

Winmostar Tutorial

Quantum ESPRESSO

Car-Parrinello MD

V8.007

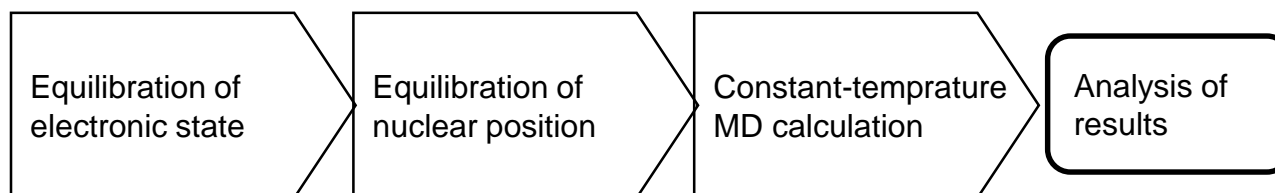
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Summary

- In this tutorial, we will calculate Car-Parrinello (CP) MD calculation of a methane molecule for a very short time. This procedure will gradually equilibrate electrons and nuclei to avoid calculation failures.



Notes:

- Number of bands, type of pseudopotential, and cutoff energy will all affect calculation results. In this tutorial, we use a setting with reduced precision for faster processing.
- The size of systems will affect calculation results.
- In order to produce data with high reproducibility, spend enough time on equilibration and set longer calculation times.

Configuration

See Quantum ESPRESSO install manual

https://winmostar.com/en/QE_install_manual_en_win.pdf

I. Molecular Modeling

Model a CH₄ molecule in the main window.

Winmostar 5 CH4 MASS=16.04 X=1.1000 Y=0.0000 Z=0.0000
2-5-1-2 Leng=1.791 Ang=35.500 Dihed=0.000 Lper=0.000 H

AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF MMOK
Winmostar

1	C	0.00000	1	0.0000	1	0.0000	1	0	0	0
2	H	1.10000	1	0.0000	1	0.0000	1	1	0	0
3	H	1.10000	1	109.0000	1	0.0000	1	1	2	0
4	H	1.10000	1	109.0000	1	120.0000	1	1	2	3
5	H	1.10000	1	109.0000	1	-120.0000	1	1	2	3

2	H	1.1	0	0	1	0	0
<input type="checkbox"/>	XYZ	1	1	1			

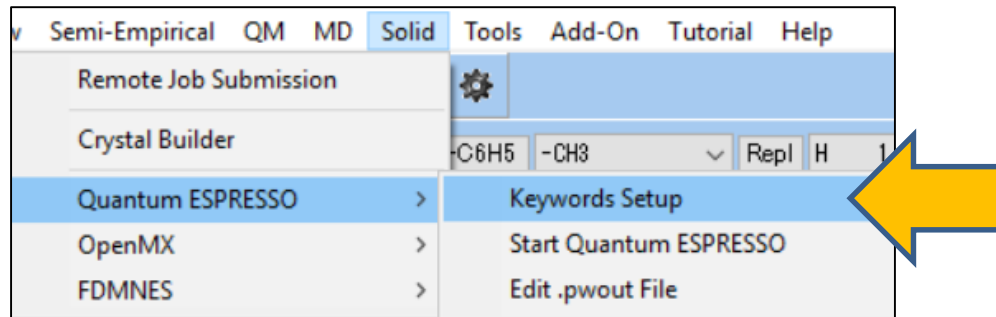
I. Molecular Modeling

1. Click **Edit | Create/Edit Cell | Create**.
2. Click **OK** in the **Create/Edit Cell** window to create cell.

The screenshot illustrates the steps to create a cell in the software. It shows the 'Edit' menu with 'Create/Edit Cell' highlighted. The 'Create/Edit Cell' dialog box is open, showing the 'Create' section with a 'Create' button. The 'Expand' section has 'Width [A]' set to 5 and 'Axis' set to Z. The 'Boundary' section has 'Periodic' selected for V1, V2, and V3. The 'OK' button is also highlighted. The final result is a 3D molecular model of a CH4 molecule in a unit cell, with a coordinate system (X, Y, Z) shown at the bottom left.

