X-Ability
クロスアビリティ

Winmostar tutorial
Quantum ESPRESSO
First-Principles Molecular Dynamics
V7.021

X-Ability Co,. Ltd.

question@winmostar.com

2017/07/06

X-Ability
クロスアビリティ

Contents

I. Molecular modeling
II. Periodic boundary condition
III. Energy minimization
IV. Energy plots
V. Relaxation
VI. MD of constant temperature
VII. Animation

X-Ability
クロスアビリティ

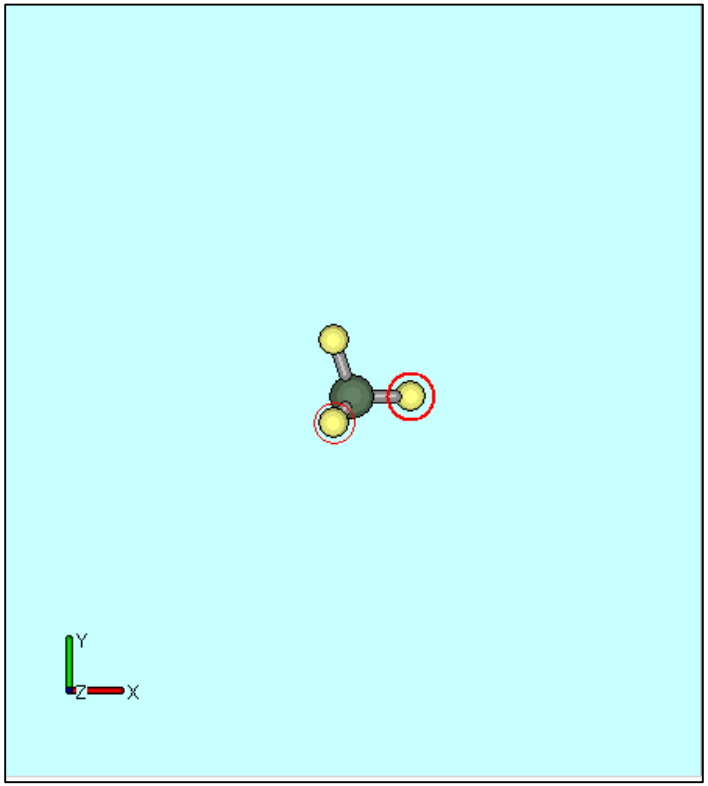
Environment setting

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

X-Ability
クロスアビリティ

I. Molecular modeling

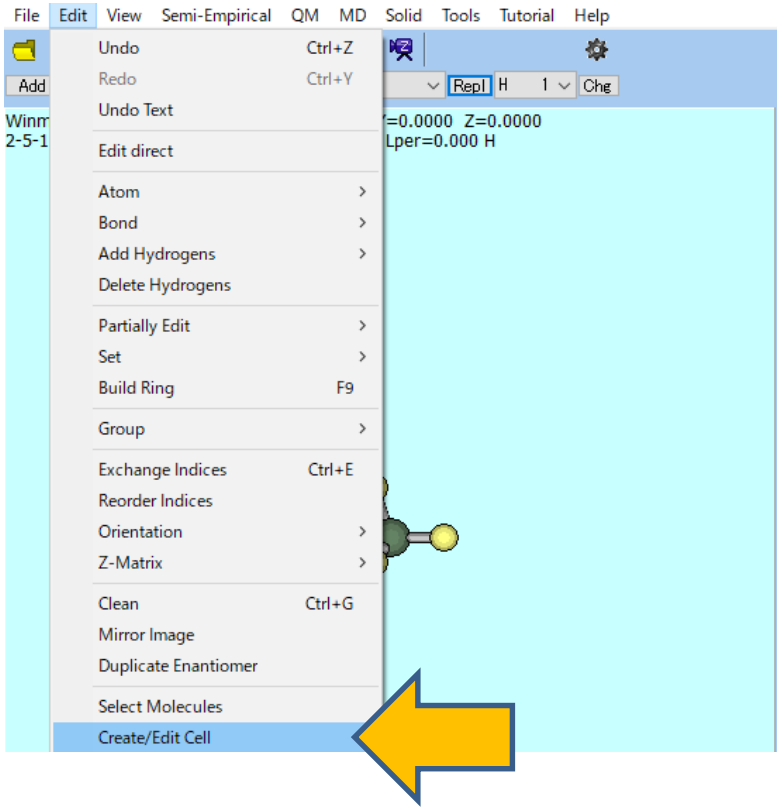
Model CH_4 on the graphics.

