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Winmostar Tutorial
Quantum ESPRESSO
Car-Parrinello MD
V8.007

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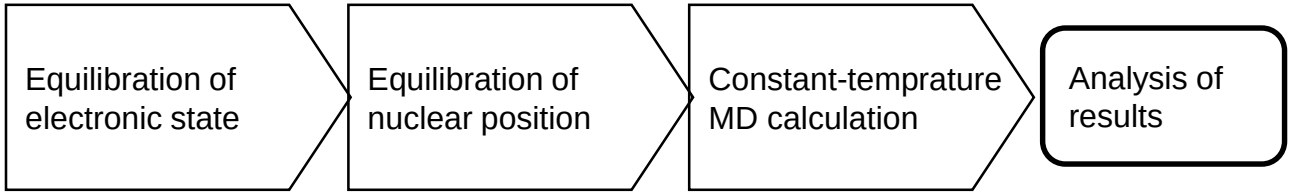
Summary

- 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.

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Configuration

See Quantum ESPRESSO install manual
https://winmostar.com/en/QE_install_manual_en_win.pdf

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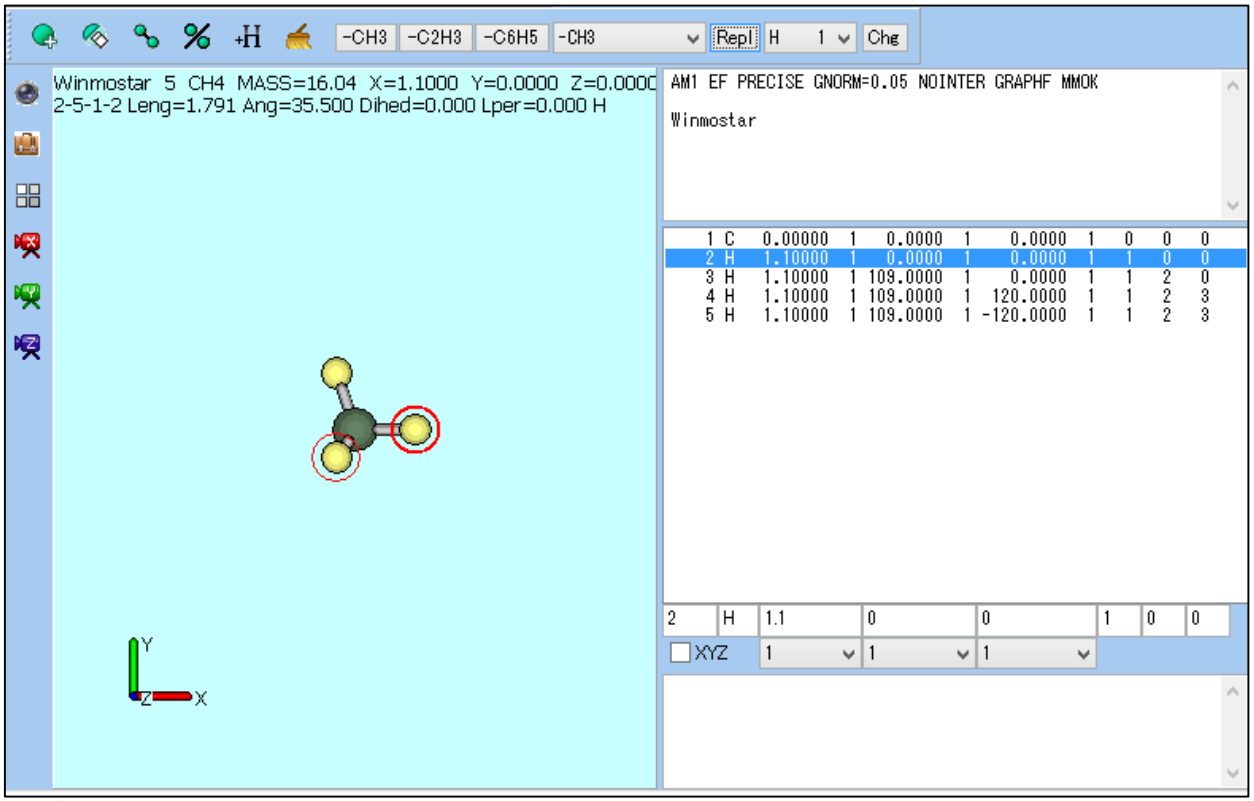
I. Molecular Modeling

Model a CH_4 molecule in the main window.



