window in crd format for CHARMM.

### 6.1.12 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.

---

### 6.1.13 Show in Explorer

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

### 6.1.14 Coordinate Format

Specify the display format in *Coordinate Viewer* and the coordinate format when saving the file in MOPAC, GAMESS, Gaussian, NWChem format.

---

**Hint:** You can also switch on tabs at the top of *Coordinate Viewer*.

---

### 6.1.15 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 Around Axis(2 Marked Atoms)* 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*.

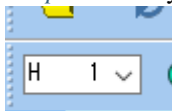
## 6.2.4 Select Element for Editing Ops


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

## 6.2.5 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  Winmostar of Toolbar.

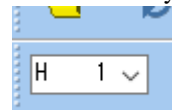
---


**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  Winmostar 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.

## 6.2.6 Delete atom

Delete the atom marked with *marker*.

---

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

---

## 6.2.7 Move atom

### Translate

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

---

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

---

### 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.

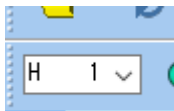
## Change Dihedral

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

## 6.2.8 Atom Properties

### Element

The element of the selected atom is changed to the element selected by the *Select element for editing ops*



pull-down menu *Winmostar* 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 of the selected atom. 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 charge (User charge) or spin density value of the selected atom. If a group is selected, all the atoms selected in the group will be covered.

---

**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.

## 6.2.9 Add Dummy Atom

By effectively arranging dummy atoms, it is possible to increase the efficiency of structure optimization calculation and IRC calculation using Z-Matrix, or to avoid errors derived from Z-Matrix.

### Along 2 marked atoms

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

### To Center of Mass of Selected Group

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

## 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

We will automatically add hydrogen to all atoms.

---

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

---

### To marked atoms (Auto)

Add one hydrogen atom to the atom with the marker.

---

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

---

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

Make 1 to 3 hydrogen added to the atom with the marker.

### 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, *cygwin\_wm 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, *cygwin\_wm 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).

---

**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* .

### 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 Around Axis(2 Marked Atoms)

Rotate a group-selected structure around a vector between two atoms with *two markers (red circle, red circle)*

---

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

---

#### 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 group selected structures to orient to a specific axis or plane. 2 atoms with markers, if oriented in a specific axis, or 3 atoms. if oriented in a specific plane, must be included in the group selected structure (It can be confirmed by *Marked Order:* in the upper left of *Viewport*).

### 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.

### Quick Optimization

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

---

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

---

### 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

Set the optimization flag of all components of the group-selected structure to “0” (fix) or “1” (free). If you want to control more finely, select *Edit* → *Change Atom Property* → *Optimization Flags*.

---

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

---

## 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.

## 6.2.18 Automatically Adjust Atoms/Bonds

### Quick Optimization

We will perform structure optimization using molecular force field.

---

**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.

---

### 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.

## 6.2.19 Change Distance/Angle Between Marked Atoms

Enter and change the distance, angle, or dihedral angle between 2 and 4 atoms with markers (red circles) (you can check with the *Marked Order:* at the top left of *Viewport*).

## 6.2.20 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 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.

## 6.2.21 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.

**Warning:** To use this function, *cygwin\_wm setup* is required.

### 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.

### Invert X/Y/Z Axis

Inverts the specified axis and recreates the coordinate system.

## 6.2.22 Chirality

### Invert Chirality

Convert the molecular structure displayed in the main window to an enantiomer. The sign of the x coordinate is inverted.

### Generate Enantiomer

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

### 6.2.23 Create/Edit Cell

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 *Box 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 *Change Density*.
  - If you want to return atoms outside the simulation cell to the simulation cell before editing, use the *Wrap Around Cell Boundary* function.
- 

### 6.2.24 Delete Cell

Delete Cell.

### 6.2.25 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 the *Display* → *Wrap Around Cell Boundary* function, only the display changes and the coordinates do not change, but in this function the coordinates actually change.
- 

### 6.2.26 Change Density

Specify to change the density and simulatively expand or shrink simulation cell and atomic coordinates. The coordinates of each atom are scaled with respect to the center of gravity of the molecule, and the relative position within the molecule does not change.

### 6.2.27 Edit Charge

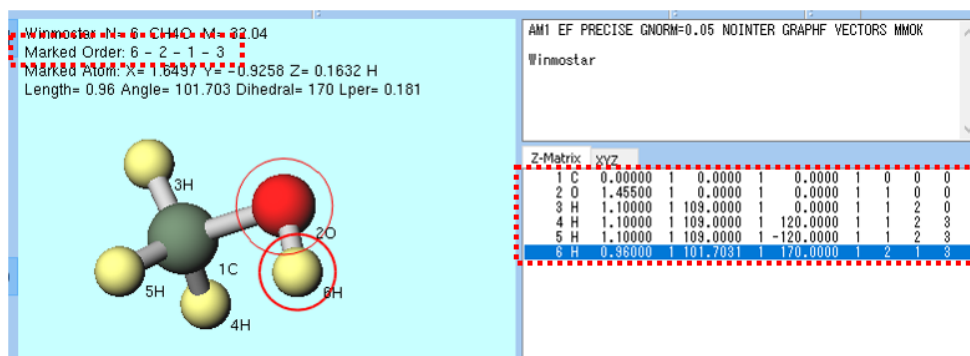
Specify the type of charge and set it to user charge. You can also delete specified charges.

## 6.3 Select menu

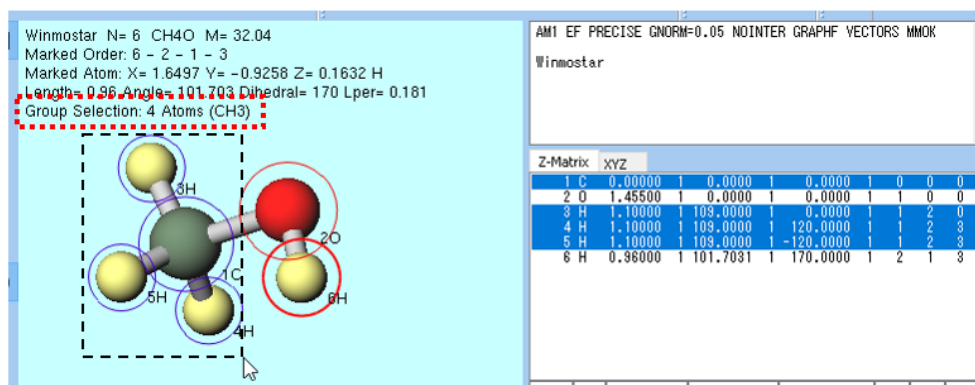
It is a menu related to the function of selecting atoms or molecules.

### 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*.

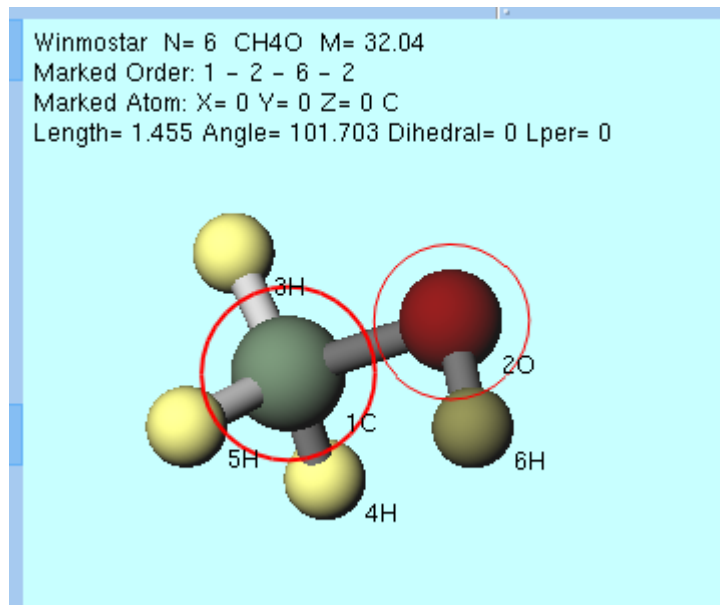


The method using group selection of the blue circle is mainly used for operations on multiple atoms. You can select a group by Ctrl+left drag, Ctrl+left click or Shift+left click in *Viewport*. You can also select a group by using the function of *Select* menu. In the example of the methanol molecule in the figure below, after Ctrl+left drag around the CH<sub>3</sub> (methyl) group, it can be confirmed that the CH<sub>3</sub> 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



*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 Around Axis(2 Marked Atoms)* is selected, the group with the last marker on the CH3 group is automatically selected (highlighted on the screen).



### 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 <i>Apply</i> button.
moleid 1-3	Select 1, 2 and 3rd molecules. You can see the numbers of molecules in the list under <i>Apply</i> 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 <i>Apply</i> button.
charge 0.5	Select the atoms whose atom name is CA. A tolerance of $\pm 0.1\%$ is provided.
resname GLY	Select the atoms whose residue name is GLY.
name CA	Select the atoms whose atom name is CA.

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.

### 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 Register Selected Group

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

### 6.3.10 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)*.

### 6.3.11 Import Groups from Index File (ndx)

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

### 6.3.12 Export Groups to Index File (ndx)

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

### 6.3.13 Add Selected Group to Index File (ndx)

Add the group selected group to the specified `ndx` file.

## 6.4 View Menu

### 6.4.1 Show Keywords & Coordinates Areas

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



### 6.4.2 Show Multi-View

Make Viewport three views.

### 6.4.3 Reset View

Return the camera to the default position.

### 6.4.4 Align View

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

### 6.4.5 Zoom In/Out

Expand or reduce the field of view.

### 6.4.6 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.

### 6.4.7 View Marked Atom

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

### 6.4.8 Pan

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

### 6.4.9 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.

#### View

Drag left in the main window to rotate the display.

### 6.4.10 Perspective

If checked here, perspective is applied to Viewport.

### 6.4.11 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*.

### 6.4.12 Items

Check the items to be displayed in Viewport.

### 6.4.13 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)
Show Number&Element	It displays the serial number of the atom and the element name.
Show Mulliken Charge	Displays the Mulliken charge read when various log files are opened.
Show ESP Charge	Displays ESP or RESP charge read when various log files are opened.
Show Lowdin Charge	Displays Lowdin charge read when various log files are opened.
Show User Charge	<i>Edit</i> → <i>Chnge Atom Property</i> → <i>Charge/Spin Density</i> and <i>MD</i> → <i>Assign Charges</i> 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 <i>Edit</i> → <i>Change Atom Property</i> → <i>Charge/Spin Density</i> .
Show Difference Density	Show Difference Density

### 6.4.14 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.

## 6.4.15 Molecular Representation

Select the expression method (model) of the molecule.

## 6.4.16 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.

## 6.4.17 Winmostar Viewer

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

## 6.4.18 External viewer

Displays the structure displayed in Viewport with various external programs.

### Jmol

Start Jmol.

### VRML

Output the VRML format file and start the VRML viewer.

### 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.

### 6.4.19 Copy Image

Copy the image of Viewport to the clipboard.

## 6.5 Semi-Empirical QM → MOPAC menu

It is a menu related to MOPAC. MOPAC 6 and MOPAC 7 are bundled with Winmostar. When using other MOPAC please purchase MOPAC body separately from distributor and set the path in Preferences window.

### 6.5.1 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
PM3	MOPAC 6, MOPAC 7, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012
RM1	MOPAC 2007
AM1 EXTER-NAL=RM1.rm1	MOPAC 7.1, MOPAC 93, MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012
PM5	MOPAC 2002, MOPAC 2006
PM6	MOPAC 2007, MOPAC 2009, MOPAC 2012
PM7	MOPAC 2012
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
MNDO-d	MOPAC 97, MOPAC 2000, MOPAC 2002, MOPAC 2006, MOPAC 2009, MOPAC 2012

**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 orbitals 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.

## 6.5.2 Import Keywords

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

### 6.5.3 (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. Difference of *Run (1) MOP6W70*, *Run (2) MOP7W70*, *Run (3) MOPACX* is the program path to start MOPAC. You can change the program path with *Tools* → *Preferences* → *Program Path*. Default setting *MOP 6W 70* is MOPAC 6, *MOP 7 W 70* is MOPAC 7, both of which are built in Winmostar. *Run (3) MOPACX* is assumed to be used by specifying a program such as MOPAC 2012. 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	In the file outputted by specifying the keyword GRAPH, Contains information used to draw molecular orbits.
Working Directory water_mop_temp\	Working directory.

### 6.5.4 Open Log File (out)

Open out file in a text editor.

### 6.5.5 Open Log File (arc)

Open arc file with a text editor.

## 6.5.6 Animation

### Optimization (arc)

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

### IRC, STEP (out)

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

## 6.5.7 Analyses

### MO & Density (mgf)

Select the mgf file and display the molecular orbital. GRAPHF must be set on *keyword*. Refer to *Energy Level Diagram window*, *MO Plot window* for how to operate the subwindow.

### Charges (arc)

Select arc file and display charge, dipole. 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.

## 6.5.8 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 Semi-Empirical 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](https://winmostar.com/jp/manual_third_party/cndos_man.pdf)>. The CNDO/S program (: file: *cn-dosw.exe*) has been compiled with gfortran.

### 6.6.1 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.

- $Z_a * Z_b / 1$
- $Z_a * Z_b * \gamma_{ab}$

**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.

### 6.6.2 Import Keywords

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

### 6.6.3 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
Ist file water.lst	Calculation log file.
Working Directory water.cnd_temp\	Working directory.

### 6.6.4 Open Log File (Ist)

Open the Ist file with a text editor.

### 6.6.5 Analyses

#### UV-Vis

Select Ist file and display UV-Vis spectrum and molecular orbital. Refer to *UV-Vis Spectrum window*, *Energy Level Diagram window*, *MO Plot 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 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 the charge.