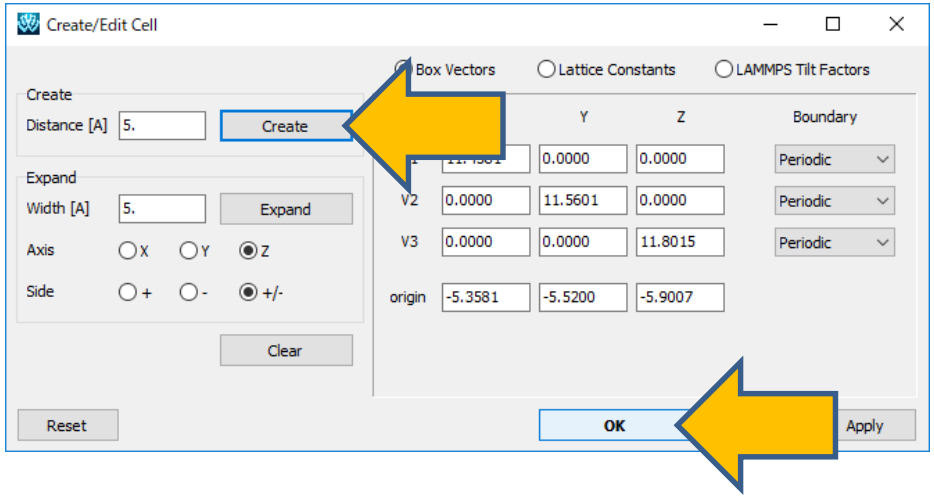


X-Ability
クロスアビリティ

II. Periodic boundary condition

1. Click **Edit** | **Create/Edit Cell**.
2. Click **Create**.
3. Click **OK**.

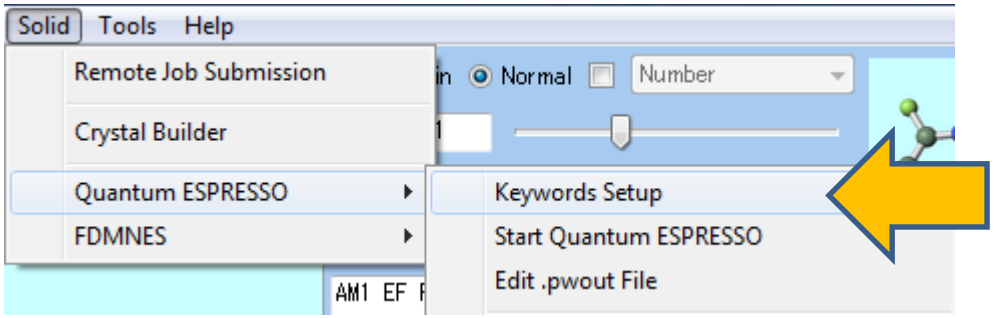




X-Ability
クロスアビリティ

III. Energy minimization 1

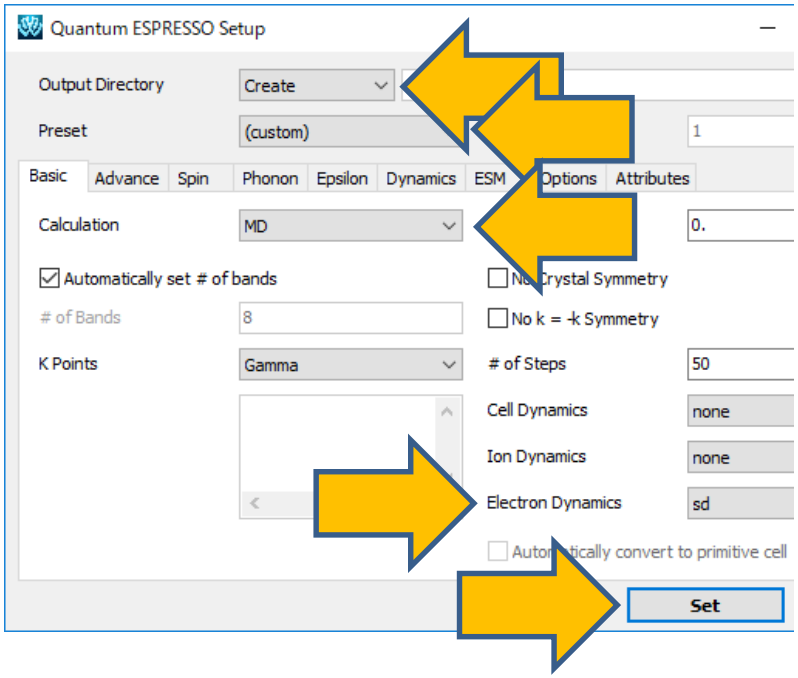
Click **Solid** | **Quantum ESPRESSO** | **Keywords Setup**.