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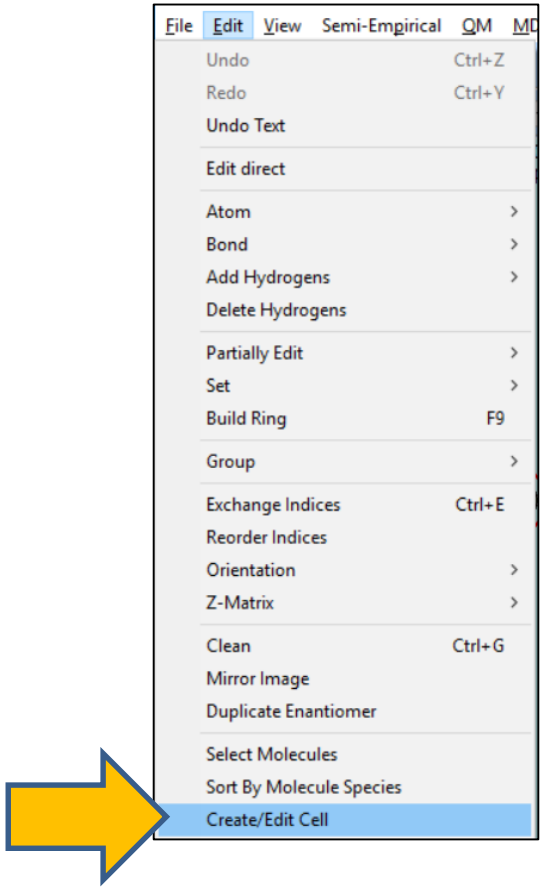
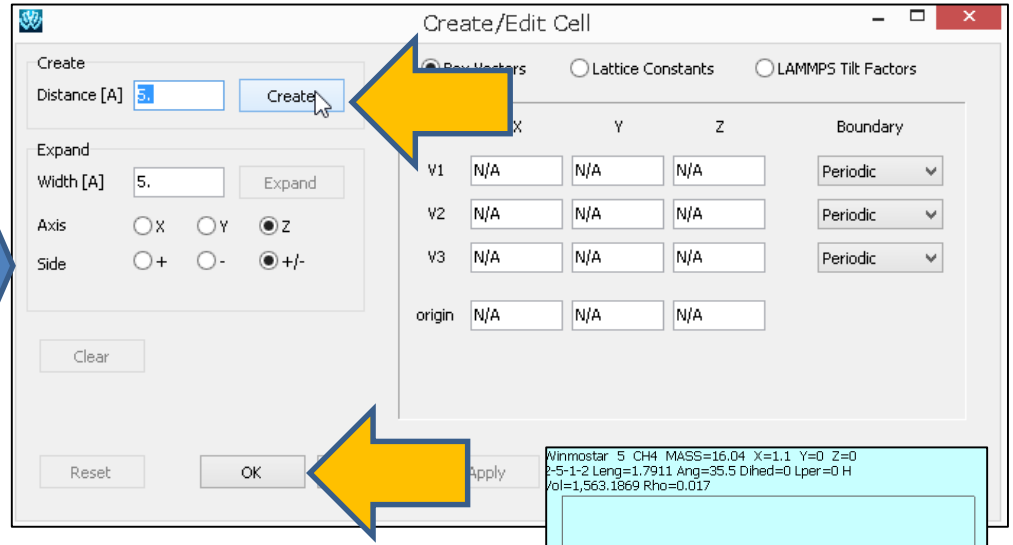
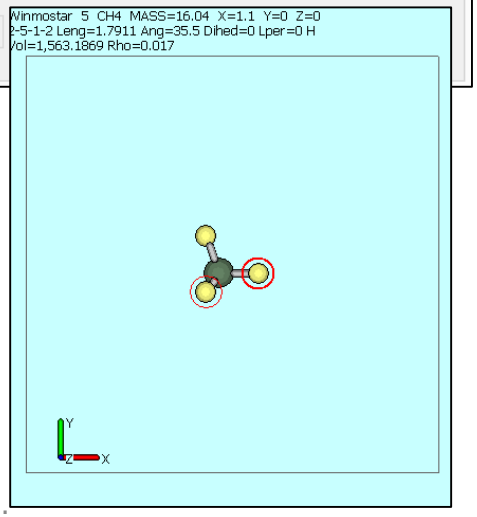
I. Molecular Modeling