**A LOT** Specify multiplicity.

**SCFTYP** Specify SCF calculation method.

- RUNTYP** Select the calculation purpose.
- COORD** Specify the format of molecular structure data.
- MAXIT** Specify the upper limit of the SCF calculation iteration number.
- NZVAR** Specify the number of internal coordinates.
- 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)
- ECP** Specify Pseudopotential.
- 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
- Others** Fill in other keywords.

#### **\$BASIS**

- Basis Set** Select the basis function system. It is reflected in GBASIS, NGAUSS, NDFUNC, NFFUNC, DIFFSP, DIFFS.
- GBASIS** Basic set of basis functions
- NGAUSS** Number of Gaussian functions
- EXTFIL** Read the basis function from an external file.
- NDFUNC** Number of added d-polarization functions
- NFFUNC** Number of added f-polarization functions
- NPFUNC** 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** Calculation time limit (default 600 minutes)
- MWORDS** Memory usage (default 1 MW)
- 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.

**Others** Fill in other keywords.

**Z-Matrix** Make Z-Matrix settings.

**DFT****\$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)

**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.

## 6.7.2 Import Keywords

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

## 6.7.3 Import from Punch File

### Import \$VEC

Import \$VEC from the punch file.

### Import \$HESS

Import \$HESS from the punch 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, output format of coordinates changes according to the selection of *Coordinate Format* choice (*Z-Matrix* or *XYZ*) and *Z-Matrix / XYZ* tab of *Coordinate Viewer*. Difference between *Run (1) GAMESS* and *Run (2) GAMESS* is the program path of GAMESS to start. You can change the program path with *Tools* → *Preferences* → *Program Path*. *Run (1) GAMESS*, *Run (2) GAMESS* is supposed to set Firefly and GAMESS of different versions etc. and use them while using them according to the scene It is. 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 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 window*.

## 6.7.7 Analyses

### MO, UV-Vis, Charge & NMR

Obtain information on molecular orbital, UV-Vis, charge, NMR from the out file information and display it. Information on the charge read can be displayed in Viewport by selecting *View* → *Labels/Charges* → *Show Mulliken Charge* and so on. Refer to *Energy Level Diagram window*, *MO Plot window*, *UV-Vis Spectrum window*, *NMR Window* for how to operate the subwindow.

## IR/Raman

Select the out file and display the vibration spectrum (IR or Raman spectrum). 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 load is required to be outputted from the calculation executed by choosing *RESP/ESP* setting in *Configure* → *Easy Setup*. Spin multiplicity is handled on the premise of 1. Internally, we create a file that can be read by Antechamber from punch file information and calculate RESP charge using Antechamber.

**Warning:** To use this function, *cygwin\_wm setup* is required.

## 6.7.8 PDB

### Edit PDB File

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

### FMOutil

Start FMOutil.

## 6.7.9 Paired Interacting Orbitals

Paired Interacting Orbitals Executes analysis. For details, see *PIO analysis window*.

## 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 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.

#### Link0

**#nproc=n** Specify the number of processors.

**#Chk=file** Specify the checkpoint file.

**# Mem = n** Specify the amount of dynamic memory in words. It is also possible to specify units of KB, MB, GB, KW, MB, GW. (Default: 6 MW)

**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.

**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.

**oniom** Perform ONIOM 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 orbitals and 5 virtual trajectories. Also output density matrix and Mulliken electron density analysis.

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

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

**opt** Perform structure optimization.

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

**opt=modredundant** redundant Add, delete, and modify the definition of internal coordinates (including search and binding 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

**irc** Track reaction path

**irc=(maxpoint=20, stepsize=20t, calcfc)** It tracks the reaction path. Specify the number of points on the route and the step size. Calculate the force constant for the first time

**MaxCyc** Sets the maximum number of optimization steps.

**Freq**

**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** Hartree-Fock Raman intensity is not obtained by analytic frequency calculation.

**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.

**Charge** Specify the value of the charge.

**Multiplicity** Specify multiplicity.

**for example,**

**for example,** Calculate excited state energy using time-dependent Hartree-Fock or DFT method

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

**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 and perform all calculations in Z-matrix orientation.

**guess=read** Read initial wave function from checkpoint file

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

**Others** Fill in other keywords.

## 6.8.2 Import Keywords

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

### 6.8.3 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. When saving the input file, output format of coordinates changes according to the selection of *Coordinate Format* choice (*Z-Matrix* or *XYZ*) and *Z-Matrix / XYZ* tab of *Coordinate Viewer*. 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 directory water_gau_tmp\	Working directory.

The job is run through *Winmostar Job Manager*.

### 6.8.4 Open Log File (log/out)

Open the log file with a text editor.

### 6.8.5 Animation

#### Optimization

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

#### IRC/modred

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

### 6.8.6 Analyses

#### MO, UV-Vis, Charge & NMR

Information on molecular orbital, UV-Vis, charge, NMR from the information of the log file is acquired and displayed. Information on the charge read can be displayed in Viewport by selecting *View* → *La-*



*bels/Charges* → *Show Mulliken Charge* and so on. Refer to *Energy Level Diagram window*, *MO Plot window*, *UV-Vis Spectrum window*, *NMR Window* for how to operate the subwindow.

## IR/Raman

Select the log file and display the vibration spectrum (IR or Raman spectrum). Refer to *IR Spectrum Window* for how to operate the subwindow.

## Archive

Read high-precision coordinates of the archive part of Gaussian's output.

## 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.

**Warning:** To use this function, *cygwin\_wm setup* is required.

## 6.8.7 FormChk

G09W, G03W Activate Formchk of utility, create formatted .fch file from .chk file and display it.

## 6.8.8 Import Fchk (Cubegen) File

G09W, G03W Start Cubegen of the utility, read the .fch file and create the Cube file. If you do not have Cubegen, use OpenCubegen from Winmostar. For how to operate the subwindow, please refer to *MO Plot 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.

## 6.8.9 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 *MO Plot 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*.

## 6.8.10 Paired Interacting Orbitals

Paired Interacting Orbitals Executes analysis. For details, see *PIO analysis window*.

## 6.9 QM → NWChem menu

It is a menu related to NWChem. In order to use NWChem, you need to install NWChem separately. The method of installing NWChem is described in *Installing Winmostar and solvers*.

### 6.9.1 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

**Title** Specify the title.

**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.

**Exchange** Specify the exchange function of DFT.

**Correlation** Specify the DFT correlation function.

#### 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.

**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** Specify the file of the initial path. It is used for restarting calculations. Print\_Shift  
Prints the path for each specified step.

**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.

#### Advanced tab

**Memory** Specify the memory usage.

**Set tolguess** Specify the precision of initial guess.

**ECP** Specify the potential of ECP.

#### Geometry

**noautoz** Set not to convert internal coordinates.

**Other Settings** Describe other input elements.

## 6.9.2 Import Keywords

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

## 6.9.3 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. When saving the input file, output format of coordinates changes according to the selection of *Coordinate Format* choice (*Z-Matrix* or *XYZ*) and *Z-Matrix/XYZ* tab of *Coordinate Viewer*. 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 Directory water.nw_temp\	Working directory.

The job is run through *Winmostar Job Manager*.

### 6.9.4 Open Log File (out)

Open the out file in a text editor.

### 6.9.5 Animation

#### Optimization

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

#### NEB/String

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

### 6.9.6 Analyses

#### MO, UV-Vis, Charge & NMR

Obtain information on molecular orbital, UV-Vis, charge, NMR from the out file information and display it. Information on the charge read can be displayed in Viewport by selecting *View* → *Labels/Charges* → *Show Mulliken Charge* and so on. Refer to *Energy Level Diagram window*, *MO Plot window*, *UV-Vis Spectrum window*, *NMR Window* for how to operate the subwindow.

## IR/Raman

out Select the file and display the vibration spectrum (IR or Raman spectrum). After loading the IR spectrum from the out file of **RUNTYP = HESSIAN**, if you subsequently read the out Raman spectrum of **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.

## 6.10 MD menu

It is a menu on the molecular dynamics method. MD pack is necessary to use the function of MD menu. Also, with almost every feature *cygwin\_wm* 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 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.

**Add .mol2 File** Add molecules previously saved in .mol2 format to the system. After pressing the button, specify the location of the .mol2 file and enter the number of molecules to be added. If the number of molecules to be added is 1, specify whether to randomly arrange the molecule or to fix it at the coordinates written in the .mol2 file. When arranging ligand molecules cut out from a PDB file, it is usually fixed. When executing MD calculation using point charge (such as RESP charge) obtained from QM calculation etc., the point charge information must be described in the .mol2 file specified here.

**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<sup>3</sup>.

**Set Distance 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.

**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.

**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.

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

**Reset** Resets the settings in this window.

**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 *Append*. The internal operation is the same as *Solvate/Build Cell*.

## 6.10.3 Assign Charges Automatically

Automatically assign charges to multiple molecules. A working folder will be created with the current file name suffixed with `_charge_tmp`, and processing using Packmol will be performed in it.

**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, monoatomic 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

### By Acpype

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.

### By Manual Entry

You can directly specify the point charge value for each atom type for the molecular (crystal) structure displayed in the main window. It is mainly for solid system.

## 6.10.5 Polymer

See *MD* → *Polymer Menu*.

## 6.10.6 Interface Builder

See *MD* → *Interface Builder menu*.

## 6.10.7 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.

## 6.10.8 Gromacs

See *MD* → *Gromacs menu*.

## 6.10.9 LAMMPS

See *MD* → *LAMMPS menu*.

## 6.10.10 Amber

See *MD* → *Amber menu*.

## 6.10.11 MODYLAS

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

## 6.11 *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 *cygwin\_wm* is required.

### 6.11.1 Assign Force Field

Assign Force Field. The choices vary depending on the type of solver.

**Automatically assign parameters** Assign new force field parameters.

**(General)** Specify the force field of molecules other than proteins and water molecules. Internally, command: *acpype* is used for GAFF, OPLS/AA-L, in-house program is used for Dreiding. The setting of Dreiding is written in: file: *polymer/dreiding.lib.txt*.

**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/Ion)** Specify the force field of the protein. At this point, atoms assigned amino acid residue names in PDB and gro format are recognized as proteins. Internally **gmx pdb2gmx** is used.

<p><b>Warning:</b> This function can not be used when reading the molecular structure from a file not including residue name.</p>
---

**(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 edit the force field information with a text editor and customize it, first save this file using this function, and edit the top file for Gromacs and the data file for LAMMPS with a text editor etc. .
  - Next, in case of Gromacs, select *Use parameters written in topology file* and click *OK* button. Then you will be asked for the location of the top file, so open the top file you saved and edited earlier.
  - In case of LAMMPS, select *Use parameters written in file opened on main window* and click: *guiabel: 'Next> button*. Then, *:guiabel: 'Select force field* appears. Select the general type of force field to use and click the *OK* button.
- 

**Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** (For LAMMPS) Select when you want to use inorganic potential, ReaxFF or DPD. After pressing the *Next >* button, specify the type of force field to be actually used.

**Use parameters written in topology file** (For Gromacs) Select to execute MD calculation using the existing top file. The corresponding gro file must be open in the main window.

**Use parameters written in file opened on main window** (For LAMMPS) Select to execute MD calculation using the existing data file. The data file to be used must be open in the main window. After pressing the *Next >* button, specify the type of force field to use.

## 6.11.2 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* 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, *Assign 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.

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

**Preset** Specify the preset of the calculation condition. The preset contents can be confirmed from each keyword.

**# 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

**gene-well** 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** Specify the group to be temperature controlled (more than one can be set with a space delimiter).

**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.

**Lines-way** 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 pos-res.itp)

### 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** Specify the group to output in xtc format. By default, the entire system is targeted.

### 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.

### Other

**Other Parameters** Specify other settings based on the description of the mdp file.

### 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.

### Options

**Make a Backup of Working Directory** Select when backing up *working directory*.

**Restore Working Directory** Click to return *working directory* to its pre-execution status, such as when a continuous job ends abnormally.

**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 Extending 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.

### 6.11.3 Run

Run Gromacs. The execution method differs depending on the situation.

- **(Default) If *Extending Simulation* is unchecked and *Automatically assign parameters* is checked on *Assign Force Field***  
Create a new coordinate file (extension: gro) and topology file (extension: top) before starting the job.
- **If *Extending Simulation* is unchecked and *:guilabel:‘ Use parameters from topology file‘* is selected for *Assign Force Field***  
Start the job using the coordinate file (extension: gro) opened in the main window and the topology file (extension: top) specified at *Assign Force Field*.
- **When *Extending Simulation* is checked** The coordinate file ( gmx\_mdrun\_tmp.gro) and the topology file ( gmx\_tmp.top) in the working directory 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.
bat file water.gro.bat	This is a batch file for executing water.sh.
Working Directory water_gmx_tmp\	Working directory.

The following files are generated in the working directory. 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_tmp.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_tmp.mdp	It is a file that specifies calculation conditions.
gmx_tmp_mdrun.tpr	Generate from gro, top, mdp file It is an input file of mdrun.
gmx_tmp_mdrun.ndx	Index file for result processing.
gmx_tmp_mdrun.edr	Temperature, pressure, energy etc. were stored It is an energy file.
gmx_tmp_mdrun.gro	It is a gro file of the final structure.
gmx_tmp_mdrun.trr	It is a trajectory file.
gmx_tmp_mdrun.xtc	Compressed trajectory file.
gmx_tmp_mdrun.log	This is the log file of mdrun.

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**Hint:** \*\* Working directory \*\*

- A working directory 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 directory 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 directory 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 directory is `aaa_gmx_tmp`, it is `aaa_gmx_tmp1`.
  - **\*\* Directories without numbers are always up to date. \*\***

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The job is run through *Winmostar Job Manager*.