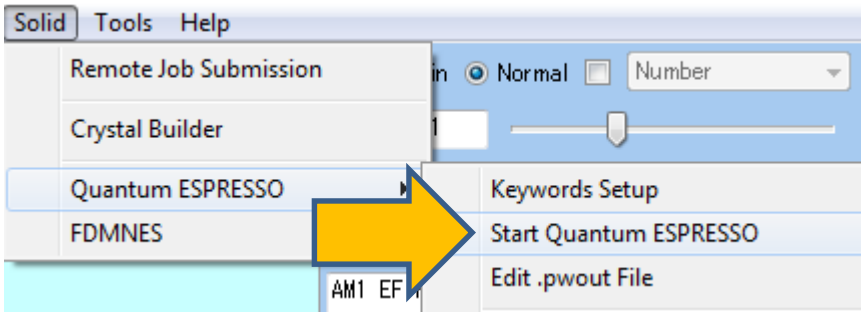


X-Ability
クロスアビリティ

III. Energy minimization 2

1. Set **Output Directory** to **Create**, **Preset** to **SCF**.
2. Set **Calculation** to **MD**, **Electron Dynamics** to **sd**.
3. Click **Set**.
4. Click **Solid** | **Quantum ESPRESS** | **Start Quantum ESPRESS**.
5. Save the file.