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







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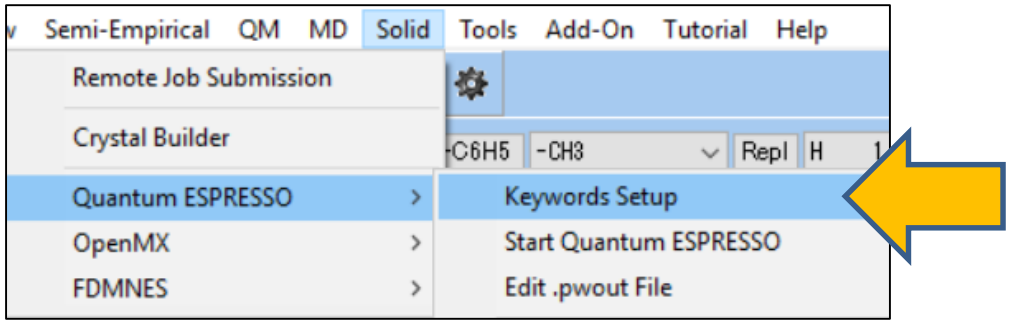
II. Equilibration of Electronic State

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



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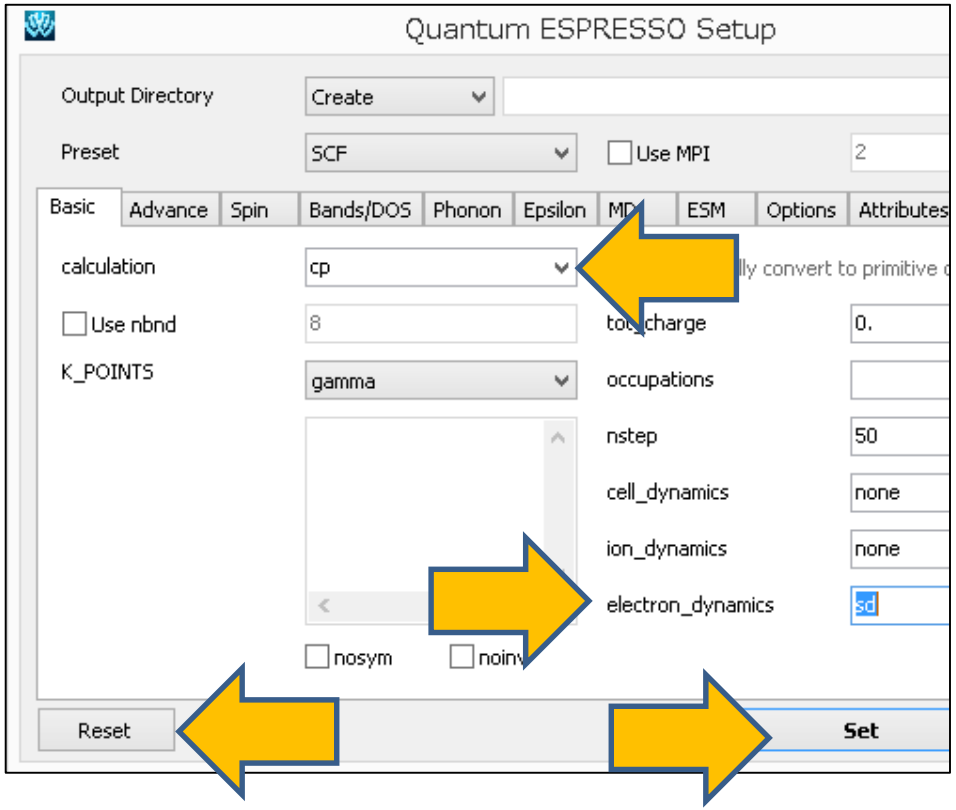
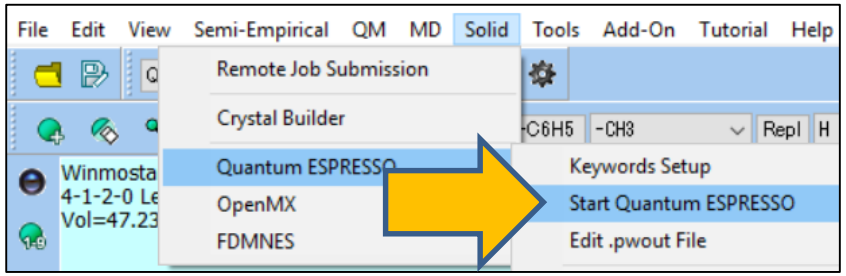
II. Equilibration of Electronic State