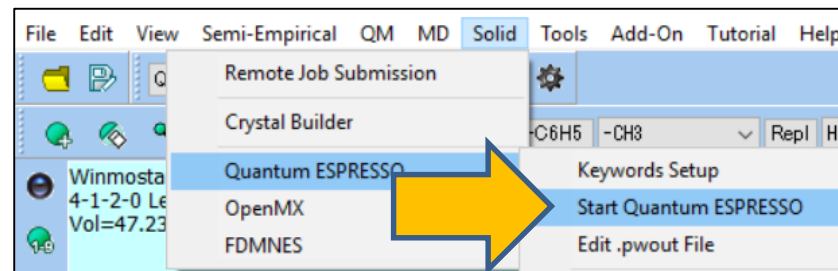
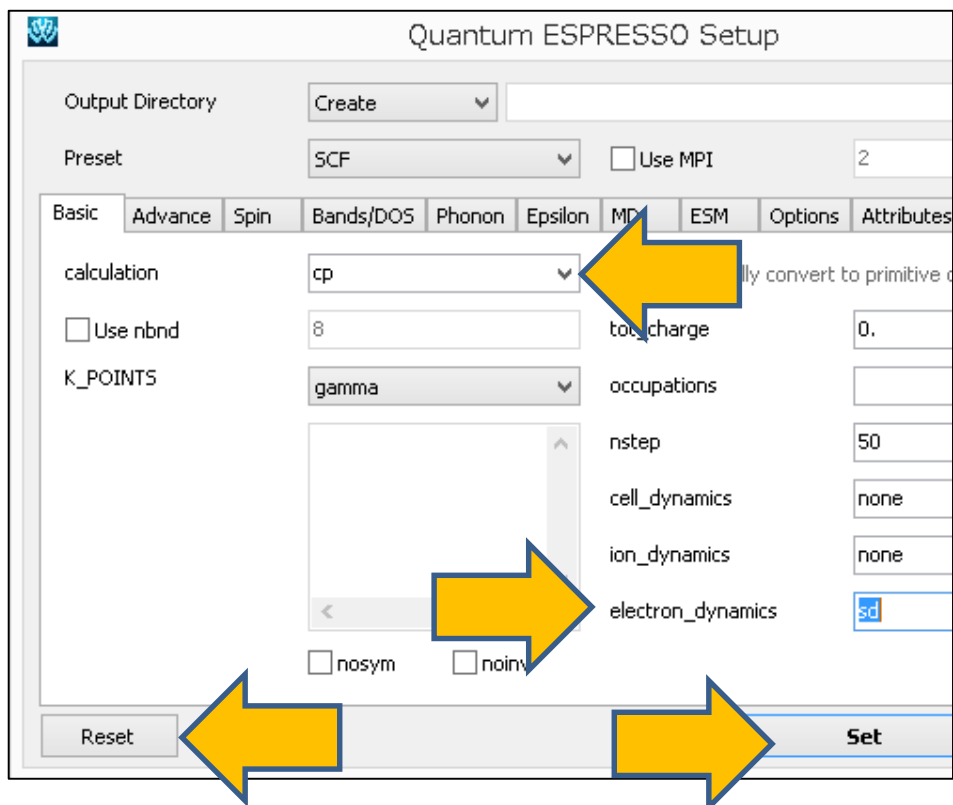
II. Equilibration of Electronic State

Click **Solid | Quantum ESPRESSO | Keyword Setup**.