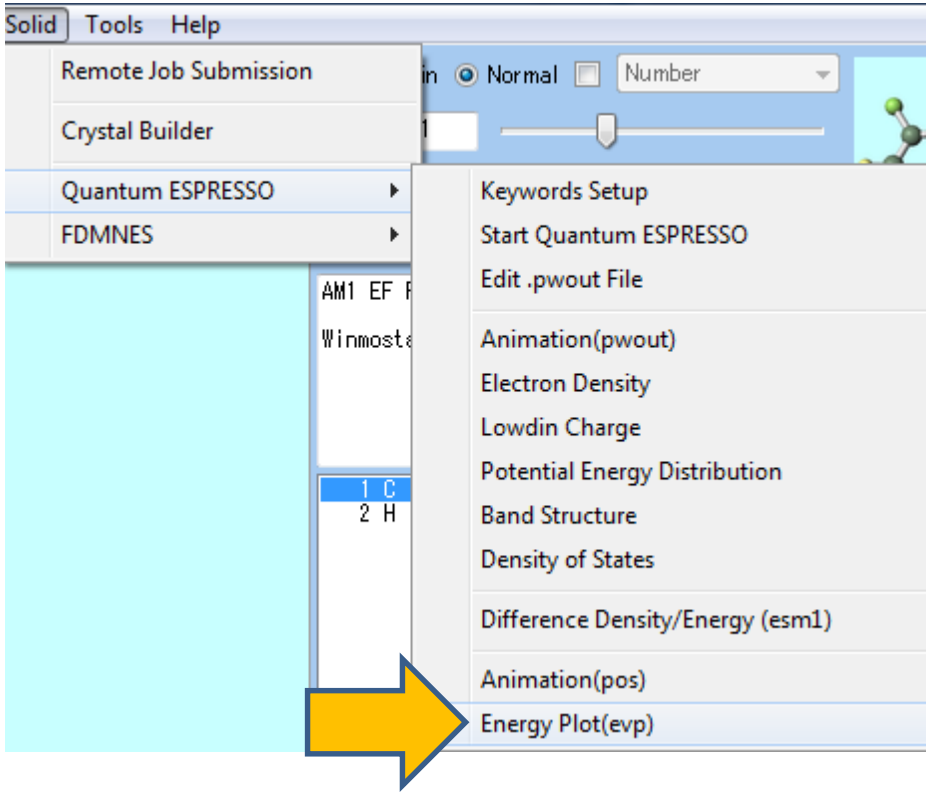




X-Ability
クロスアビリティ

IV. Energy plots 1

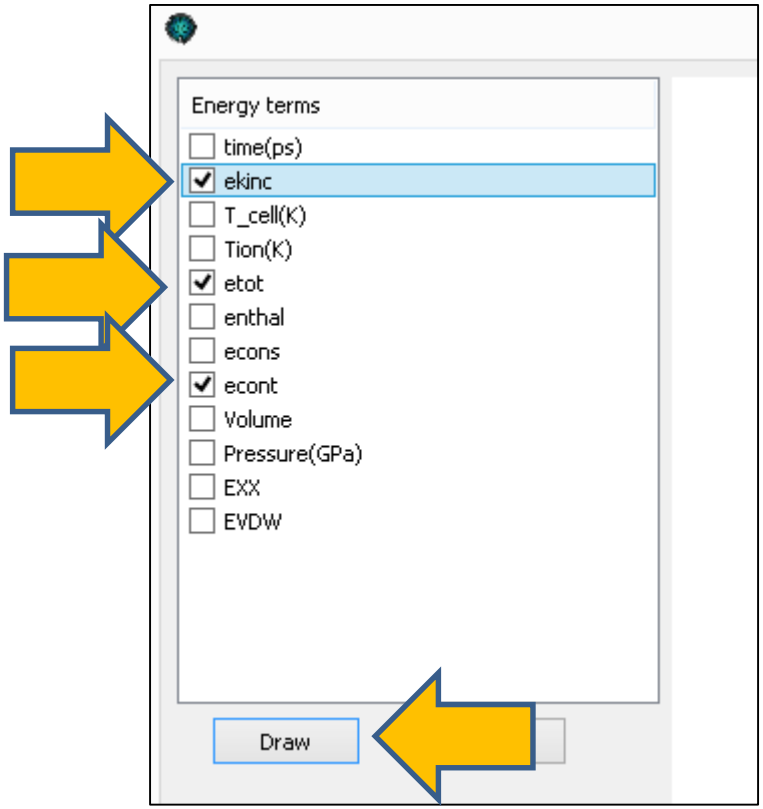
1. After the calculation,
   click **Solid** | **Quantum ESPRESSO** | Energy Plot(evp).
2. Select the default path.