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.





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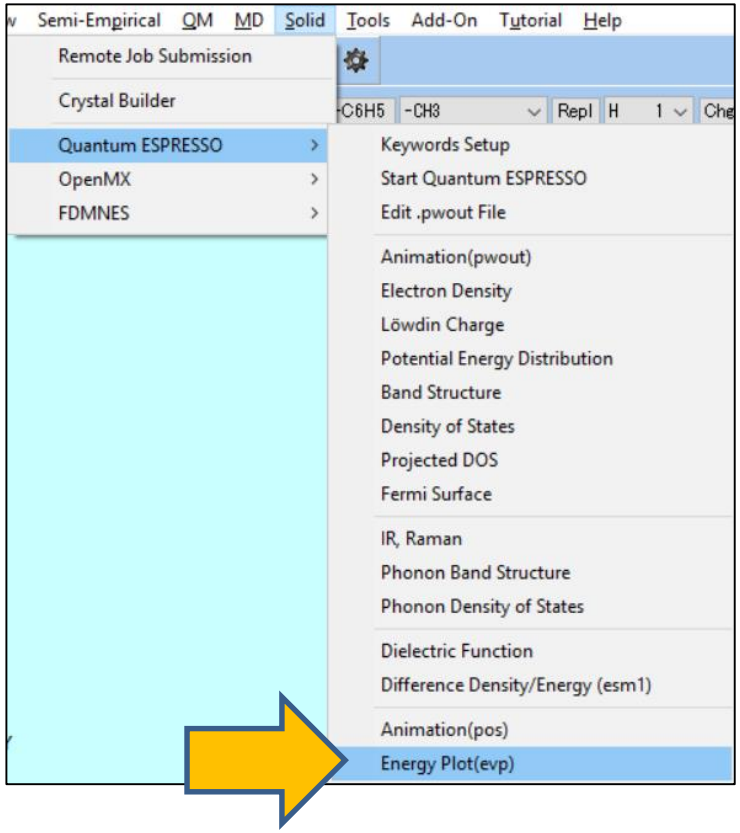
II. Equilibration of Electronic State