#### 6.11.4 Open Log File (log)

Open the log file (`* _ gmx_tmp gmx_tmp_mdrun.log`) of **gmx mdrun** with a text editor.

#### 6.11.5 Open Stdout File

Open the standard output (`* . Out`) of the shell script when running Gromacs with a text editor.

#### 6.11.6 Animation

Select the gro file and trr 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 window*.

#### 6.11.7 Energy Plot

Select theedr file output by Gromacs and display a graph of various thermodynamic quantities such as energy, temperature and pressure. Internally the **gmx energy** command is executed. Please see *Energy Plot window* for how to operate subwindow.

#### 6.11.8 Import Last Coordinate (gro)

`* _ gmx_tmp \ gmx_tmp_mdrun.gro`. When using this function, the file name of the main window does not change.

#### 6.11.9 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.

### 6.11.10 Run Sequential Job

Run Gromacs sequentially based on the contents of *Configure Sequential Job*.

### 6.11.11 Analyses

#### Radial Distribution Function

Select the trr, tpr, ndx file output by Gromacs and display the radial distribution function. Internally the **gmx rdf** command is executed. The radial distribution function is calculated between *Reference Group* and *Target Group*.

##### Definition

**Atom** Set the calculation target to atomic coordinates.

**Center of geometry** Make the calculation target geometric mean coordinates of the molecule.

**Center of mass** Make the calculation target the molecular centroid position.

##### 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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs and display mean square displacement and diffusion constant. Internally the **gmx msd** command is executed.

**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*.



**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 the trr, tpr, ndx file output by Gromacs and display the scattering function. Internally the **gmx saxs** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs, and display speed correlation function and vibration spectrum. Internally the **gmx velacc** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx file output by Gromacs and display distribution and histogram of relative dielectric constant or dipole moments. Internally the **gmx dipoles** command is executed.

**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.

**Histogram of total dipole momen** Plot the distribution of dipole moments for molecules belonging to the Target Group.

**Autocorrelation functino 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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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* command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs and display the density distribution. Internally the: command: *gmx density* command is executed.

**Group** The density distribution is output for the components that are checked here.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs and display the density distribution. Internally the **gmx freevolume** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs and display the density distribution. Internally the: command: *gmx density* command is executed.

**vdwtype** 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.

**Target group** Calculate the distance, angle, or dihedral angle using the NDX file selected in the Target Group.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD* → *Gromacs* → *Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 trr, tpr, ndx files output by Gromacs and display RMSD (mainly for proteins). Internally the **gmx rms** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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 the trr, tpr, ndx file output by Gromacs and display the turning radius (mainly for proteins). Internally the **gmx gyrate** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**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, ndx file output by Gromacs and display the Ramachandran plot of each amino acid residue. Internally the **gmx rama** command is executed.

**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*.

**Create Group** Register a new group from the atom name written in the gro file. To define atoms group selected in the main window as a group, use *MD → Gromacs → Add Selected Group to Index File (ndx)*. 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.

**First Frame** Specify the start time when trajectory is read in ps units.

**Draw** Execute the result analysis program and display the graph.

For how to operate the graph drawing area, see *How to operate the graph*.

### 6.11.12 Modify Trajectory File

For trajectory data of trr or xtc file output by Gromacs, perform operations such as thinning, rotation, calculation of spatial distribution function, etc. Internally the **gmx trjconv** command is executed. Start processing with *Execute* button.

**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 reference in *Roate and Trans*.

**Group for SDF** Specify which group to calculate SDF calculated when *Spatial distribution function* (SDF) is selected in *Postprocess*.

### 6.11.13 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 directory. 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 directory 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. If necessary, specify MPI parallel number at free energy calculation from *Options* button.
6. 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.
7. 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](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.
8. After calculating the free energy calculation, to display the result, select the *Import ER* menu.

### 6.11.14 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.

### 6.11.15 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 directories 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*.

### 6.11.16 Import BAR

The result of processing by *Start BAR* is displayed. After selecting the menu, please specify the output destination folder specified by *Start BAR*. In the background **gmx bar** is executed and the result is displayed. You can specify units for displaying energy in *Unit*. When you press the *Log* button, the log file of **gmx bar** is displayed. The displayed graph shows how the free energy varies between the state where the solute is not interacting with the solvent ( $\lambda = 0$ ) and the state where the solute interacts ( $\lambda = 1$ ).

## 6.12 MD → LAMMPS menu

It is a menu related to LAMMPS. The method of installing LAMMPS is described in *Installing Winmostar and solvers*.

### 6.12.1 Assign Force Field

Set the force field. The choices vary depending on the type of solver.

**Automatically assign parameters** Assign a new force field parameter.

**(General)** Specify the force field of molecules other than proteins and water molecules. Internally **acpype** is used for GAFF, OPLS/AA-L, in-house program is used for Dreiding. The setting of Dreiding is written in `polymer/dreiding.lib.txt`.

**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/Ion)** Specify the force field of the protein. At this point, atoms assigned amino acid residue names in PDB and gro format are recognized as proteins. Internally **gmx pdb2gmx** is used.

<p><b>Warning:</b> This function can not be used when reading the molecular structure from a file not including residue name.</p>
---

**(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 edit the force field information with a text editor and customize it, first save this file using this function, and edit the top file for Gromacs and the data file for LAMMPS with a text editor etc. .
  - Next, in case of Gromacs, select *Use parameters written in topology file* and click *OK* button. Then you will be asked for the location of the top file, so open the top file you saved and edited earlier.
  - In case of LAMMPS, select *Use parameters written in file in main window* and click *Next >* button. Then, *Select the type of force field* appears. Select the general type of force field to use and click the *OK* button.
- 

**Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** (For LAMMPS) Select when you want to use inorganic potential, ReaxFF or DPD. After pressing *Next >* button, specify the type of force field to be actually used.

**Use parameters written in topology file** (For Gromacs) Select to perform MD calculation using the existing top file. The corresponding gro file must be open in the main window.

**Use parameters written in file opened on main window** (For LAMMPS) Select to execute MD calculation using the existing data file. The data file to be used must be open in the main window. After pressing *Next >* button, specify the type of force field to use.



## 6.12.2 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.

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

**Preset** Specify the preset of the calculation condition. The preset contents can be confirmed from each keyword.

**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.

**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.

**Together** 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.

**Pressure Control** Specify how cells are moved during pressure control.

**Pressure** Specify the target pressure.

**Pdamp** Specify the time constant parameter of pressure control.

### 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).

**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** Choose a method to freeze motion of the center of gravity of the whole system during MD calculation.

**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.

**Constrain hydrogen atoms** We restrict hydrogen atoms by SHAKE method.

**SHAKE tolerance** Specify the truncation error of the SHAKE method.

**Calculate as rigid body** We treat molecules as rigid bodies.

**Set “box tilt large”** Specify the allowable degree of deformation of the simulation cell.

## 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.

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

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

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

**Calculate Thermal Conductivity** Output thermal conductivity calculated from autocorrelation function of atomic flow velocity.

**Calc Interval** Specify the calculation frequency of autocorrelation function in thermal conductivity calculation.

**ACF Length** Specify the length of autocorrelation function in thermal conductivity calculation.

**Calculate viscosity** Viscosity is calculated on-the-fly from the autocorrelation function of the pressure tensor and the Green-Kubo equation.

**Calc Interval** Specify the calculation frequency of autocorrelation function in thermal conductivity calculation.

**ACF Length** Specify the length of autocorrelation function in thermal conductivity calculation.

## 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.

**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-equilibrium (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.

### 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, .

#### 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.

**Manual entry** The contents of the generated LAMMPS input script (in file) are displayed. You can also edit directly at this location.

#### Options

**Make a Backup of Working Directory** Select this when backing up the working directory.

**Restore Working Directory** Click this button to return the working directory 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.

Set the force field. The choices vary depending on the type of solver.

**Automatically assign parameters** Assign a new force field parameter.

**(General)** Specify the force field of molecules other than proteins and water molecules. Internally **acpype** is used for GAFF, OPLS/AA-L, in-house program is used for Dreiding. The setting of Dreiding is written in `polymer/dreiding.lib.txt`.

**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/Ion)** Specify the force field of the protein. At this point, atoms assigned amino acid residue names in PDB and gro format are recognized as proteins. 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 edit the force field information with a text editor and customize it, first save this file using this function, and edit the top file for Gromacs and the data file for LAMMPS with a text editor etc. .
  - Next, in case of Gromacs, select *Use parameters written in topology file* and click *OK* button. Then you will be asked for the location of the top file, so open the top file you saved and edited earlier.
  - In case of LAMMPS, select *Use parameters written in file in main window* and click *Next >* button. Then, *Select the type of force field* appears. Select the general type of force field to use and click the *OK* button.
- 

**Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** (For LAMMPS) Select when you want to use inorganic potential, ReaxFF or DPD. After pressing *Next >* button, specify the type of force field to be actually used.

**Use parameters written in topology file** (For Gromacs) Select to perform MD calculation using the existing top file. The corresponding gro file must be open in the main window.

**Use parameters written in file opened on main window** (For LAMMPS) Select to execute MD calculation using the existing data file. The data file to be used must be open in the main window. After pressing *Next >* button, specify the type of force field to use.

### 6.12.3 Run

Execute LAMMPS. The execution method differs depending on the situation.

- **(Default) *Extending Simulation* is unchecked and *Automatically assign parameters* or *Use parameters defined in external parameter file***  
Create a new data file (file containing coordinates and topology) and start the job.
- ***Extending Simulation* is unchecked and *Use parameters written in file opened on main window*” in *Assign Force Field* is checked**  
Start the job using the data file opened in the main window.
- **When *Extending Simulation* is checked** Start the job using the `lmp_tmp_final.data` located in the working directory 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 It is a batch file.
Working Directory water_lmp_tmp\ 	Working directory.

The following files are generated in the working directory. Only the main files are shown here.

type	Description
lmp_tmp.data	It is the initial state file of the calculation specified by read_data.
lmp_tmp.in	It is a file that specifies calculation conditions.
lmp_tmp.log	It is a log file. It is the same as: file: <i>water.log</i> .
lmp_tmp.dump	It is a trajectory file in dump format.
lmp_tmp.restart	It is a restart file containing information on the final state.
lmp_tmp_final.data	It is a data file containing information on the final state. It is generated from the restart file.
postproc.sh	lmp_tmp_final.data LAMMPS generated is insufficient for the execution of LAMMPS, It is a script that performs processing to compensate for insufficient information.
lmp_tmp.xtc	To use the Gromacs tool for processing results, It is a trajectory file of xtc format.
lmp_tmp.xtc	To use the Gromacs tool for processing results, It is a trajectory file of xtc format.
lmp_tmp.gro	To use the Gromacs tool for processing results, It is a gro format coordinate file. Convert from the data file specified as the input file
6.12. MD → LAMMPS menu	It will be created.

---

**Hint: Working directory**

- A working directory 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 directory 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 directory 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 directory 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*.

### 6.12.4 Open Log File

Open the LAMMPS log file (`*.log`) with a text editor.

### 6.12.5 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 window*.

### 6.12.6 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.

### 6.12.7 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.

### 6.12.8 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*.

## Static Dielectric Function

Select the xtc file output by LAMMPS and the gro, ndx file automatically generated by Winmostar and display the scattering function. 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. 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. See *Free Volume* for details.

## Autocorrelation Function

Displays the autocorrelation function that is output when calculating the thermal conductivity and viscosity using the Green-Kubo equation.

## 6.12.9 Dissipative Particle Dynamics

### DPD Cell Builder

Create a simulation cell for dissipative particle dynamics.

**Monomers Available** Select the monomer (particle) that constitutes the polymer chain.

**# of Monomers** Specify the number of selected monomers.

>> **Add** >> Add selected monomers.

#### 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.

<< **Delete** << Delete the added monomer.

**# of Polymers** Specify the number of polymer chains.

**>> Add >>** Add the listed polymer chain to the calculation target.

**Polymers Used** The composition and number of added polymer chains are listed.

**<< Delete <<** Delete the added polymer chain.

**Density** Specify the density (dimensionless) of the system.

**Build** Build a simulation cell.

**Reset** Restore all settings to default.

**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).

**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.

## 6.13 MD → Amber menu

It is a menu related to Amber. Since Winmostar runs Amber on the Cygwin environment, in order to use this function, you need to set up `cygwin_wm` is required.

### 6.13.1 Configure LEaP

Use tLEaP to set conditions for creating coordinate (crd) and topology (prmtop) files. Select each item, specify it, and click the [OK] button.

**Force Field** Select the type of force field.

**Add Na +** Specify whether to add Na ion, and specify the number.

**Add Cl-** Specify whether to add Cl ions and specify the number.

**Solvate** Specify whether to add water molecules.

**Box/Octahedron** Specify the box type.

**Solvent** Specify the type of solvent.

**Distance** Specify the distance between the solute and the box boundary.

**Other LEaP Commands** Write other LEaP commands.

### 6.13.2 Run LEaP

Create coordinates (crd) file and topology (prmtop) file using tLEaP. (Crd file name except extension)  
Create a working folder named \_leap\_tmp, and processing will be done in that folder.

### 6.13.3 Configure sander

Set conditions for executing calculation by sander. Select each item, specify it, and click the [OK] button.

