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Winmostar tutorial

Gromacs

Vapor Pressure・Surface Tension

V7.025

X-Ability Co., Ltd.

question@winmostar.com

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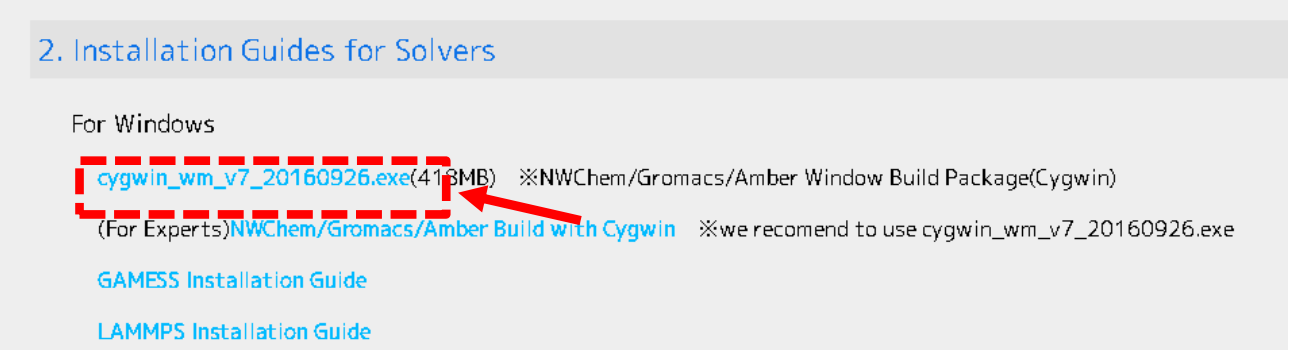
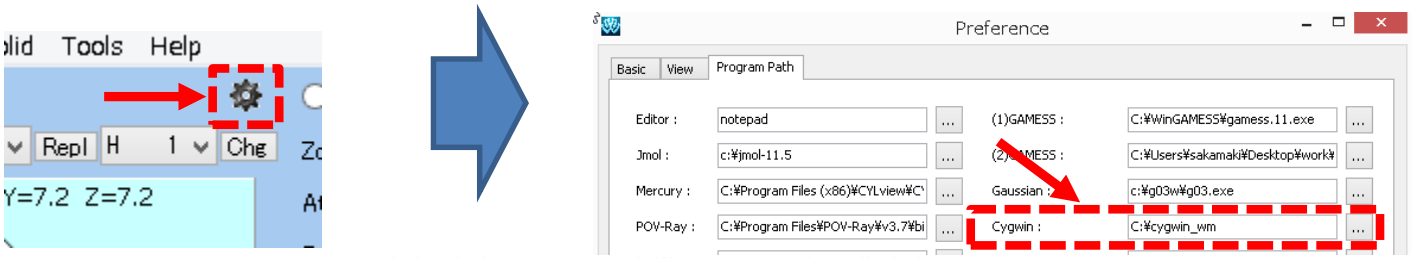
Configure

You must set up Cygwin to use Gromacs on Winmostar.

- Obtain the installer for Cygwin, which contains the all programs needed by Winmostar, at https://winmostar.com/en/manual_en.html.



- When you change the installation path for Cygwin from the default one, specify it on the preference panel.



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Note

- The simulation steps required are dependent on molecular species and initial density.
- To obtain accurate and reproducible results, you have to set long simulation time.
- The method for interaction calculations and/or the force field also affect the simulation results.
- Insert vacuum layer as needed before executing calculations for equilibrium.