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



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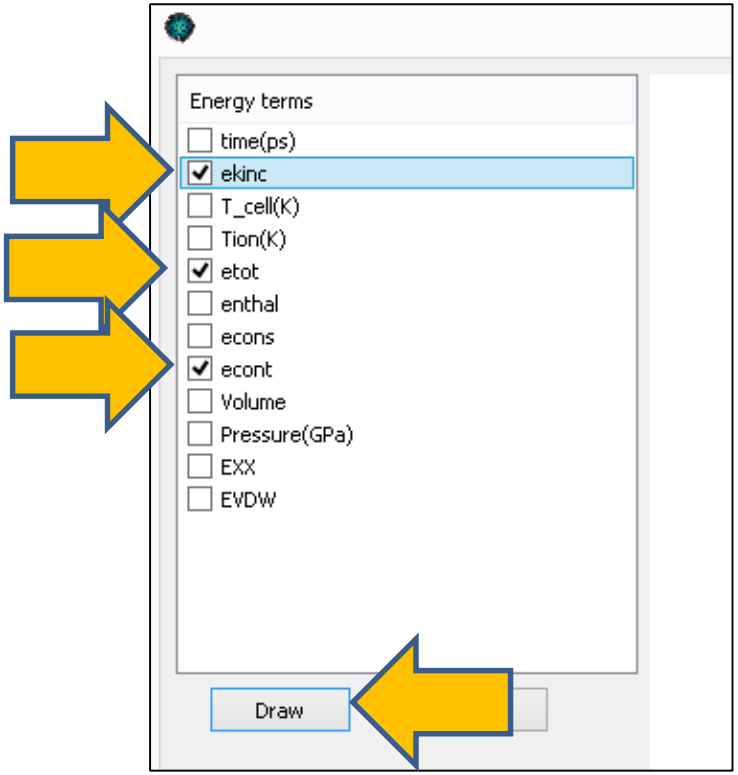
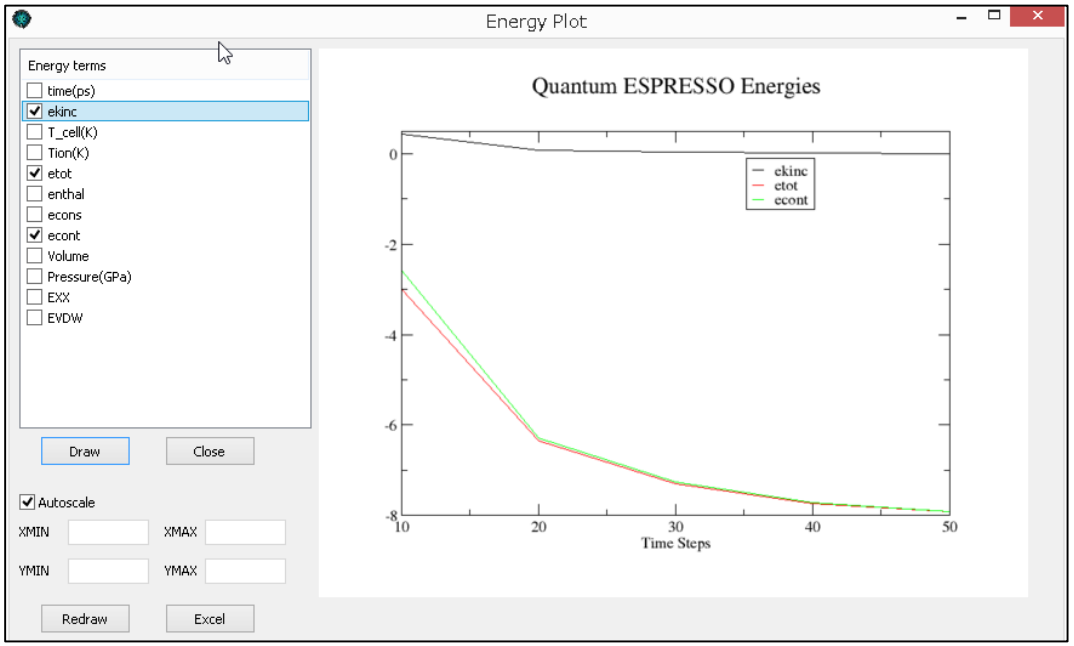
II. Equilibration of Electronic State

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.