#### Basic

**imin** Specify whether to perform energy minimization.

**igb** Specify the solvent model.

**ntb** Specify whether it is a periodic boundary condition or not.

**ntt** Specify temperature scaling.

**times** Specify the initial temperature.

**temp0** Specify the reference temperature.

**I NSTL** Specify the number of MD steps.

#### Advanced

**maxcyc** Specify the maximum number of cycles.

**NCYC** Specify the number of cycles using the maximum gradient algorithm.

**gamma\_In** Specify the collision frequency  $\gamma$ .

**DT** Specify a time step.

**cut** Specify the cutoff distance.

**ntpr** Specify output frequency such as energy value, temperature.

**ntwx** Specify how often the coordinates are output to the trajectory file.

#### QM/MM

**Use qmmm** Set ifqnt = 1, add &qmmm namelist, and enable the setting for QM/MM/MD calculation.

**qm\_theory** Select the calculation method used in the QM region.

**qmcharge** Specify the net charge of the QM area.

**qmshake** Specify the application of the SHAKE method to the H atom in the QM region.

**qm\_ewald** Specify the application of the Ewald method to the QM region.

**qm\_pme** Specify the application of the PME method to the QM region.

**qmmask** When you press the [Set] button, the atom selected on the main window is set as the QM area. Blue atoms selected by Ctrl + drag on the main window are targeted.

#### Misc

**Other Settings** Write the other settings.

### 6.13.4 Run sander

Run sander. (Crd filename excluding extension) Create a working folder named `_amb_tmp`, and processing will be done in that folder. The job is run through *Winmostar Job Manager*.

### 6.13.5 Animation

Import the coordinates of the trajectory from the PDB file converted from mdcrd file with ptraj. For the animation display operation method, see *Animation window*.

### 6.13.6 Energy Plot

Display the energy graph from the calculated log file. Please see *Energy Plot window* for how to operate subwindow.

### 6.13.7 Import Coordinate File

Load Amber coordinates (crd) file and topology (prmtop) file and display them in the main window.

## 6.14 MD → Polymer Menu

The procedure for preparing the polymer system is as follows.

1. Model the monomer and execute *Register Monomer*.
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*.

### 6.14.1 Register Monomer

register the monomer 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 monomer (repeating 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.

**[Name]** Enter the name of the monomer to be registered.

**[OK]** Register the monomer and close the window. A monomer file is created.

**[Cancel]** Discard the settings and close the Register Monomer window.

### 6.14.2 Homo Polymer builder

Create a homo polymer for use with *Polymer Cell Builder* from the monomers registered with *Register Monomer* 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 (repeating unit) used and the degree of polymerization. Charges for atoms deleted by polymerization are equally allocated to the atoms of the whole polymer.

**[Polymer Name]** Enter the name of the polymer to be registered.

**[Polymerization Degree]** Specify the degree of polymerization.

**[Monomer List]** Select the monomer to use.

**[Display]** The selected monomers are displayed in the main window.

**[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 <math>\leq x <math>\leq 1.0).

**[Head/Tail Configuration]**

**[Head to Tail]** Combine the head atom of the monomer and the tail atom by overlapping.

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

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

**[Close]** Close the window.

### 6.14.3 Block Polymer Builder

Create a block polymer for use with *Polymer Cell Builder* from the monomers registered with *Register Monomer* 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*.

**[Polymer Name]** Enter the name of the polymer to be registered.

**[Polymerization Degree]** Specify the degree of polymerization.

**[First Monomer]** Select the first monomer from the monomer list.

**[Last Monomer]** Select the last monomer from the list of monomers.

**[Internal Monomer]** Select an intermediate monomer from the monomer list. In [Number], enter the number of monomers.

**[Number]** Specify the number of intermediate monomers.

**[Add]** Reflect the set intermediate monomer name and number in the Internal Monomer List.

**[Display]** Display the set intermediate monomer on the main window.

**[Delete wmo File]** Delete the specified monomer file.

**[Delete From List]** Remove the selected intermediate monomer from the list in the list.

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

**[Close]** Close the window.

#### 6.14.4 Random Polymer Builder

Create a random polymer for use with *Polymer Cell Builder* from the monomers registered with *Register Monomer* 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*.

**[Polymer Name]** Enter the name of the polymer to be registered.

**[Polymerization Degree]** Specify the degree of polymerization.

**[First Monomer]** Select the first monomer from the monomer list.

**[Last Monomer]** Select the last monomer from the list of monomers.

**[Internal Monomer]** Select an intermediate monomer from the monomer list. In [Number], enter the number of monomers.

**[Ratio]** Specify the appearance rate (0 <math>x</math> <math>1.0</math>) of the selected intermediate monomer.

**[Add]** Reflect the set intermediate monomer name and appearance rate in the Internal Monomer List.

**[Display]** Display the set intermediate monomer on the main window.

**[Delete wmo File]** Delete the specified monomer file.

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

**[Delete From List]** Remove the selected intermediate monomer from the list in the Internal Monomer List.

**[Definition of Ratio]**

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

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

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

**[Close]** Close the window.

### 6.14.5 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 it 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.

#### [Box Configuration]

**[Density]** Specify the density.

**[X-Axis Length]** Specify the rectangular parallelepiped cell's X direction length in Å. Or the length is displayed in Å.

**[Y-Axis Length]** Specify the length of rectangular parallelepiped cell in Y direction in Å. Or the length is displayed in Å.

**[Z-Axis Length]** The length of rectangular parallelepiped cell in Z direction is displayed in Å.

**[Cubic Cell]** Specify a cube cell.

#### [Periodic Boundary Condition]

**[X],[Y],[Z]** Toggle in the direction that imposes periodic boundary condition.

#### [Polymer Available]

**[Number]** Specify the number of selected polymers.

**[Display]** The selected polymer is displayed on the main window.

**[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.

**[Build]** Create a simulation cell.

**[Close]** Close the window.

### 6.14.6 Monomer allocation

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

### 6.14.7 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.

## 6.15 MD → *Interface Builder* menu

Join the two simulation cell files (mol2 or cif format) prepared in advance to create an interface model.

**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 Constraints

**[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.

## 6.16 Solid Menu

It is a menu related to first principle (band) calculation. Solid pack is required to use the functions of the solid menu.



## 6.16.1 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.

**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).

**Add** Add an atom that becomes an asymmetric element.

**Remove** Delete the atom which becomes the asymmetric element selected on the list.

**Atom** 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.

## 6.16.2 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.

**View menu** It is the same as *Crystal Builder*.

## 6.16.3 Cleave Plane

Specify the mirror surface and redefine the unit cell. When creating a slab model, execute *Insert Vacuum* after executing this function.

**View menu** It is the same as *Crystal Builder*.

### Step 1/2 Cutting

**Cleave Plane** Define the Miller index (hkl) of the surface.

**Offset** Specify the position of the surface by the relative position (percentage) from the upper end to the lower end of the unit cell.

**Next >>** Go to *Step 2/2 Transform Unit Cell*.

### Step 2/2 Transform Unit Cell

**View Configuration** Set the drawing range.

**Lattice Choice** Select the grid definition.

**Manual** Specify atom on the origin, a axis, b axis, c axis with *Set* button.

**Filter (Ortho)** Choose from *Lattice*. Only rectangular candidates will appear in *Lattice*.

**Filter (All)** Choose from *Lattice*.

**Lattice** The grid definition choices are displayed.

**Filter** Specify the narrowing condition of *Lattice*.

**OK** Perform the processing.

## 6.16.4 Insert Vacuum

Insert a vacuum layer above and below the crystal structure and construct a slab model.

**View menu** It is the same as *Crystal Builder*.

**Axis** Select the direction in which the vacuum layer is to be inserted from the X, Y, and Z axes.

**Bulk** Indicate the thickness of the original cell in Å. (Display only)

**Vacuum** Define the vacuum layer thickness in Å.

**Total Width** Indicates the sum of *Bulk* and *Vacuum*. (Display only)

**Automatically shift to center** When this check box is checked, the original crystal structure is fixed at the center of the slab model. When not checked, the Shift function becomes available.

**Shift** You can specify the location of the surface structure in the expanded cell. Numeric values in the edit box indicate the position of the reference plane in fractional coordinates.

**Reference Plane** Specify the position of the reference plane. For Base, the reference plane is the bottom of the crystal structure. At the center, the reference plane is the center of the crystal structure.

**Terminate dangling bonds with hydrogen atoms** The dangling bond is capped with hydrogen on the surface in contact with the vacuum. If you want to modify with a functional group, check this function, return to the main window, and use *Replace with Fragment* to replace the hydrogen with any functional group.

**OK** Perform the processing.

### 6.16.5 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 center point of the cluster in terms of fraction coordinates. With an atom on the graphic window selected, click Set to specify the selected atomic position as the center point. **Cluster Radius** Specify the radius of the cluster in angstrom units.

**Hydrogen** Define the vacuum layer thickness in Å.

**OK** Perform the processing.

### 6.16.6 Convert Lattice

For cells displayed in the main window, perform conversion between primitive cells and conventional cells.

### 6.16.7 Quantum ESPRESSO

See *Solid* → *Quantum ESPRESSO menu*.

### 6.16.8 OpenMX

See *Solid* → *Quantum ESPRESSO menu*.

### 6.16.9 FDMNES

See *Solid* → *FDMNES menu*.

## 6.17 *Solid* → *Quantum ESPRESSO menu*

It is a menu related to Quantum ESPRESSO. The way to install Quantum ESPRESSO is described in *Installing Winmostar and solvers*.

## 6.17.1 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* 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 destination folder for the data. outdir is set as a new folder.

**Continue** Continue the job of QE that was loaded on the main window and executed immediately. outdir is set to outdir of the job executed immediately before.

**Select** Specify the folder specified in the opened dialog as the output destination and continue the job from the data of that folder. Outdir will be set to what you specify here.

**Preset** Select preset for setting.

**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

**calculation** Select the type of calculation.

**Use nbnd** Specify the number of bands. If not checked, it will be set automatically. When selected in parentheses, the number of valence electrons when pseudopotential is used is displayed. If the calculation of the number of valence electrons fails, it is displayed as N/A.

**K\_POINTS** Select the specification method of point K from the pull-down and specify K point in QE format in the text box below. In the case of gamma, it is calculated only with the  $\Gamma$  point. In the automatic case, “(number of divisions in the kx direction) (division number in the ky direction) (number of divisions in the kz direction) (shift flag in the kx direction) (shift flag in the ky direction) (shift flag in kz direction)” Enter a delimiter. When the shift flag is 0, there is no shift (the k point includes the  $\Gamma$  point), when it is 1, there is a shift (k point crosses the  $\Gamma$  point). For details, please refer to doc/brillouin\_zones.pdf under pw.x manual or QE installation folder.

**Set default k-path** The default k-point path of the Bravais 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.

**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.

**tpnfor** 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.

**diagonalization** Specify diagonalization algorithm.

**lspinorb** Pseudopotential file with spin orbit interaction can be used during calculation of non-colinear.

**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.

**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 spin polarization calculation setting.

**Use tot\_magnetization** When checked, specify the magnetization of the whole system here. If you do not check it, specify starting\_magnetization.

**starting\_magnetization** Give the initial value of magnetization of each atom type.

**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 phonon calculation. Specifically, execute ph.x after executing pw.x. In order to make this item effective, you need to choose SCF or relax for Calculation. I/O files such as ph.x are created in the working directory.

**Threshold** Specify the censored error of phonon calculation.

**Calc Macroscopic Dielectric Constant** Calculate the dielectric constant obtained from phonon calculation.

**Calc Non-resonant Raman** Include calculation of Raman spectrum.

**Acoustic Sum Rule** Specify how to give Acoustic Sum Rule at the time of spectrum calculation (dynmat.x) after phonon calculation. It does not affect phonon calculation itself.

**Calc Phonon Dispersion** Calculate phonon dispersion. In order to acquire phonon band structure, phonon density of states you need to specify this.

**K Points (Dispersion)** Specify the number of K points when computing phonon variance.

#### 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).

#### 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.

**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.

**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.

**Other 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.

#### Options

**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.

**Make a Backup of Working Directory** When Output Directory is Create, if the `_qe_data` folder to be created already exists, add a number to the end of the folder name to back up the existing folder.

**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`.

**Use RISM-enabled QE** Check if you want to use QE with RISM installed.

### 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.

### Pseudo Potentials 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.

**Pseudo Potential** Pseudopotentials of the type common to all the elements in the system can be selected by pulldown. (Manual) is selected, the user separately sets the pseudopotential for each element in the list below. Pseudopotential files are searched from folders specified in pseudo Directory. The one written at the top of `UserPref/qe_pseudo_priority_list.txt` is preferentially selected.

**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`.

## 6.17.2 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 directory 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 directory then.
- If the case of *Output Directory = Select*, use the selected folder as the working directory (`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 <code>si.pwout</code>	Calculation log file.
bat file <code>si.bat</code>	It is a batch file for running Quantum ESPRESSO.
Working Directory <code>si_ge_data\</code>	Working directory.

The following files are generated in the working directory. Only the main files are shown here.

type	Description
Pseudopotential file *.UPF	The pseudopotential file used for calculation is Copied here, the ESPRESSO_PSEUDO environment variable It is set to the working directory.
gmx_tmp.mdp	It is a file that specifies calculation conditions.
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	In post processing, use phonon calculation with <b>ph.x</b> It is an input file for execution.
ph.out	This is the log file of ph.in.

**Hint:** \*\* Working directory \*\*

- A working directory 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 directory 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 directory 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 directory is `aaa_gmx_tmp`, it is `aaa_gmx_tmp1`.
- **\*\* Directories without numbers are always up to date. \*\***

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Job is run through *Winmostar Job Manager*.

### 6.17.3 Open Log File (pwout)

Open the log file with a text editor.

### 6.17.4 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)*. For the animation display operation method, see *Animation window*.

#### CPMD(pos)

Specify CPMD's pos and cel files and display animation. To display the result of pw.x, use *Optimization, BOMD(pwout, out)*. For the animation display operation method, see *Animation window*.

### 6.17.5 Energy Plot

#### SCF Energy Change (pwout)

Select the log file and display a graph of total energy. For CPMD use *CPMD Energy Plot (evp)*.