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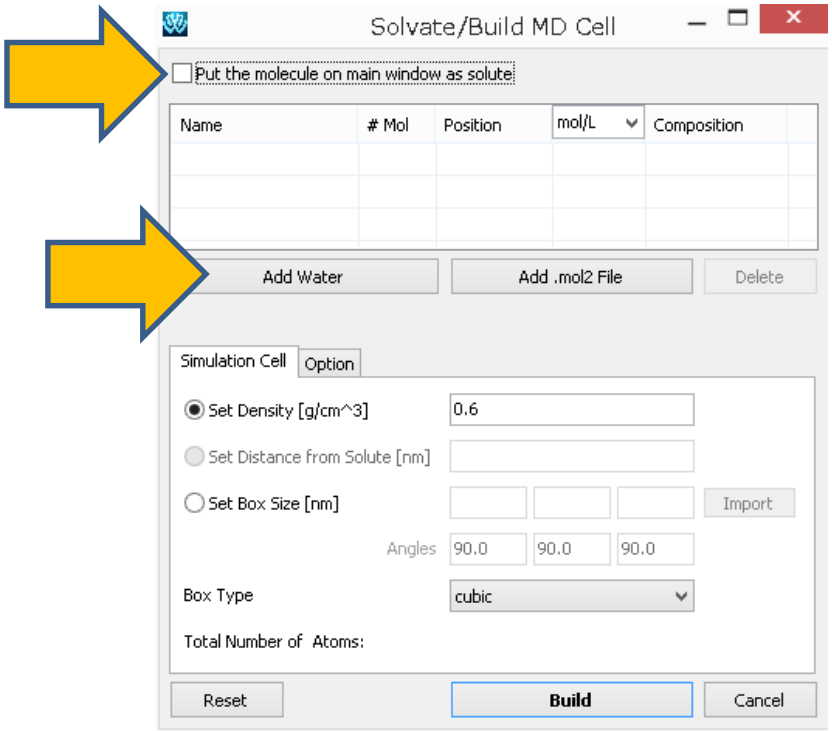
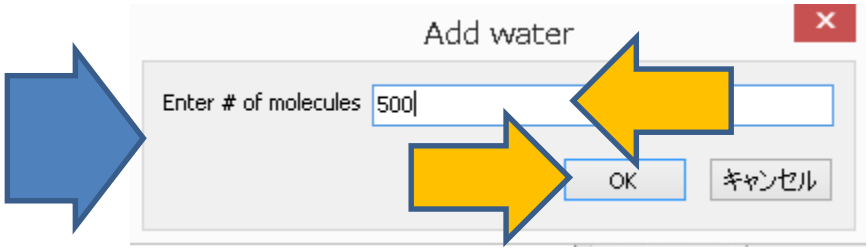
I. Build a simulation cell

In this tutorial, we'll calculate the saturated vapor pressure and surface tension with a vapor–liquid equilibration.

1. Click **MD | Solvate/Build Cell**.
2. Uncheck **Put the molecule on main window as solute**.
3. Click **Add water**. Set **Enter # of molecules** to **500**.
4. Click **OK**.