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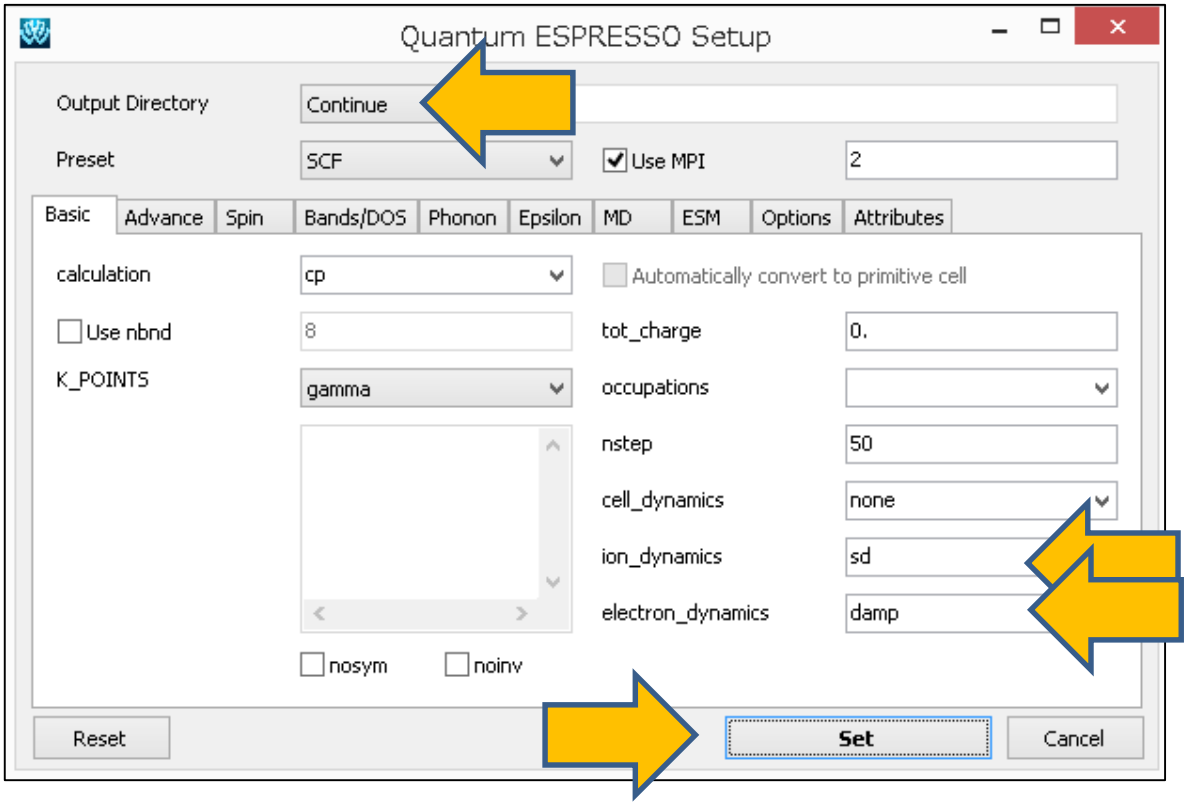
III. Equilibration of Nuclei

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.



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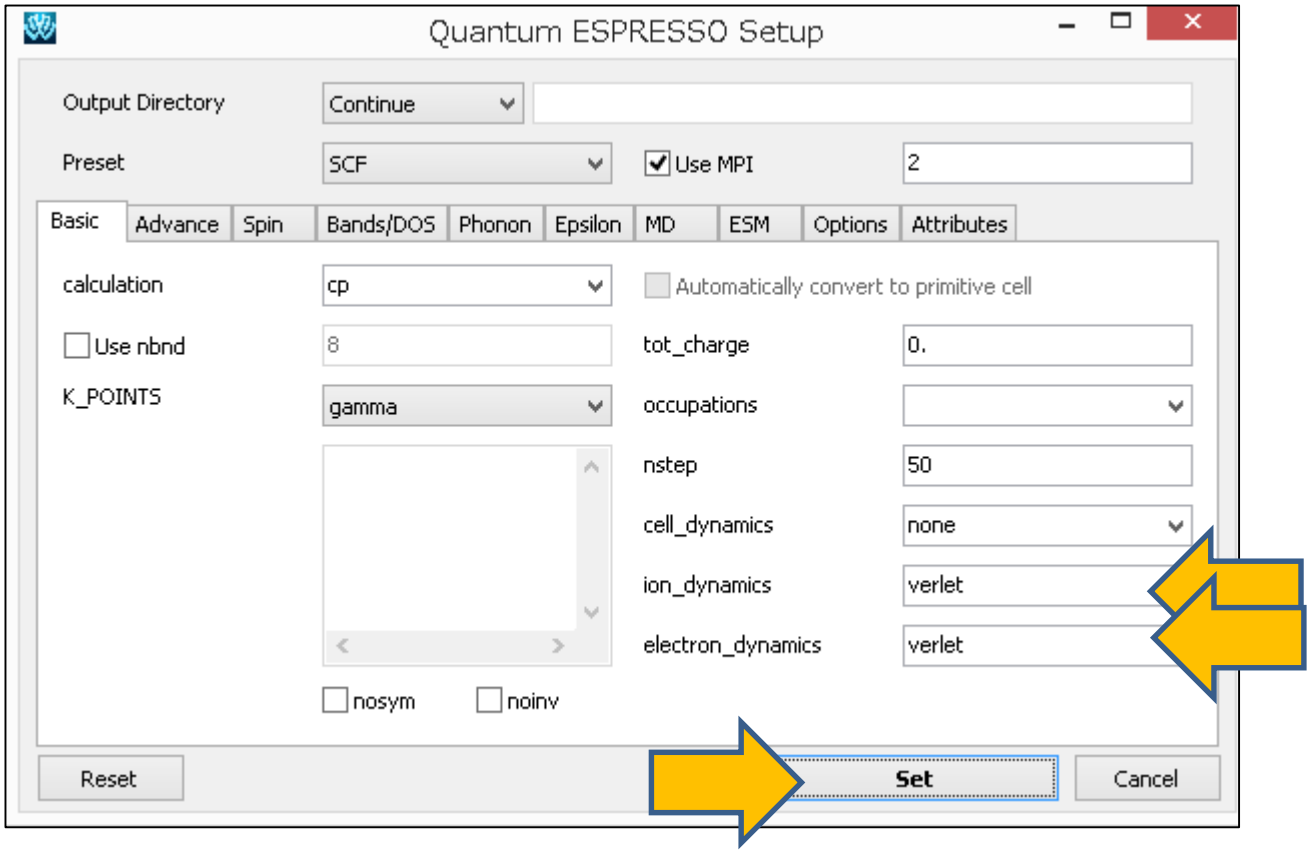
IV. Constant-Temprature MD Calculation