**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*.

## 6.17.6 Analyses

### Electron Density

Specify working directory (outdir) and display isoelectric density surface. In the background, pp.x flows, and a cube file is generated. Refer to *MO Plot window* for how to operate subwindow.

### Lowdin Charge

Specify the working directory (outdir), calculate and display the point charge. Projwfc.x flows in the background.

### Potential Energy Distribution

Specify the working directory (outdir) and log file for SCF calculation and display the potential energy distribution in the z-axis direction. Fermi energy is acquired from the log of SCF calculation. The difference between the Fermi energy and the maximum value of the potential 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*.

### Band Structure

Specify the working directory (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 flows 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*.

### Density of States

Specify the working directory (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 flows 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*.

### Projected DOS

Specify the working directory (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 flows 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* <<http://fermisurfer.osdn.jp/>>. 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 directory 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*.

## IR/Raman

Specify the working directory 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 directory 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  $2\pi/a$ , 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 directory 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*.

### 6.17.7 Generate MOL File

Create a MOL file of the solvent used in the RISM calculation (`trism = .True.`). Please call this function after creating one molecule in the main window. When entering LAMMPS data format, please check *Use parameters in displayed file*. 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.

### 6.17.8 Nudged Elastic Band

#### Configure

Set conditions for NEB calculation. Please set in the state that the structure optimization calculation of each of the start state and the end state has been completed.

#### Run

Perform NEB calculation using `neb.x`.

#### Transition Path

Specify the file after NEB calculation and display the change in energy and atomic structure along the reaction coordinates. For the animation display operation method, see *Animation window*.

### 6.17.9 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 directory 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, calculate expansion coefficient.

*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 directory (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.

### 6.17.10 Phonopy

Phonopy calculates in the following three steps.

1. Create a supercell based on the given Quantum ESPRESSO input file. (Pre-processing)
2. Execute Quantum ESPRESSO for all generated super cells.
3. Create ForceSets file from Quantum ESPRESSO output file and calculate Phonon band, DOS, thermodynamic properties, etc. (Post processing)



## Configure & Run

Set calculation conditions for pre-post processing using Phonopy and execute 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 directory.

The following files are generated in the working directory `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

Open the conf file with a text editor. Use when you want to edit the keywords set on the Configure window.

### Run QE for Phonopy

Execute Quantum ESPRESSO for all super cells generated in Configure & Run window. Quantum ESPRESSO will run in the local environment.

### Run Phonopy

Executes post processing of Phonopy. 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 of States

Displays the density of states based on total\_dos.csv included in the working folder.

### Thermodynamic properties

Displays thermodynamic properties based on thermal\_properties.csv included in the working folder.

## 6.18 Solid → OpenMX menu

Menu related to OpenMX.

### 6.18.1 Configure

Set the OpenMX calculation conditions. Click the *Run* button to execute the calculation immediately after setting, or the: *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* 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.

### SCF tab

**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.

**SpinPolarization** Specify non-spin polarization or spin polarization of the electron system. Specify “ON” to calculate spin polarization and “OFF” to calculate non-spin polarization. In addition to the above two options, specify the option “NC” for non-collinear DFT calculations.

**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”.

**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.

**ElectronicTemperature** Set the electronic temperature (K).

**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).

**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.

**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.

**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 (“RMM-DIIS”), Kerker method (“Kerker”), or RMM-DIISK method (“RMM-DIISK”) or RMM-DIISH method (“RMM-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  $0 < \text{Init.Mixing.Weight} < 1$

**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 (Hamiltonian) 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.

**criterion** Specify the convergence condition for the SCF calculation (in Hartree). The SCF iteration ends when the condition  $dU_{ele} < scf.criterion$  is met. Here  $dU_{ele}$  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).

#### SCF.Hubbard tab

**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”.

#### OrderN tab

**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.

#### MD tab

**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.

**maxIter** Specify the maximum number of iterations for MD and structural optimization calculations.

**TimeStep** Specify time step (fs).

**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.

**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.

### File 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.

#### Bands/DOS tab

##### Band

**dispersion** Set to “ ON ”to evaluate band dispersion.

##### DOS

**fileout** Set to ON to evaluate the total density of states (DOS) and projected partial density of states (PDOS).

**Erangle** 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 tab

**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.

**Atoms.Coord.Unit** Specify the unit of the atomic coordinate.

## 6.18.2 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 cygwin_wm.
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 directory.
Working directory dia_mx_data\	Working directory

The following files are generated in the working directory. 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.
6.18. <b>Solid</b> → <b>OpenMX</b> menu wm.tden.cube	The total electron density in Gaussian cube format is stored.

---

**Hint: Working directory**

- A working directory 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 directory 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 directory 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 directory is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
    - \*\* Unnumbered directories are always up to date. \*\*
- 

Job is run through *Winmostar Job Manager*.

### 6.18.3 Open Log File (mxout)

Open the log file with a text editor.

### 6.18.4 Animation (md)

Create and display animations such as structure optimization and molecular dynamics calculations from md file information. Please refer to *Animation window* for how to operate the animation.

### 6.18.5 Analyses

#### Density/Spin/Energy Distribution

Specify the cube file and display the electron density, spin density, and energy distribution. See *MO Plot window* for how to operate subwindows.

#### Band Structure

Specify the working directory (`dia_mx_data\`) and display the band structure. Calculation must be completed with `Band.dispersion=on`

#### Density of of States

Specify the working directory (`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 directory (`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.

## Fermi Surface

Specify the working directory (`dia_mx_data\`) and display the fermi surface. Use *FermiSurfer* [<http://fermisurfer.osdn.jp/>](http://fermisurfer.osdn.jp/) 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.

## 6.19 Solid → FDMNES menu

It is a menu related to FDMNES. The method of installing FDMNES is described in *Installing Winmostar and solvers*.

### 6.19.1 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.

### 6.19.2 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*.

### 6.19.3 Opem Log File (log)

Open the log file with a text editor.

### 6.19.4 Analyses

#### XANES Spectrum

Select the conv file ( \*\_conv.txt ) and display the XANES spectrum.

## 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

Register the molecular structure displayed in the main window as a part. Atom replaced with marker (heavy red circle) is set as the connection part when replacing.

#### Delete Fragment

Delete the registration of the parts selected by *select a fragment* by pull down menu | repl | of *toolbar*.

### 6.20.3 Conformation Search (Balloon)

We will search for conformation using Balloon. Click *Search* button to start processing. An intermediate file is created in the working folder \*\_balloon\_tmp.

### 6.20.4 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  $\Leftrightarrow$  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.

### 6.20.5 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 Molecular 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)

Ovality (Ovality) is calculated by the following formula. Molecule surface/Minimum surface area =  $S/4\pi(3V/4\pi)^{2/3}$  Minimum surface area =  $4\pi(3V/4\pi)^{2/3}$  (surface area of a true sphere having the same molecular volume)

### 6.20.6 Aspect Ratio

Calculate the aspect ratio of the molecule. The aspect ratio is defined as the ratio L/D of the length L and the diameter D of the cylinder of the smallest diameter inscribed by the molecule.

### 6.20.7 Radius of Gyration

Calculate the inertial radius of the molecule.

### 6.20.8 Sterimol Parameters

Calculate the Sterimol parameter for the substructure selected for the group on the main window. Click *Calculate* button to start the calculation.

### 6.20.9 Project Browser

Opens a window for managing files in the project.

### 6.20.10 Job Manager

Start Winmostar Job Manager that manages local jobs.

### 6.20.11 Submit Remote Job

Opens a window for executing and managing remote jobs. For details, see *Each function of the Submit Job window*.

### 6.20.12 Cygwin

Start the terminal window (terminal) of *cygwin\_wm*.

### 6.20.13 Unit Converter

Opens a unit conversion tool specialized for atomic and molecular systems.

### 6.20.14 Search String

It searches character strings in various log files and outputs the hit line to Excel or text file.

### 6.20.15 Batch Queue

We run Gaussian and GAMESS bat files in succession.

1. First, run Gaussian or GAMESS using normal operation method. Confirm that there is no error on the console window (DOS window) during execution, and then press the X button on the console window to forcibly terminate processing.
2. Next, activate this function. The bat file of the job executed in 1. is displayed in the list on the left side of the window.
3. Select the bat file and press the => button to add it to the list on the right side of the window.
4. When you press the *Run* button, continuous execution of jobs registered in the list on the right starts. When you press the *Run at* button, continuous execution starts at the specified time. Continuous execution jobs are saved in winmos\_batjob\*.bat. *Save* and :guilabel:' Load' button to save and load settings.

### 6.20.16 Superimpose Molecules

Multiple molecules are superimposed and displayed.

1. First, select the file with the *Add* button and select the molecule to be superimposed. File types are various input files that can be read with Winmostar and output files of MOPAC, GAMESS, NWChem, and Gaussian. You can select multiple files simultaneously. You can also load files by drag & drop. *Import From Main Window* button allows you to capture molecules displayed in the main window.
2. Selecting the filename displayed in the list will highlight that molecule blue.
3. Delete selected molecule with *Delete* button, *Clear* button to delete all molecules.
4. You can align the orientation of each molecule with *Align All* 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 structure of the molecule is close, press X,:guilabel:'Y, Z' button to shift the surface to be superimposed.
6. You can display it with *Winmostar Viewer* by pressing *Open Viewer* button.

## 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 directory 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.

#### Edit tab

**Bonding Factor** Set the threshold for judging the presence or absence of covalent bond from inter-atomic 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 and press the *Delete* button.

**Move markers to pasted atoms.** If checked, move the marker to the pasted atom when using *Paste*.

**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.

#### Calculation tab

**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.

**Timeout** Set the time-out period of time-consuming processing.

**Default extensions** Set the extension set by default when creating input files for each solver.

**Use Gnuplot as default plotting tool** If you check, use Gnuplot for some graph drawing functions. Otherwise, use Grace. From V9, the graph drawing function using Grace or Gnuplot will gradually replace the graph drawing function of Winmostar native. The Gnuplot file can be saved from the *Export* button of the Winmostar native graph drawing function.

**Confirm before starting calculation** If checked, a confirmation dialog will be displayed when executing each solver.



**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 directory for Remote Job Submission.

**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.

#### 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.

**VDW radius of selected atom** Change the VDW radius for the element of the atom with marker in Viewport.

**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*.

**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.

**Depth cue** Adjusts the fog density used for depth expression.

**Items to be drawn** Check the items to be displayed in Viewport. You can also be set from *View → Items*.

**View center after opening file** Check *View Marked Atom* automatically when opening a file.

**For patent application** Display in black and white and no gradation, which can be used when applying for a patent.

**Program Path Tab** Specify the install path of various programs.

## 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 Check cygwin\_wm

Click *Check Now* button to check the installation of *cygwin\_wm*. 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 *cygwin\_wm* may be obstructed when installing *cygwin\_wm*, so you can check it easily with this function.

### 6.23.6 Open Preferences Folder

Open the UserPref folder under the Winmostar installation folder.

### 6.23.7 Debug Mode

Switch to debug mode.

## 6.24 Animation window

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. About animation (trajectory) data It is also possible to analyze results directly from this window. For details, please refer to the *Tools* menu.

#### File menu

**Realod** Read the animation from the original file again. You can also operate from the *Reload* button.

**Export GIF Animation** Write a GIF animation file. You can also operate from the *Export* button.

**Export JPEG Images** Export serial number JPEG file. You can also operate from the *Export* button.

**Export Animated GRO File** Output animation gro file. It can be used for linking with VMD etc. You can also operate from the *Export* button.

**Close** Close this window. To reopen it, select *Window menu* → *Animation*. You can also operate from the *Close* button.

**Control menu**

**Go to First Frame** Move to the first frame. You can also operate from the buttons in the window.

**Play/Pause** Play/pause the animation. You can also operate from the buttons in the window.

**Go to Last Frame** Move to the last frame. You can also operate from the buttons in the window.

**Tools menu**

**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.

**Distance/Angle Change** Analyze the bond length, bonding angle, dihedral angle between specified atoms in the trajectory.

1. On the *Bond/Angle Change* window, select: guilabel:‘ Type‘.
2. List the atoms that define the bond length, bond angle, and dihedral angle you want to calculate in *Target Atoms* separated by commas. Clicking *Set* button you can automatically enter atoms with markers in the main window.
3. In *Plot*, choose whether to output time change ( *Time Change* ) or histogram ( *Histogram* ).
4. Click the *Draw* button.

**Mean Square Displacement/Diffusion Constant** Calculate 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 equivalent functions may be provided in the solver menu.

**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.

**Extract Trajectory for Selected Group** In the main window, create a trajectory file extracting only the atoms selected from the group.

**Up/Down slider** Drag to move between frames.

**Speed slider** Adjust the playback speed.

**Loop check box** If it is checked, the loop will be played.

**Dynamics Bond check box** 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.).

**Open Viewer button** Display the currently open animation using *Winmostar Viewer*.

**Excel button** Output the contents of the list in csv format, start Excel and load it.

**Excel button** 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 reflected 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 MO Plot 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 and open the file.

**File** → **Open Jmol menu** It displays with Jmol.

**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*.
- **ESP(Population Charge)/Surface** Display *ESP(Population Charge)* information on the molecular surface.
- **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.

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**Hint:** You can display the ESP on the surface of the molecule corresponding to *ESP/Surface* by following the steps below.

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*.

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## 7. Click *Draw* button

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**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.

---

**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.

**Open Excel** Output the csv file and open it.

**Save 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.

**Open Excel** Output the csv file and open it.

**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.

**Open Excel** Output the csv file and open it.

**Copy Image** Copy the graph to the clipboard.

**Close** Close the window.

## 6.30 PIO analysis window

Set up and execute PIO (Paired Interacting Orbitals) analysis by GAMESS or Gaussian.