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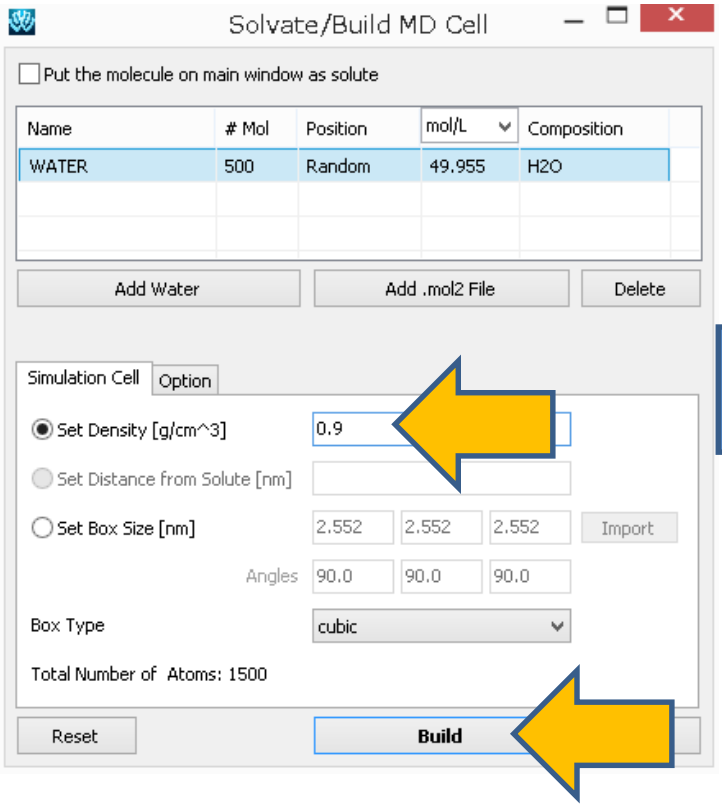
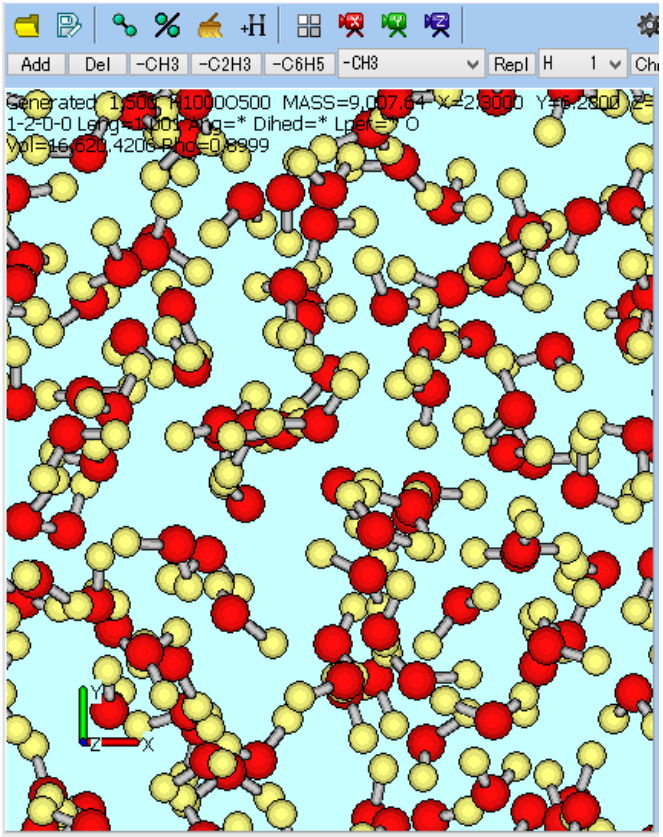
I. Build a simulation cell