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.



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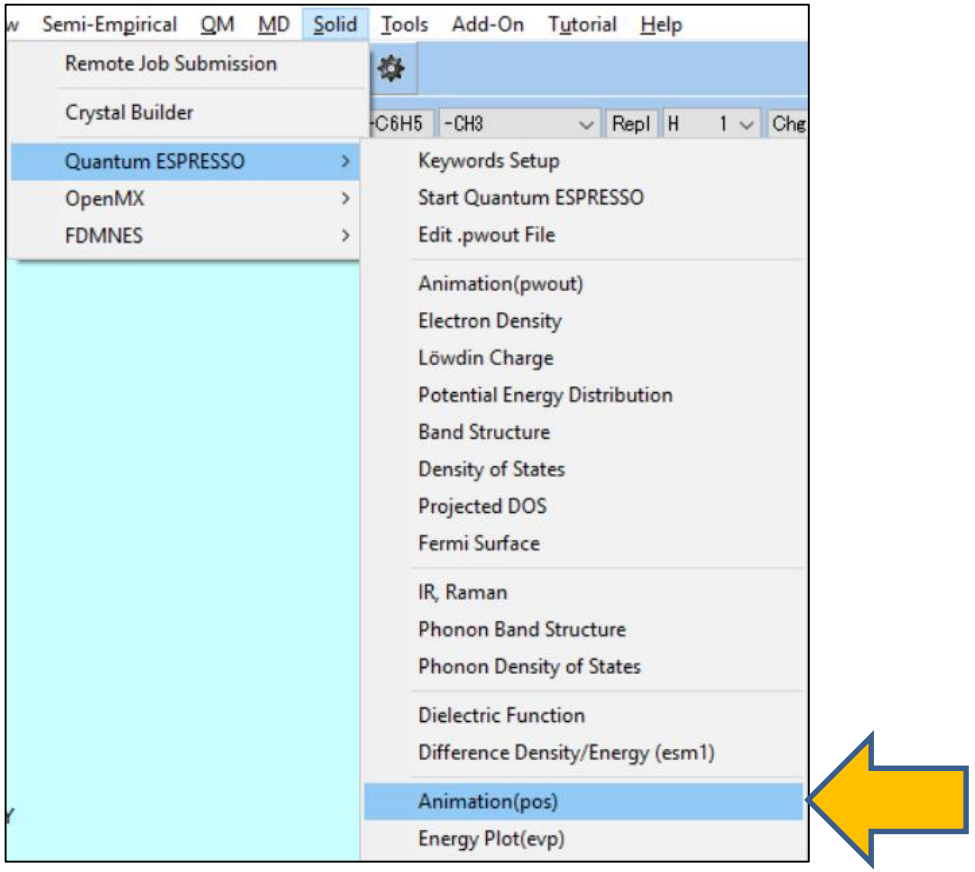
V. Analysis

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



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V. Analysis

Click the **play button** (|>) to view each step.
To view in an external viewer such as VMD, click **gro**.