(1) Click the fragment

**Set** Specify a fragment. Click A to select it, then click B, then click the Set button.

**Reset** Release the setting of the fragment.

(2) Save ab.inp

**Save** Outputs and saves data files for coalescing AB and solitary systems A and B.

**Edit** Edit the data file.

(3) Gamess/GAMESS Exec

**Gauss/GAMESS** Perform calculation by Gaussian/GAMESS.

**GenG** Create a batch file.

**GENP** Create a data file for PIO.

(4) PIO

**PIO** Perform PIO calculation.

**ISPC** For the specified number of peaks, enter the wavelength and oscillator strength values in the figure. (From long wavelength side)

**0** We will make PIO using all molecular orbits of A and B fragments.

**1** We will create PIO using only occupied molecular orbital of both A and B fragments. It expresses overlap repulsion (closed-shell repulsion) working between both fragments.

**2** We will create a PIO using only the occupied molecular orbital of A and the empty molecular orbital of B. It expresses the delocalization of electrons from A to B.

**3** We will create PIO using only A 's empty molecular orbital and B occupied molecular orbital. It expresses the delocalization of electrons from B to A.

**Edit** Edit the output file (extension out) by PIO.

**Sum.** Display summary.

**Edit** Edit the output file (extension log) by PIO.

**MO** Opens a command window for displaying molecular orbits. For information on the molecular orbital display function, please see *MO Plot window*.

**Close** Close this window.

## 6.31 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*.

**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.

**Calc Ave** The average value of each item is output as a text file. 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.

## 6.32 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.

### X/Y Axis

**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.

**Open Excel** Output csv file and open Excel.

**Export Gnuplot File** Output Gnuplot file.

## 6.33 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.

### 6.33.1 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.



## 6.33.2 Menu operation

### File menu

**Open** Read gld and MOLDA format files.

**Save GLD** Save the currently open GLD format file with a name.

**Save MOLDA** Save the structure displayed in the window in MOLDA format.

**Save JPEG** Save the contents displayed in the window as a JPEG file.

**Save JPEG (Stereo)** Save the left and right screens for stereoscopic viewing as a JPEG file.

**StereoPhoto Maker** Start StereoPhotomaker.

**Exit** Quit Winmostar 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.

### 6.33.3 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.

**JPEG** When playing with checked, the displayed contents are saved in JPEG format

**GIF** When you play with the checked, the displayed contents are saved in GIF format

**Close** Close this panel.

### 6.33.4 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 *l* in the middle of this window *9* is assigned to each molecule.

**Composition** Assign *9* from *l* 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)

**X, Y, Z** 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.

## 6.34 Winmostar Job Manager

Winmostar Job Manager (Winmostar/JM) is job management software for multi-core Windows PC.

We can automatically schedule the execution of various solvers such as GAMESS, Gaussian etc. on PC ( *local machine* ) which works as an auxiliary program of Winmostar and has Winmostar installed.

### 6.34.1 Basic actions

In Winmostar, if you choose to execute a job (called *local job*) on the local machine, the JM window as shown below will be launched and registered in the first queue. :guilabel: *Status* of the queued job is first *WAIT* (queued for execution), in order of registration, *Priority*, sequential considering the number of executed cores *RUN*, and the job is started. The *Status* of the job that has finished processing switches 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 × (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.

*MaxCores* is the maximum number of cores that JM can use and defaults to the number of cores of the machine. While this value is large, many jobs are executed in parallel, but setting it more than the number of cores on the local machine does not improve efficiency.

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**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.

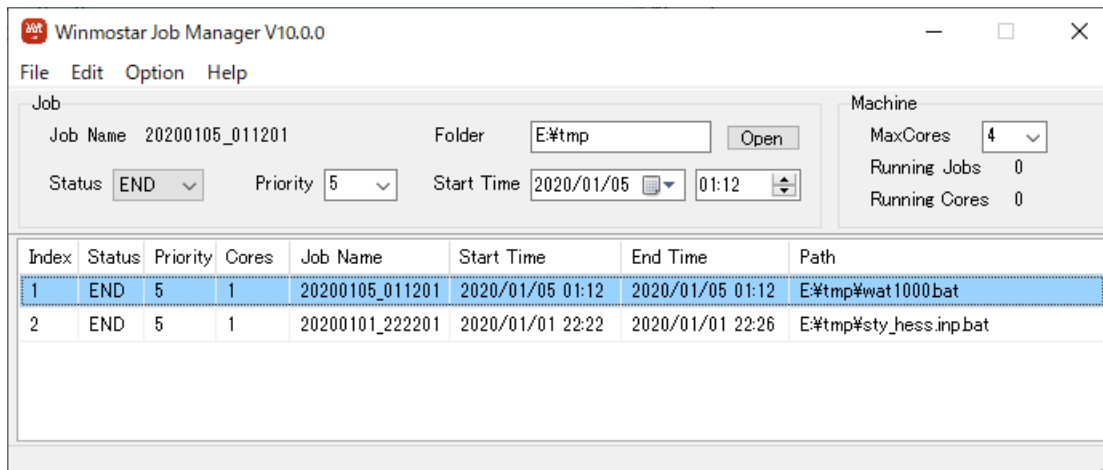
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Jobs are basically executed in the order of old jobs in the *WAIT* state, but you can adjust their order by changing *Priority*. *Priority* has a lower value job execution with higher priority.

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.



**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 .

### 6.34.2 How to forcibly terminate/cancel a job

If you want to forcibly terminate the job in *RUN* state (running), press the × (close) button in the job's prompt (DOS) window. On JM you can also finish by clicking on the line of the job in the guilabel: *run* state and changing the *Status* to *END*, but in some solvers such as MOPAC 2009 That operation does not work.

In JM, click on the row of the job in *RUN* state, the DOS window for that job will be displayed in the foreground.

If you want to cancel the job in the *WAIT* state, select the line of that job with JM and press *Edit* → *Delete Job* or keyboard *Delete* key. If you do not want to execute it without deleting it from the queue, change *Status* from *WAIT* to *END*.

### 6.34.3 How to specify start time specified

The start time displayed in the window is the time registered in the execution queue when *WAIT*, but it changes to the time when it becomes *RUN*.

By setting the time of the future at the start time, execution can be delayed. Once you have made a *RUN* state, also forcibly terminate the job using the *How to forcibly terminate/cancel a job* method, then change the start time and change the *Status* to *WAIT* , It is also possible to execute the job again. (For example, using this method, you can check the operation of the job you want to execute later in advance.)

### 6.34.4 How to force a job to start

You can forcibly start processing ignoring other conditions by changing the *Status* of the job in the *WAIT* state to *RUN*. Likewise you can also resume the job with the *END* status changed to *RUN*.

### 6.34.5 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.

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 job schedulers

Winmostar supports following job schedulers. It is also possible to add additional support to your desired job scheduler with customize service [Winmostar for you](#) .

- TORQUE (PBS)
- SGE, UGE
- SLURM
- T2SUB
- lsubmit
- NQS
- NQS2
- ST
- NSUB
- Rescale
- Winmostar Job Manager

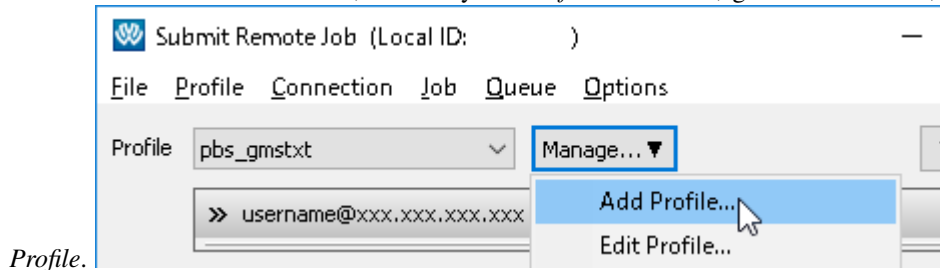
When using T2SUBAME 3.0, select SGE. If the corresponding job scheduler is not installed on the remote server, you can execute the remote job in the following way.

1. 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.
2. Select Run with *Queue* setting.

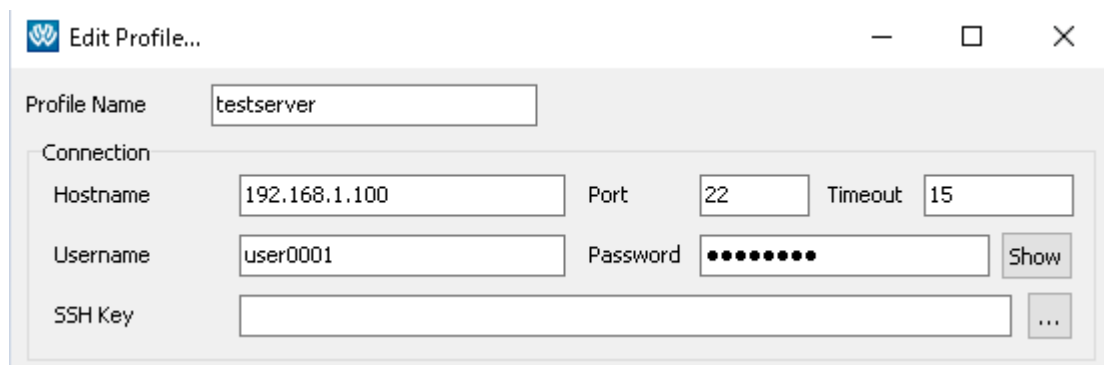
## 7.2 Submitting remote job

For details of each function, see *Each function of the Submit Job window*.

1. Set up the job scheduler and solver on the server you want to calculate. If you are planning to install it now, please refer to [here](#). When executing a job without using job scheduling, setup of the job scheduler is unnecessary, and select “Run” in the setting of *Queue*.
2. Follow steps 1 and 2 on *Basic Operation Flow* to create initial conditions and set keywords and close the Configure window with the *OK* button.
3. Click *Submit Remote Job* button | toolbar\_submit | on the tool bar.
4. On *Submit Remote Job* window, if already set *Profile* is selected, go to [here](#). If not, select *Manage* → *Add*



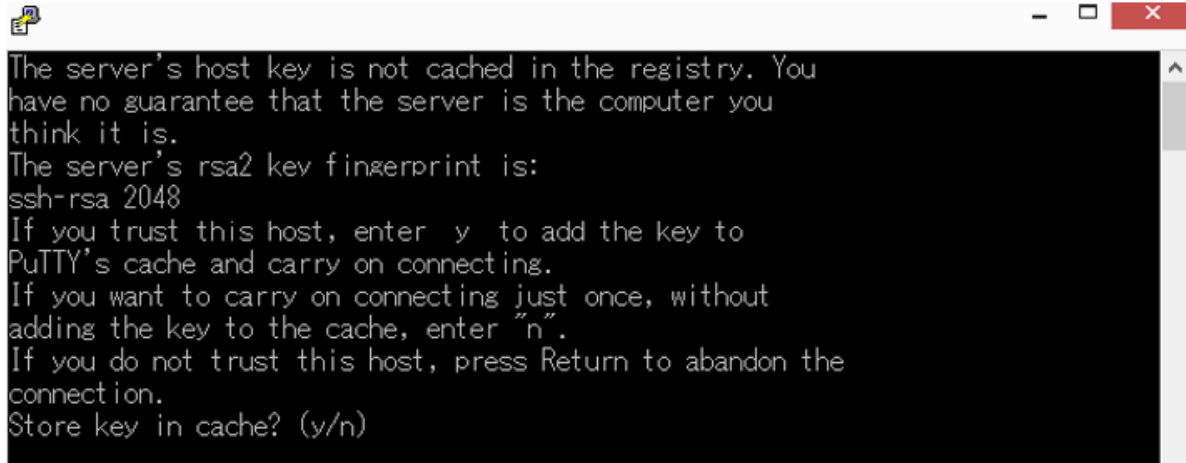
5. Enter the following contents on the top of window of *Edit Profile*.
  - Profile Name
  - Connection
    - Hostname
    - Port (normally 22 is used)
    - Timeout (Use default value if you do not know)
    - Username
    - Password
    - SSH Key (Set as required)



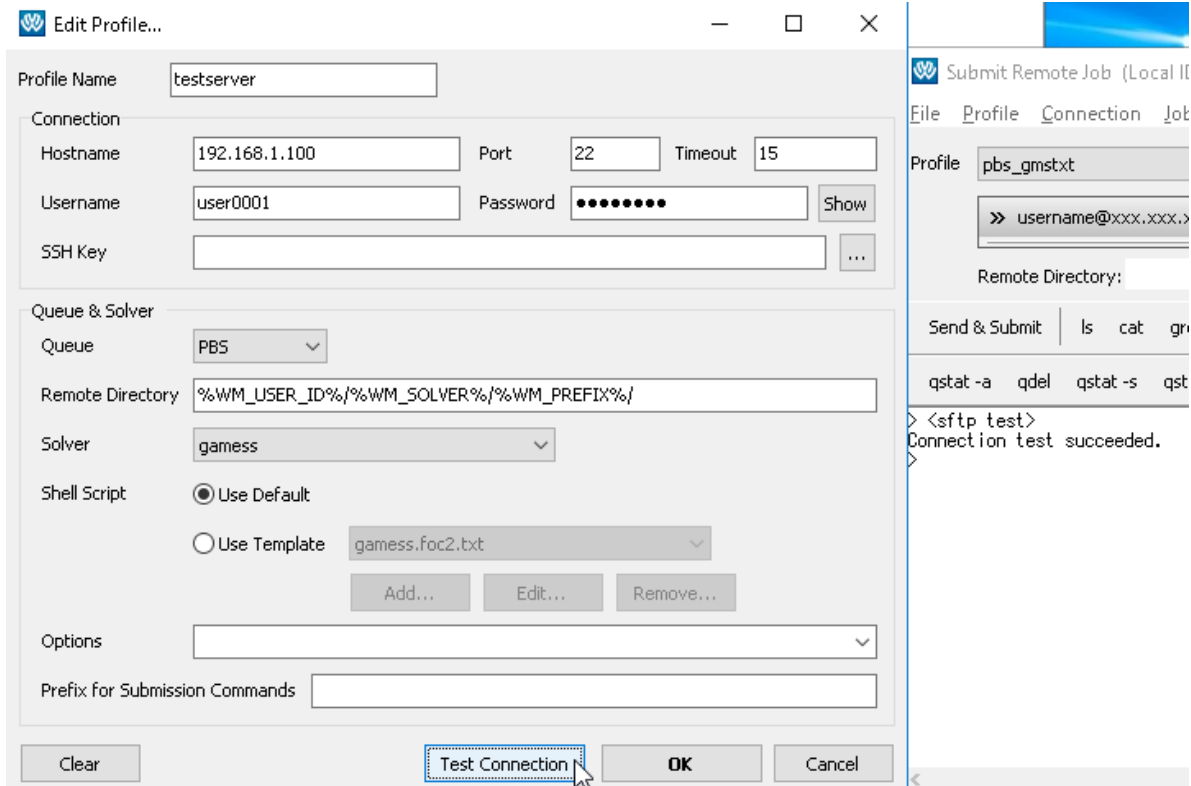
Please

ask us to make multi-stage SSH connection to TSUBAME, FOCUS, etc.