1. Set **Set Density** to **0.9**.
2. Click **Build**.





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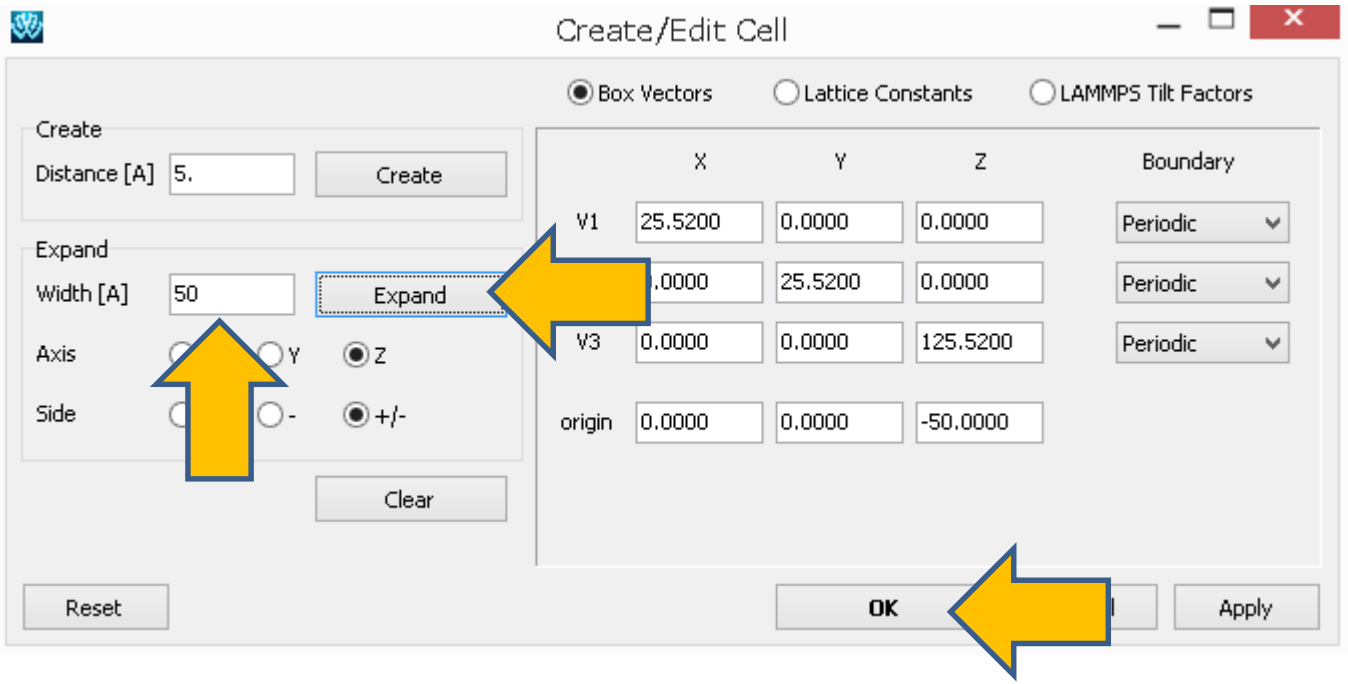
I. Build a simulation cell

1. Click **Edit | Solvate/Build Cell**.
2. On **Expand**, set **Width** to **50**, then click **Expand**.
3. Click **OK**.



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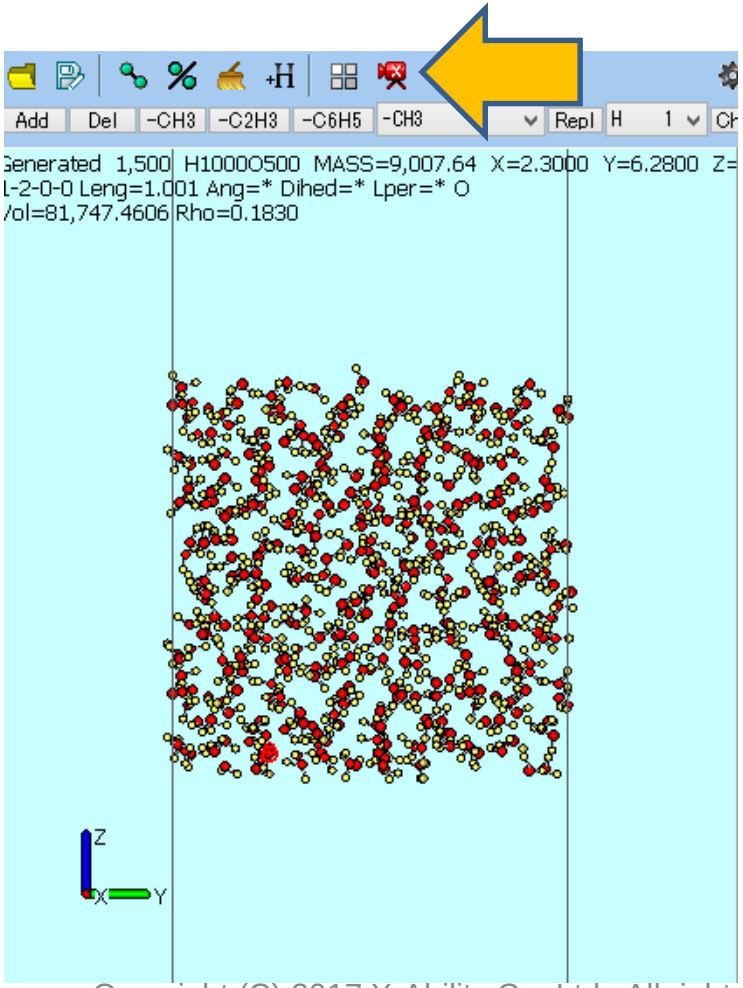
I. Build a simulation cell