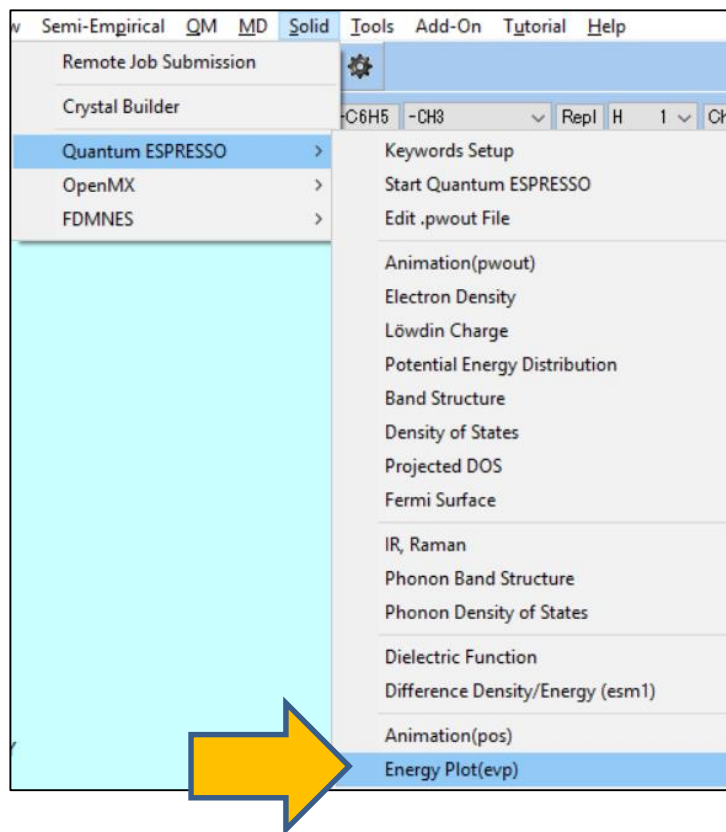
II. Equilibration of Electronic State

1. First click **Reset**. Set **calculation** to **cp**, **electron_dynamics** to **sd**, then click **Set**.
2. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
3. Save file to start calculation.



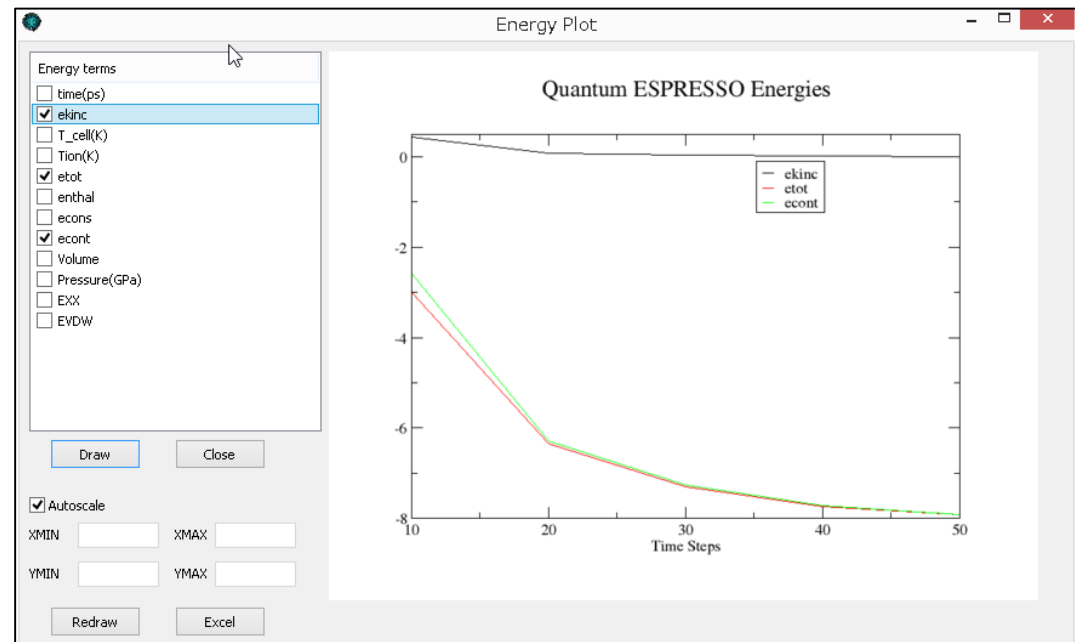
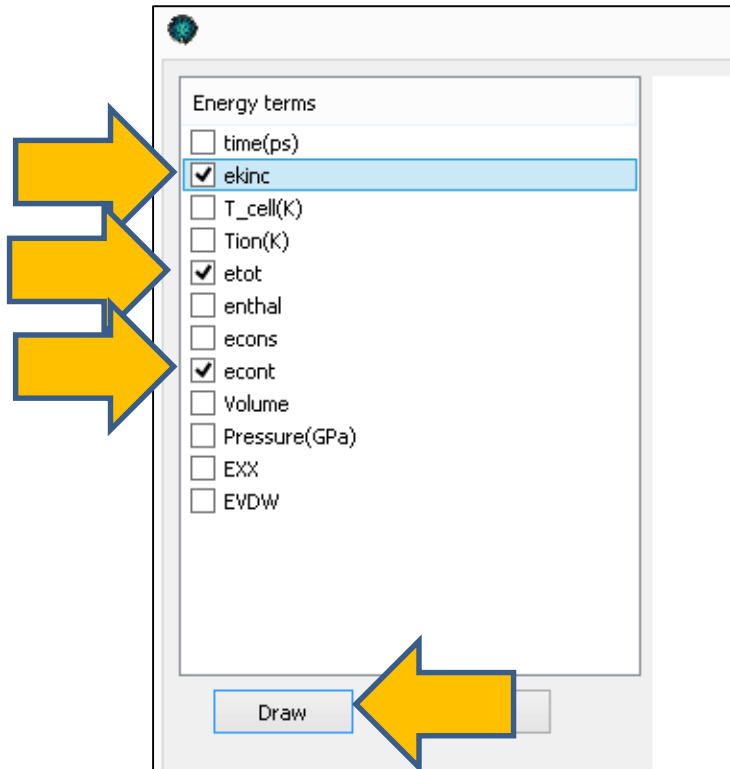
II. Equilibration of Electronic State