6. After input, click the *Test Connection* button under the *Edit Profile* window to test the SSH connection. 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*.



If the connection is successful, you will see Connection test succeeded. At the bottom of the previous: `Submit Remote Job` window.



If user settings etc. are wrong, you will see `Access denied ***@***'s password:` in the terminal window. Even if you enter the correct password on the spot, please re-enter the password again 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.

7. Enter the following contents at the bottom of the window of *Edit Profile*.

- Queue & Solver
  - Queue
  - Solver
  - Shell Script

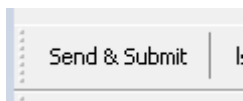


- Options (command arguments for submitting jobs such as **qsub**)

First se-

lect *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. 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](#).

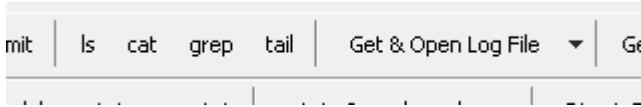
8. Press the *OK* button to close the *Edit Profile* window.
9. In the *Submit Remote Job* window, click the *Queue* → *Show Usage of Each Queues* menu and make sure the remote server information is displayed at the bottom of the window. If it is not displayed correctly, review the setting with *Manage* → *Edit Profile*.
10. To start the job, click the *Send & Submit* button. The operation method here is the same as the 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`.

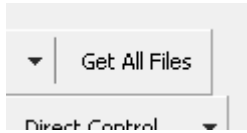
11. Check the status of the submitted job with *Queue* → *List Submitted Jobs*. If all jobs are completed, --- will be displayed.  
If the submitted job ends too soon, --- will be displayed even if you submit it.
12. To check the status of a specific job on a remote server, please do the following.
  - *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.

13. If you want to analyze the result of the job that ended on the remote server on the local machine, click the: guilabel: *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.

14. After file acquisition, result analysis can be performed by the same operation method as local job.

## 7.3 Each function of the Submit 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 directory 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 Queuing Commands** When executing commands such as qsub, if you need the prefix of those commands, set them here. Normally it is empty.

**Test Connection** We will test the connection of SSH. Please note that the job scheduler will not be tested.

### Connection Menu

**Test Connection Using SFTP** We will test the connection of SSH. The same operation is possible with the *Test Connection* button in the window.

**Share SSH Connection Once Established** Used to maintain SSH connection. If you execute it once before the operation involving SSH connection, the operation after that will be lightened.

**Open Putty** Open the Putty setting window and make detailed settings for connection.

**Do Not Use Putty for Connection(experimental)** Do not use Putty for Putty connection. Since the connection is maintained, the operation becomes light. When connecting with key authentication, it is also necessary to specify the public key.

### 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. 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.

**Restart 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

**Enable Admin Mode** Used to access the remote server with root privilege

## 7.4 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 CPU (MPI) parallel number
%WM_NUM_THREAD%	Thread side by side
%WM_NUM_PARALLEL%	Product of% WM_NUM_PROC% and% WM_NUM_THREAD%

## 7.5 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 fol-

lowing order of priority. UserPref\winmos\_profile.ini > UserPref\winmos\_server.ini > wm\_system\RemoteJobdefault\_profile.ini

## 7.6 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 ID, start date/time, end date/time, and batch file.
- If you want to cancel the job with the *Delete Job* button, enter the job ID.

## 8.1 CONFLEX

Set and execute the calculation condition of CONFLEX.

## 8.2 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.

### 8.2.1 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.

## 8.2.2 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 inserions 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.

### 8.2.3 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.

### 8.2.4 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.

### 8.2.5 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.

## 8.3 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*.

### 8.3.1 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*.

**Extending 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:\winmos10\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 *Extending 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 Directory** Click to return the working directory to its pre-execution status, such as when a continued job ends abnormally.

### 8.3.2 Run

To run DCDFTBMD, open *Remote job*. See *Remote job* for detailed instructions. The execution method depends on the situation.

- **(Default) If *Extending 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 *Extending 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 directory, 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 <code>water.dco</code>	DCDFTMD standard output file. A copy of <code>dftb.out</code> in your working folder.
Shell script <code>water.sh</code>	To perform DCDFTBMD and its pre/post processing shell script.
conf file <code>water_conf.sh</code>	Contains variables used in the above shell script file.
Working directory <code>water_dc_data\</code>	working directory.

The following files are generated in the working directory. Only the main files are shown here.

Type	Explanation
<code>dftb.inp</code>	Input file actually passed to DCDFTMD
<code>dftb.out</code>	Standard output file
<code>dftb.dat</code>	Detailed output file
<code>traject</code>	Trajectory file in MD calculation
<code>restart</code>	Restart file

---

**Hint:** **\*\* Working directory \*\***

- A working directory 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 directory 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 directory with the same name for continued jobs, by default, a backup of the previous job's working directory 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 directory is `aaa_gmx_tmp`, it will be `aaa_gmx_tmp1`.
    - **\*\* Unnumbered directories are always up to date. \*\***
- 

### 8.3.3 Open Log File (dco)

Open the dco (standard output) file with a text editor.

### 8.3.4 Open Detailed Data File (dat)

Open the detailed output file in a text editor.

### 8.3.5 Animation

#### OPT (dco)

Select a dco file and animate optimization calculation trajectory. Please refer to *Animation window* for how to operate the animation.

#### MD (traject)

Select dci and traject files and animate MD calculation trajectory. The main window file name does not change. Please refer to *Animation window* for how to operate the animation. You can calculate mean square displacement, self-diffusion coefficient, and radial distribution function from *Tools* → *Mean Square Displacement/Diffusion Constant* and *Tools* → *Radial Distribution Function* in Animation window. See *Diffusion Constant/Mean Square Displacement* or *Radial Distribution Function* for details.

### 8.3.6 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.

## 8.4 Hansen SP & QSPR model

Hansen solubility parameter (HSP) is calculated by atomic group contribution method. Various physical properties are calculated by atomic group contribution method and QSPR (structural property correlation). Purchase of add-on is necessary for using. It is also possible to process multiple molecular structures automatically and continuously using a batch file from the command line (see below).

1. After creating the molecule for which HSP is desired in the main window, click this menu. In the case of a polymer, make a repeat unit (eg ethane molecule in case of polyethylene) and left click on two points to be combined with the next report unit. This behavior is the same as Register Monomer of Polymer Builder function.
2. Click *Calc Hansen SP* button in the case of molecules, or *Calc Hansen SP for Polymer* button for polymer.
3. A csv file with HSP and various physical properties is created. The meaning of each item in the csv file is as follows. The unit of each physical property is written in the csv file.

Display name	Meaning
totHSP	$\text{Sqrt}((\text{dD14})^2+(\text{dP14})^2+(\text{dH14})^2)$ (Equivalent to Hildebrand solubility parameter)
dD14	HSP variance term
dP14	HSP polarization term
dH14	HSP hydrogen bond term
dHdo14	HSP hydrogen bond term (donor)
dHac14	HSP hydrogen bond term (acceptor)
polym_totHSP	$\text{Sqrt}((\text{polym\_dD14})^2+(\text{polym\_dP14})^2+(\text{polym\_dH14})^2)$ (Equivalent to Hildebrand solubility parameter)
polym_dD14	HSP dispersion term (for polymers)
polym_dP14	HSP polarization term (for polymers)
polym_dH14	HSP hydrogen bond term (for polymers)
polym_dHdo14	HSP hydrogen bond term (donor) (for polymers)
polym_dHac14	HSP hydrogen bond term (acceptor) (for polymers)
Boiling Point	Boiling Point
Melting point	Melting point
Log10(Viscosity)	Logarithmic viscosity
Standard enthalpy of formation	Standard generation enthalpy
Standard Gibbs free energy of formation	Standard Gibbs energy
Surface tension	surface tension
Thermal conductivity	Thermal conductivity

The calculated HSP and various physical properties are calculated by the group contribution method. The total number of atoms can be calculated up to 250, and the number of atoms excluding hydrogen can be calculated up to 120. The difference between the function for monomer and the function for polymer is, for example, in the case of polyethylene, whether the terminal is CH<sub>3</sub> or CH<sub>2</sub>. If you want to process multiple molecular structures automatically and continuously, use a batch file from the command line. For command line syntax, see *How to launch from the command prompt*. When you use the command line, a

csv file and a working folder are created in the original file folder. If you want to calculate the value for the polymer from the command line, change the atomic type of the two locations that bind to the adjacent repeat unit in the original file to At. For example, if you create a batch file as shown below and place a mol2 file in the same hierarchy as the batch file, then double-click the batch file to execute calculations continuously for the molecules in the mol2 file.

```
cd %~dp0
for %%F in (*.mol2) do (
  C:\winmos10\winmostar.exe %%F -s -hsp
)
pause
```

However, when calculating for a long time using a batch file, Warnings may appear such as “Do you want to stop running this script?”, “The script on this page is slowing down your web browser”, “If you keep running the script, your computer may stop responding”. In that case, please refer to the [Microsoft page here](#) and follow “Let me fix it myself” way to avoid the warning.

## 9.1 Integration with ChemDraw

Molecules modeled in ChemDraw can be loaded into Winmostar.

### 9.1.1 When reading 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.

### 9.1.2 When reading 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 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.

Execution of MOPAC	-mopac1, -mopac2, -mopac3 These correspond to the three MOPAC binaries selected in <i>Tools</i> → <i>Preferences menu</i> → <i>Program Path</i> .
Calculation of molecular surface area and volume	-molsv
Calculation of aspect ratio	-aspect
Coordinate Adjustment	-adjust
Add Hydrogens	-hadd
Delete All Hydrogens	-hdel
Quick Optimization	-clean
Change file type and save	-o output_file_extension
Save as specified file name	-outfile output_file_name

Use case:

```

"C:\winmos10\winmostar.exe" "C:\winmos10\samples\dbt.dat" -s -mopac1
"C:\winmos10\winmostar.exe" "C:\winmos10\samples\dbt.dat" -s -molsv 1 2.0 0.02
"C:\winmos10\winmostar.exe" "C:\winmos10\samples\dbt.dat" -s -o pdb "C:\winmos10\winmostar.exe"
"C:\winmos10\samples\dbt.dat" -s -adjust -hadd -clean -o gif

```



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.

## 10.2 cygwin\_wm

cygwin\_wm is Cygwin for Winmostar. It is called internally by Winmostar in the processing described in this manual as follows.

**Warning:** To use this function, *cygwin\_wm setup* is required.

Installation method is described in *cygwin\_wm setup*.

**Warning:**

- Some security countermeasure software may automatically delete or interfere with normal module in cygwin\_wm due to malfunction.
- If you download and install the cygwin\_wm installer from the Winmostar official HP, you can easily check for missing files in cygwin\_wm by using *Help* → *Check cygwin\_wm* function. (Only the existence of the file is checked.)
- If trouble occurs with the function that uses cygwin\_wm, please also check the activity report of security countermeasure software.

If you select *Tools* → *Cygwin*, you can start the console of cygwin\_wm directly.

- *If you start Winmostar with administrator privileges, you can not open files with drag-and-drop.*
- *Some software does not work if you enable the Windows “Use Unicode UTF - 8 for worldwide language support” option.*
- *Opening some subwindows such as Animation, Submit Job and so on, it will not appear even if you try to open again after closing.*
- *The graph display at the bottom of the Animation window collapses. Other UI display collapses.*
- *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.*
- *I can not calculate the RESP charge when using Firefly.*
- *Gromacs freezes while running Gromacs on local machine.*
- *Gromacs Chi or DPD parameter calculation function outputs 0.5 times the original definition.*
- *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.*
- *When outputting an animated GIF from the animation window, an error may occur if the number of frames is large.*

### **11.1 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)

## 11.2 Some software does not work if you enable the Windows “Use Unicode UTF - 8 for worldwide language support” option.