Click the icon of red X camera, then zoom out the camera.
Vapor – liquid equilibration system has been built.



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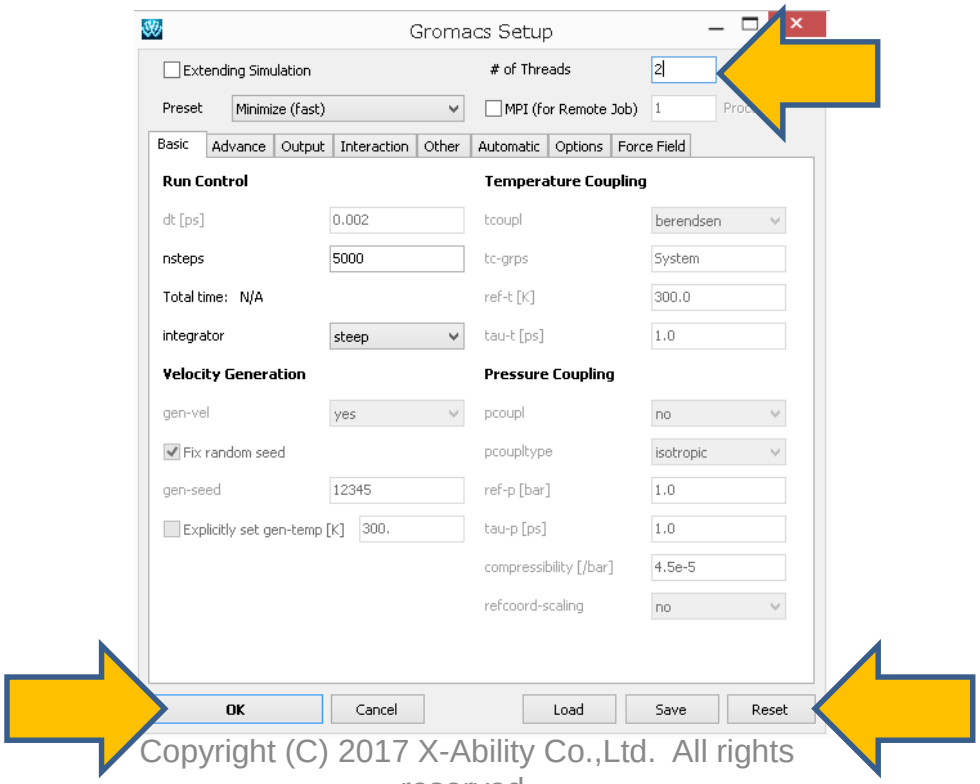
II. Equilibration

1. Click **MD | Gromacs | Keywords Setup**.
2. Click **Reset**.
3. Click **# of Threads** to parallel number, then click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.
5. Save the coordinate file as **spce500k.gro**, the topology file as **spce500k.top**.