1. When calculation is complete, click **Solid | Quantum ESPRESSO | Energy Plot (evp)**.
2. Select directory suggested by default.



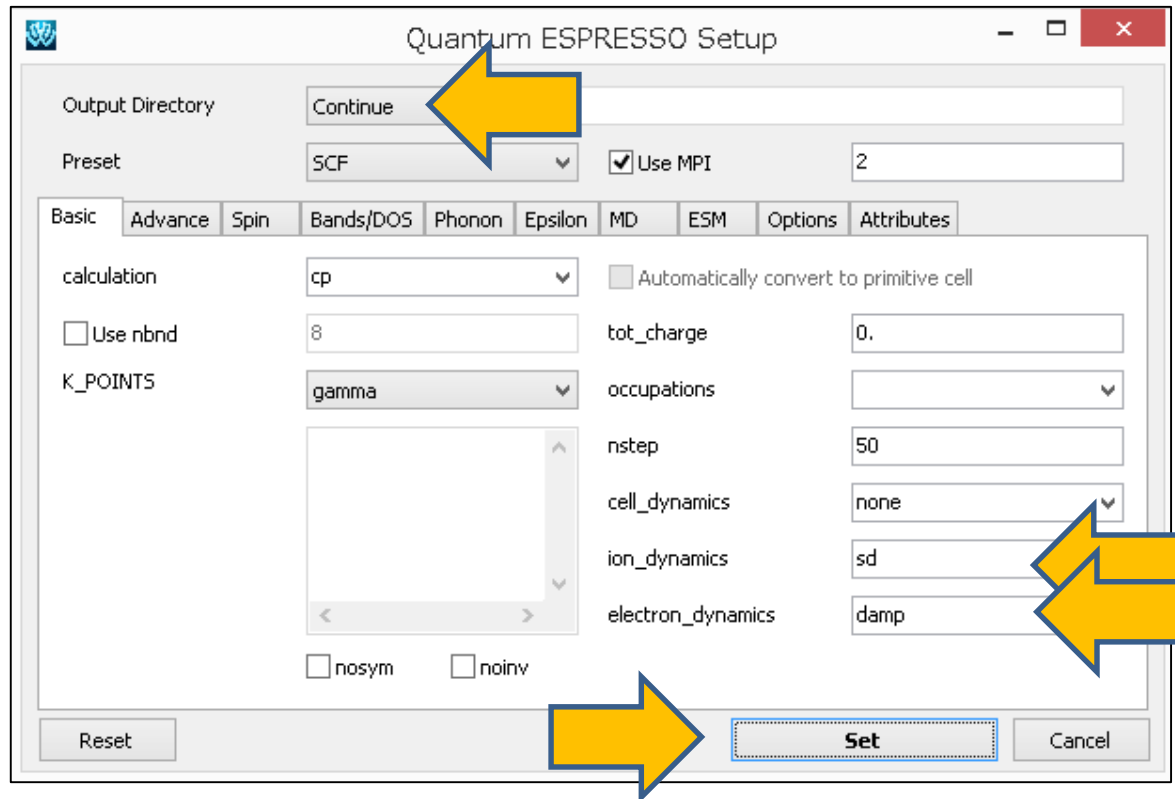
II. Equilibration of Electronic State

1. In the Energy Plot window, click the check boxes for **ekinc** (hypothetical kinetic energy of electrons) , **etot** (electrostatic potential energy of electrons), **econt** (total energy).
2. Click **Draw** to obtain a graph showing reducing energy levels.