In English version Windows 10 (1803), if the check box is checked in [Control Panel] - [Region] - [Administrative] - [Change system locale . . .] - [Use Unicode UTF - 8 for worldwide language support] There was a report that FDMNES execution failed. This is a problem caused by fdmfile.txt being read at FDMNES execution being output with BOM. Winmostar is sequentially corresponded at the timing of the problem, but please contact us if similar problems occur with other functions. (Reported on May 25, 2018)

## 11.3 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)

## 11.4 The graph display at the bottom of the Animation window collapses. Other UI display collapses.

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)

## 11.5 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)

## 11.6 I can not calculate the RESP charge when using Firefly.

As Winmostar’s RESP charge calculation has been developed as a target for GAMESS (US), at present, please use GAMESS (US) only for calculation at RESP charge calculation after structure optimization using Firefly etc. In the future we plan to calculate RESP charge using Firefly. (Reported on July 31, 2018)

## 11.7 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. (Reported on July 31, 2018)

## 11.8 Gromacs Chi or DPD parameter calculation function outputs 0.5 times the original definition.

If you are a V9 or V8 user, please update to 9.0.2 or later or 8.027 or later where the bug has been fixed. Since V7 is outside the support period, please be careful about the calculated value. (Reported on June 2, 2019)

## 11.9 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 (Ifcpopt = .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)

## 11.10 When outputting an animated GIF from the animation window, an error may occur if the number of frames is large.

Use *Export JPEG Images* to output serial JPEG files, and then create animation files using various movie creation software. (Reported on January 29, 2020)

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### Frequently asked questions · Troubleshooting

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- *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?*
- *Terms and conditions of use of each license*
  - *Q. Please tell me how to use it in the lecture. Please tell me the terms of use of lecture license.*
  - *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?*
- *License Code*
  - *How do I change an already entered license code?*
  - *Q. Please tell me how to display the MAC address.*
- *Support and Maintenance*
  - *Are there any precautions when asking a question?*
  - *How to pronounce Winmostar.*
  - *Q. How long do you plan to support and maintain the previous version?*
  - *Q. Is it possible to update/upgrade version of the Winmostar I am using?*
- *Software operations*
  - *Q. I can not create a model as I expected. It can not calculate. It does not work.*
  - *Q. Please tell me the minimum and recommended specifications of PC for Winmostar.*

- *Q. Is it possible to install Winmostar on a PC that is not connected to the network?*
- *Q. "ERROR: I/O error 32" is displayed and the processing fails.*
- *Q. Is it possible to use the created molecular model etc for academic presentations and papers? How should I quote at conference presentations and paper submissions?*
- *Q. Process using Cygwin will end abnormally. / tools → diagnose cygwin\_wm function will display ... ERROR ... / Cygwin's black window shows child\_info\_fork :: abort: ... Loaded to different address: parent ... != Child ...*
- *Q. Tools → Check cygwin\_wm function will display WARNING ... some files are missing.*
- *The job registered in Job Manager is not executed.*
- *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. Does Winmostar work in an offline environment without internet connection? Is Winmostar software that requires an Internet connection?*
- *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 I open a file or model a molecule, the bonds no longer appear or a lot of extra bonds have come to appear.*
- *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.*
- *MPI on local machine, parallel execution*
  - *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.*
- *Remote Jobs*
  - *Q. Please tell me how to submit a job to a supercomputer or a linux server in my company or my campus.*
  - *Remote Job Submission is not working.*
  - *Q. The connection test with Test Connection succeeds, but the job submission fails.*
- *MOPAC, CNDO/S, GAMESS, NWChem, Gaussian*
  - *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. It can not be calculated when Method=INDO is used in CNDO/S.*
  - *Q. Is it possible to speed up 3D display of ESP (electrostatic potential) of GAMESS, Gaussian, and NWChem?*

- *Q. I can not run NMR calculation with GAMESS.*
  - *Q. When running GAMESS, “\* ERROR: MEMORY REQUEST EXCEEDS AVAILABLE MEMORY” etc. will be output to the log and the calculation will end abnormally.*
  - *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 parallel execution of NWChem, the calculation outputs “Please specify an authentication passphrase for smpd:” to the log and does not run.*
  - *Q. I read the Gaussian out file, but the orbital (eigen) energy etc. are not written.*
  - *Q. How do I calculate the chk file read in Gaussian?*
  - *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”.*
- *Gromacs, LAMMPS*
    - *Q. How can we equilibrate the system in molecular dynamics calculation?*
    - *Q. Even if Gromacs ER method result loading is executed, the result can not be displayed / an error will appear.*
    - *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 after MD calculation?*
    - *Q. Can I calculate dielectric constant from Gromacs or LAMMPS (Molecular Dynamics Calculation)?*
    - *Q. When loading the final structure or animation in Gromacs, the molecules are sometimes displayed in pieces.*
  - *About Quantum ESPRESSO, OpenMX*
    - *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. 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. 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. When executing Phonon calculation using Quantum ESPRESSO, ph.x output (ph.out) displays “The phonon code with US-PP and raman or elop not yet available” and the calculation result can not be acquired .*
- *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)?*
- *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.*

## 12.1 Purchase

### 12.1.1 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.

### 12.1.2 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.

### 12.1.3 Q. How do I place an order other than an end user, such as an agency?

A.

Please use a designated agent. For more information, please visit [Pricing](#).



## 12.2 Terms and conditions of use of each license

### 12.2.1 Q. Please tell me how to use it in the lecture. Please tell me the terms of use of lecture license.

A.

The lecture license is available only for lecture purposes at educational institutions, and for all students participating in teachers and classes.

Please check the following notes when applying.

- Please contact directly from the teacher who is lecturing.
- Please enter the name of the lecture, period, approximate number of students in the detail entry field.
- I am pleased to share the lesson materials later.

You can apply for lecture a license [here](#).

### 12.2.2 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).

### 12.2.3 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 move from your institutional affiliation at the time of purchase, you cannot use it, even if it is a permanent right.

## 12.3 License Code

### 12.3.1 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.

### 12.3.2 Q. Please tell me how to display the MAC address.

A. In Windows 10, start the command prompt by clicking on *Start menu* → *Windows System Tools* → *Command Prompt*. Then, in a command prompt window, type `ipconfig /all` and press the Enter key. Look for the “Physical Address” line among the various information that will be output. That content is 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.

## 12.4 Support and Maintenance

### 12.4.1 Are there any precautions when asking a question?

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.

### 12.4.2 How to pronounce Winmostar.

win·mo·str

### 12.4.3 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.

### 12.4.4 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.

## 12.5 Software operations

### 12.5.1 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 and cygwin\_wm 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, 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)

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.

- 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 cygwin\_wm, and solvers including MPI from monitoring.
- If you are using cygwin\_wm, run *Help* → *Check cygwin\_wm* and perform a simple diagnosis of cygwin\_wm.
- Reinstall Winmostar, cygwin\_wm 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 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 occurred 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](#).

### 12.5.2 Q. Please tell me the minimum and recommended specifications of PC for Winmostar.

A. See [Hardware requirements](#).

### 12.5.3 Q. Is it possible to install Winmostar on a PC that is not connected to the network?

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.

### 12.5.4 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.

**12.5.5 Q. Is it possible to use the created molecular model etc for academic 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*.

**12.5.6 Q. Process using Cygwin will end abnormally. / tools → diagnose cygwin\_wm 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) 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 `cygwin_wm` on the same machine.
- `cygwin1.dll` may be included in various freeware etc even if you do not install Cygwin in other location.

- 4) With all Cygwins on the machine being used terminated, at the [Run] of Windows `C:\cygwin_wm\bin\ash.exe` (when `cygwin_wm` is installed in `C:\cygwin_wm`), execute the `/bin/rebaseall -v`, and restart the machine.
- 5) 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)*.
- 6) Temporarily disable security software.
- 7) Disable software that tends to cause problems described in [Cygwin FAQ](#).
- 8) In addition, try the method described in [Cygwin FAQ fork\(\) related failures](#).
- 9) Install a new version of Cygwin from the [Cygwin official site](#) and check if you can start a terminal.

**12.5.7 Q. Tools → Check cygwin\_wm function will display WARNING ... some files are missing.**

A. Please reinstall `cygwin_wm`.

If it is displayed even after the reinstallation, temporarily disable the security software, or exclude installation destination and installer from monitoring.

### 12.5.8 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.

### 12.5.9 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.

### 12.5.10 Q. Does Winmostar work in an offline environment without internet connection? Is Winmostar software that requires an Internet connection?

A. Winmostar works in an offline environment. Also, only a few features require an Internet connection. As of V10.0.1, only the download function of pseudopotential file for Quantum ESPRESSO requires an Internet connection. This function does not start unless the user explicitly operates it, so it does not operate in the background.

### 12.5.11 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. Check if the line feed code or encoding has changed.

### 12.5.12 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. The value of *Bonding factor* in *Tools* → *Preferences* → *Edit* may not be appropriate. Return to the default value or set a value around 1.15.

## 12.6 On the modeling of molecules and creation of systems

### 12.6.1 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.

## 12.6.2 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. If you still can not do it, reinstall internally used Gromacs in the following procedure.

1) Comment out or delete the line of

```
source /usr/local/gromacs_sse/bin/GMXRC
```

Or

```
source /usr/local/gromacs_avx/bin/GMXRC
```

in `/etc/profile.d/winmostar.sh` under `cygwin_wm` installation folder.

2) Click *Tools* → *Cygwin* of Winmostar and try 1-2. [Gromacs of Installation procedure of solvers for Winmostar](#) on the installed cygwin.

3) Click *Tools* → *Cygwin* and run **gmx**. Rebuild will be successful if a message indicating *GROMACS: gmx, VERSION...*, etc. is displayed.

There are cases where the number of molecules is large (depending on the case, but it is about 10,000), since it is currently the limit of processing of **gmx solvate**, which is used in internal processing, *Edit* → *Modify Selected Group* → *Replicate*. In future it is also planned to handle cases where the number of molecules is large with this function.

## 12.7 MPI on local machine, parallel execution

### 12.7.1 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 ready, 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.

**12.7.2 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.

## 12.8 Remote Jobs

**12.8.1 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.

**12.8.2 Remote Job Submission is not working.**

——— 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.)

### 12.8.3 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 .

## 12.9 MOPAC, CNDO/S, GAMESS, NWChem, Gaussian

### 12.9.1 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 also supports MOPAC2016.

MOPAC2016 has no limit on the number of atoms, and is free for those who belong to a institution for academic degrees.

*MOLSIS web page* <<https://www.molsis.co.jp/en/>>

### 12.9.2 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.

### 12.9.3 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*.

### 12.9.4 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.

### 12.9.5 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.

### 12.9.6 Q. I can not run NMR calculation with GAMESS.

A. First of all, please take action of *general errors*.

It is necessary to set DIRSCF=.F. in \$SCF and NCPUS=1 because parallel calculation is not supported.

(The details are listed as follows at the end of the calculation result output.)

```
INCOMPATIBLE OPTION CHOSEN WITH RUNTYP=NMR ***
NMR MAY BE COMPUTED ONLY FOR SCFTYP=RHF,
NO CORRELATION OPTION (DFTTYP, CITYP, CCTYP, MPLEVL) MAY BE CHOSEN
NO SEMI-EMPIRICAL OPTION (GBASIS=AM1/PM3/MNDO) MAY BE CHOSEN
DIRECT AO INTEGRAL CALCULATION (DIRSCF) IS NOT ENABLED,
AND/OR PARALLEL EXECUTION IS NOT ENABLED.
```

**12.9.7 Q. When running GAMESS, “\* ERROR: MEMORY REQUEST EXCEEDS AVAILABLE MEMORY” etc. will be output to the log and the calculation will end abnormally.**

A. It means that the allocated memory capacity of GAMESS is insufficient. You can avoid errors by increasing the value of MWORDS in the input file.

**12.9.8 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.

**12.9.9 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.

**12.9.10 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.

**12.9.11 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.

**12.9.12 Q. I read the Gaussian out file, but the orbital (eigen) energy etc. are not written.**

A. It is not output if pop=full or pop=regular is missing in the Gaussian input file.

### 12.9.13 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.

### 12.9.14 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.

## 12.10 Gromacs, LAMMPS

### 12.10.1 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.

### 12.10.2 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.

### 12.10.3 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.

### 12.10.4 Q. Why do molecules sometimes come out of the cell when in the trajectory or the final structure after MD 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*.

### 12.10.5 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.

### 12.10.6 Q. When loading the final structure or animation in Gromacs, the molecules are sometimes displayed in pieces.

A. This problem is caused by a minor bug in Gromacs. Considering the periodic boundary condition, the shape of the molecule is maintained, and it is properly processed as a molecular dynamics calculation, so there is no problem in analyzing the results. To modify the appearance, select *display* → *periodic boundary condition format* to *relocate atomically inside the cell*.

## 12.11 About Quantum ESPRESSO, OpenMX

### 12.11.1 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](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>>.

### 12.11.2 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.

### 12.11.3 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*.

- Check if it tends not to converge really.
- 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.
- Up / down gives the arrangement of spins.
- Constrain the magnetic moment of the whole system.
- Use a reasonable initial structure.
- Use structures obtained by experiments and other calculation methods.
- If there are arbitrary atoms (placement of light elements, solid solutions, defects, non-integral components etc. which can not be seen with X rays) in the calculation, try different arrangements.
- 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`.
- Change the type of pseudopotential.
- Adjust the initial value of spin polarization. (Atomic unit or whole system)
- 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).
- Adjust the parameters of matrix calculation (review only settings that are difficult to converge).
- If large dipole moment occurs in the system, such as molecules are adsorbed on the slab, correct the dipole.

Try in balance with calculation time / calculation precision:

- Take a large cutoff energy.
- Take a lot of K points.
- Adjust smearing (type / width).
- Reduce the degree of update of the wave function (`mixing_beta` in QE).

Try with balance with calculation accuracy:

Loosen the convergence parameter of the SCF.

#### **12.11.4 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).

**12.11.5 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.

**12.11.6 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.

**12.11.7 Q. When executing Phonon calculation using Quantum ESPRESSO, ph.x output (ph.out) displays “The phonon code with US-PP and raman or elop not yet available” and the calculation result can not be acquired .**

A. Use a norm preserving pseudopotential.

**12.11.8 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.

**12.11.9 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)?*.

## 12.12 Addons

**12.12.1 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.

**12.12.2 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.