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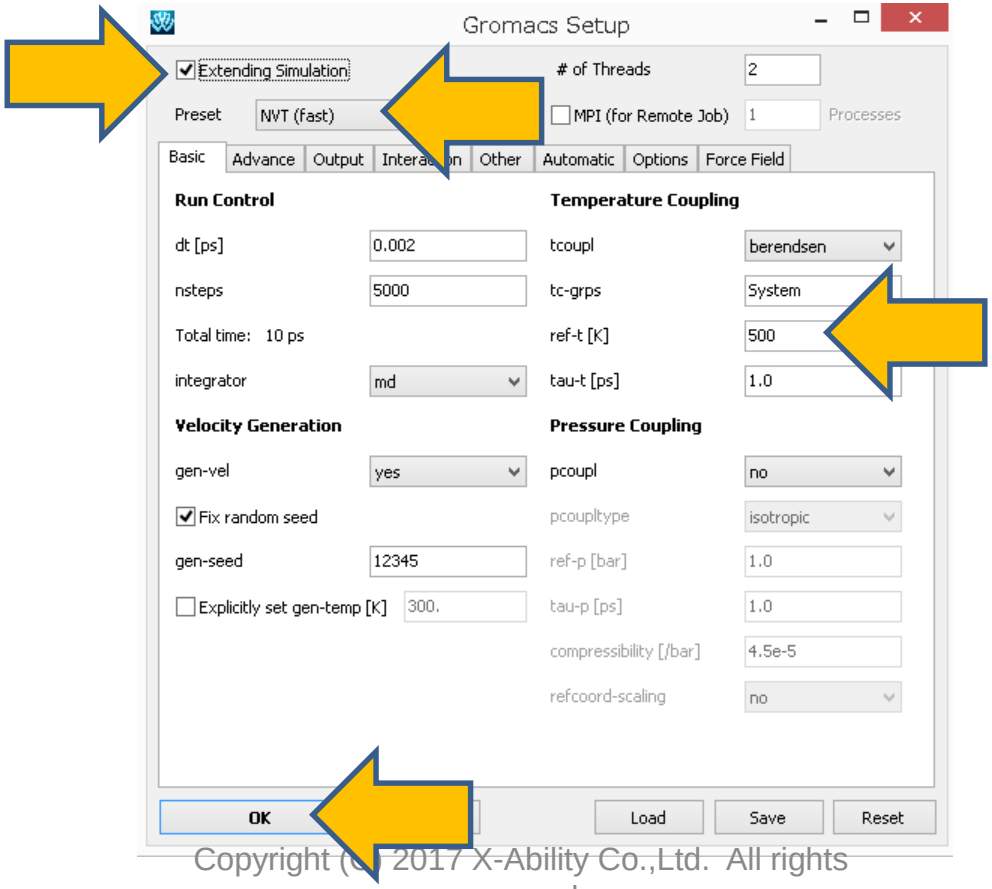
II. Equilibration

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Check **Extending Simulation**.
3. Set **Preset** to **NVT (fast)**, **ref-t [K]** to **500**, then click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



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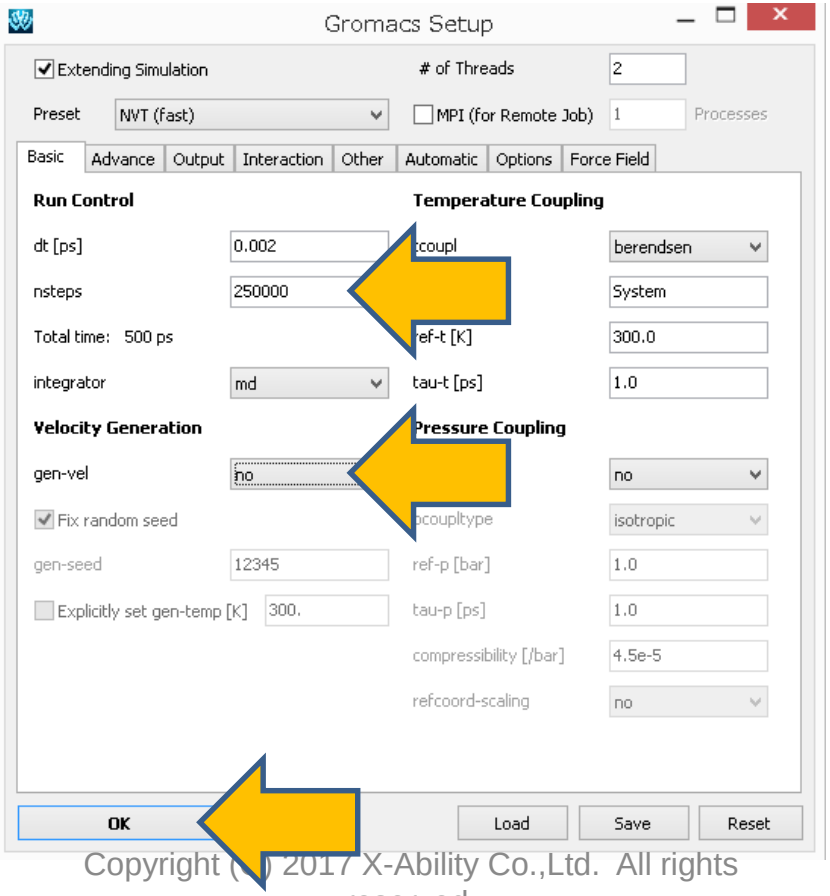
III. Product run