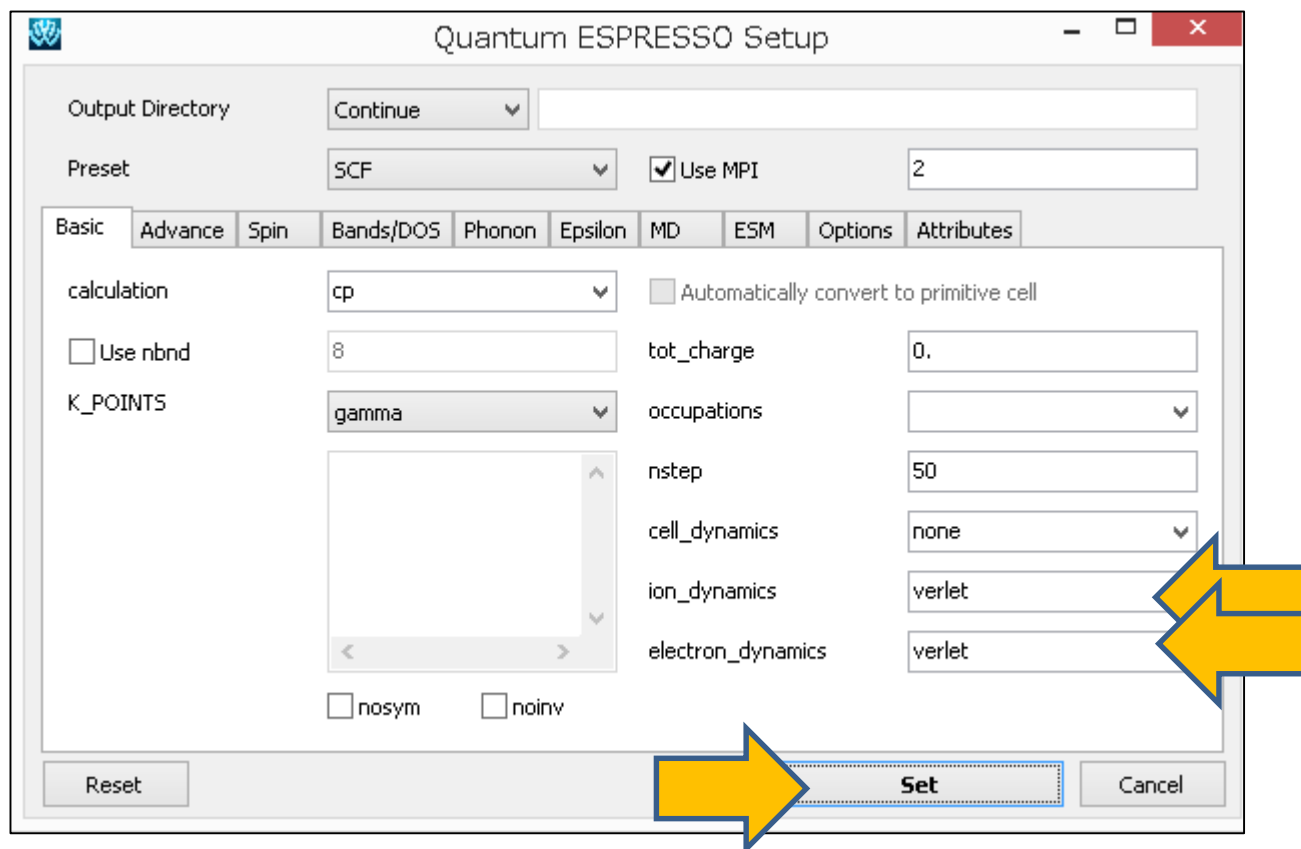
III. Equilibration of Nuclei

1. Click **Solid | Quantum ESPRESSO | Keyword Setup**.
2. Set **Output Directory** to **Continue**, **ion_dynamics** to **sd**, and **electron_dynamics** to **damp**, then click **Set**.
3. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO** to begin calculation.



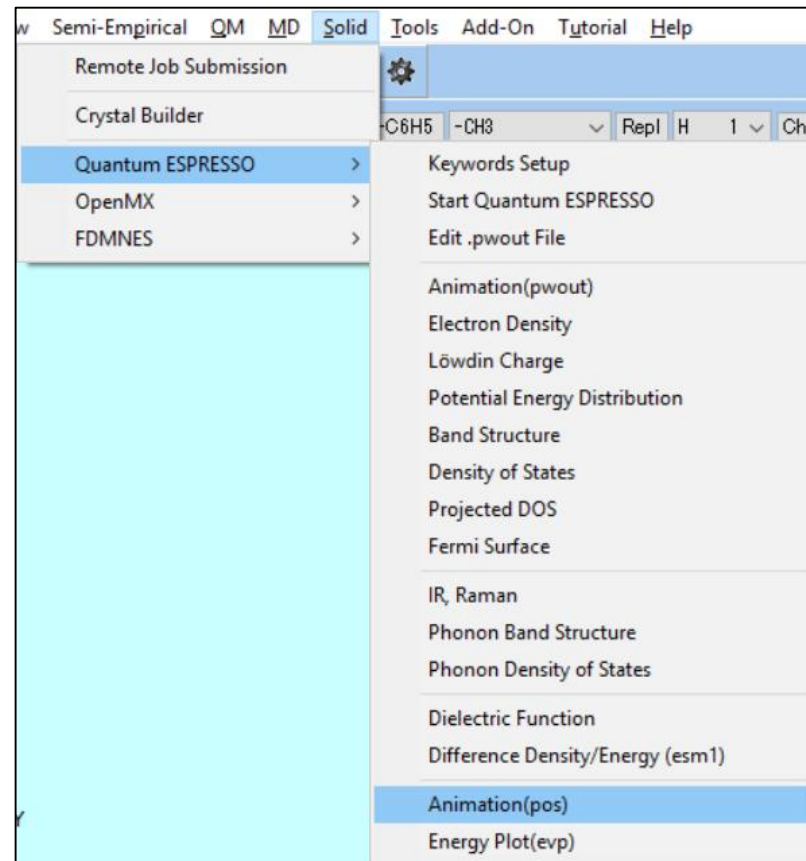
IV. Constant-Temperature MD Calculation

1. Click **Solid | Quantum ESPRESSO | Keyword Setup**.
2. Set both **ion_dynamics** and **electron_dynamics** to **verlet**, then click **Set**.
3. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO** to begin calculation.



V. Analysis

1. When calculation is complete click **Solid | Quantum ESPRESSO | Animation (pos)**.
2. Select the three files suggested by default.



V. Analysis

Click the **play button** (\triangleright) to view each step.

To view in an external viewer such as VMD, click **gro**.