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **nsteps** to **250000**, **gen-vel** to **no**, then click **OK**.
3. Click **MD | Gromacs | Start Gromacs**.



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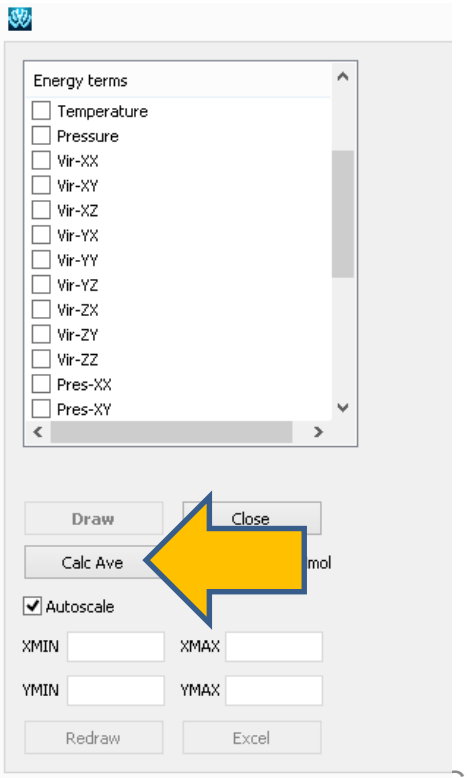
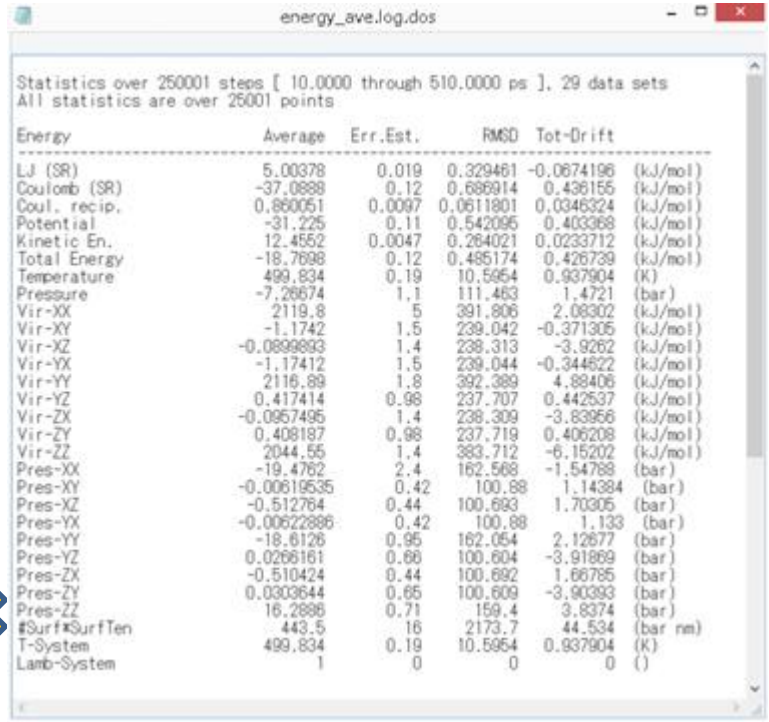
IV. Analyze

1. Click **MD | Gromacs | Energy Plot**.
2. Open the edr file selected by default.
3. Click **Calc Ave**, then open the gro file selected by default.

[Pres-ZZ] indicates vapor pressure (vapor-liquid pressure, the unit is bar),
[#Surf*SurfTen] indicates the product of number of interfaces (2 in this case) multiplied by surface tension (the unit is bar*nm).




energy_ave.log.dos

Statistics over 250001 steps [10.0000 through 510.0000 ps], 29 data sets
All statistics are over 25001 points

Energy	Average	Err.Est.	RMSD	Tot-Drift	
LJ (SR)	5.00378	0.019	0.329461	-0.0674196	(kJ/mol)
Coulomb (SR)	-37.0888	0.12	0.686914	0.436156	(kJ/mol)
Coul. recip.	0.860051	0.0097	0.0611801	0.0346324	(kJ/mol)
Potential	-31.225	0.11	0.542095	0.403368	(kJ/mol)
Kinetic En.	12.4552	0.0047	0.264021	0.0233712	(kJ/mol)
Total Energy	-18.7698	0.12	0.485174	0.426739	(kJ/mol)
Temperature	499.834	0.19	10.5954	0.937904	(K)
Pressure	-7.26674	1.1	111.463	1.4721	(bar)
Vir-XX	2119.8	5	391.806	2.08302	(kJ/mol)
Vir-XY	-1.1742	1.5	239.042	-0.371305	(kJ/mol)
Vir-XZ	-0.0899893	1.4	238.313	-3.9262	(kJ/mol)
Vir-YX	-1.17412	1.5	239.044	-0.344622	(kJ/mol)
Vir-YY	2116.89	1.8	392.389	4.88406	(kJ/mol)
Vir-YZ	0.417414	0.98	237.707	0.442537	(kJ/mol)
Vir-ZX	-0.0957495	1.4	238.309	-3.83956	(kJ/mol)
Vir-ZY	0.408187	0.98	237.719	0.406208	(kJ/mol)
Vir-ZZ	2044.55	1.4	383.712	-6.15202	(kJ/mol)
Pres-XX	-19.4762	2.4	162.568	-1.54788	(bar)
Pres-XY	-0.00619535	0.42	100.88	1.14384	(bar)
Pres-XZ	-0.512764	0.44	100.693	1.70305	(bar)
Pres-YX	-0.00622886	0.42	100.88	1.133	(bar)
Pres-YY	-18.6126	0.95	162.054	2.12677	(bar)
Pres-YZ	0.0266161	0.66	100.604	-3.91869	(bar)
Pres-ZX	-0.510424	0.44	100.692	1.66785	(bar)
Pres-ZY	0.0303644	0.65	100.609	-3.90393	(bar)
Pres-ZZ	16.2886	0.71	159.4	3.8374	(bar)
#Surf*SurfTen	443.5	16	2173.7	44.534	(bar nm)
T-System	499.834	0.19	10.5954	0.937904	(K)
Lamb-System	1	0	0	0	()

Reference: R. Sakamaki *et al.*, J. Chem. Phys., 134, 124708 (2011).

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IV. Analyze

1. Click **MD** | **Gromacs** | **Density Profile**.
2. Open default files for 3 times.
3. Click **Draw** to draw Density distribution toward the z axis.

If you need the density of liquid or gas phase respectively, click **Excel** to obtain csv file. Try distribution fitting configurations on various graphing softwares.