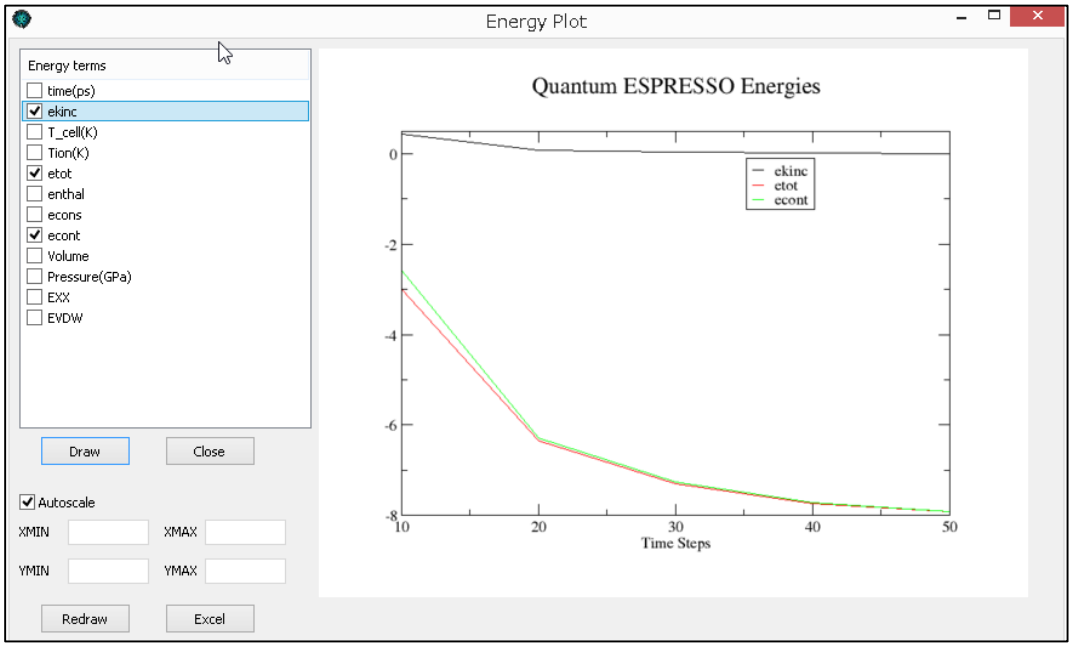


X-Ability
クロスアビリティ

IV. Energy plots 2

1. On the Energy Plot window,
   check **ekinc** (imaginary kinetic energy of electrons)
   check **etot** (Electric potential energy of electrons)
   check **econt** (Total energy)
2. Click **Draw** to get the following graph.

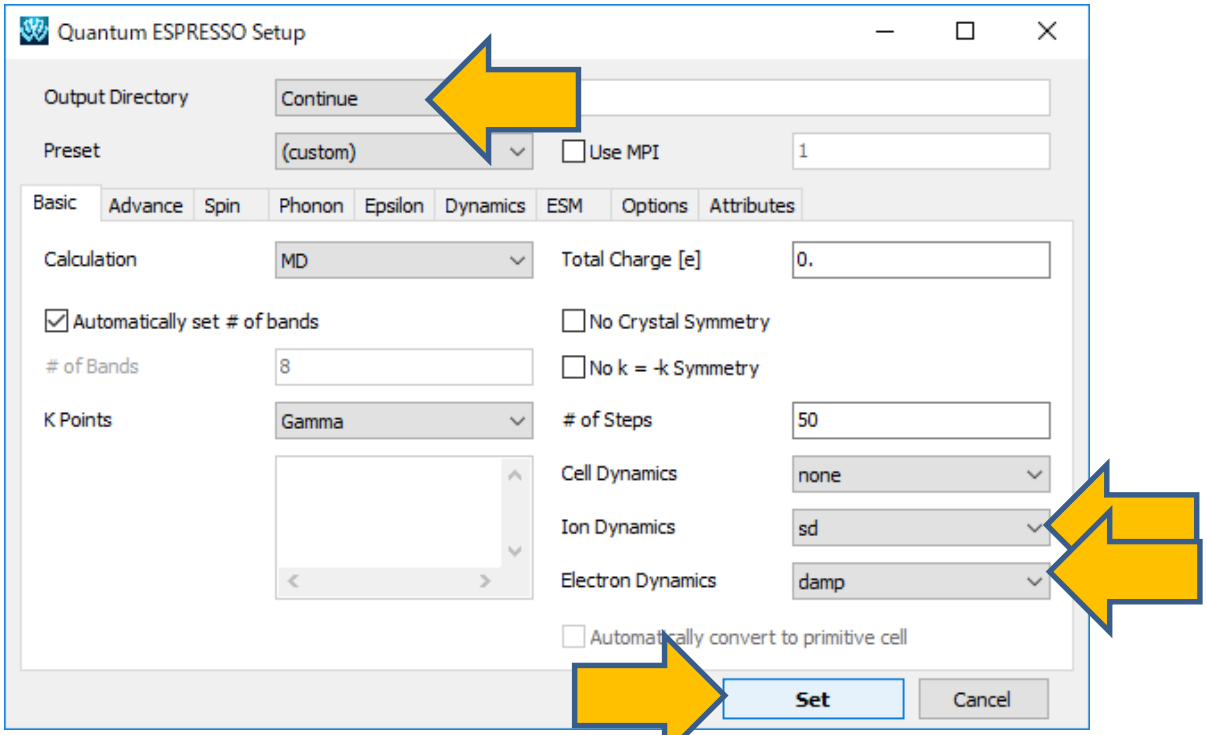




X-Ability
クロスアビリティ

V. Relaxation

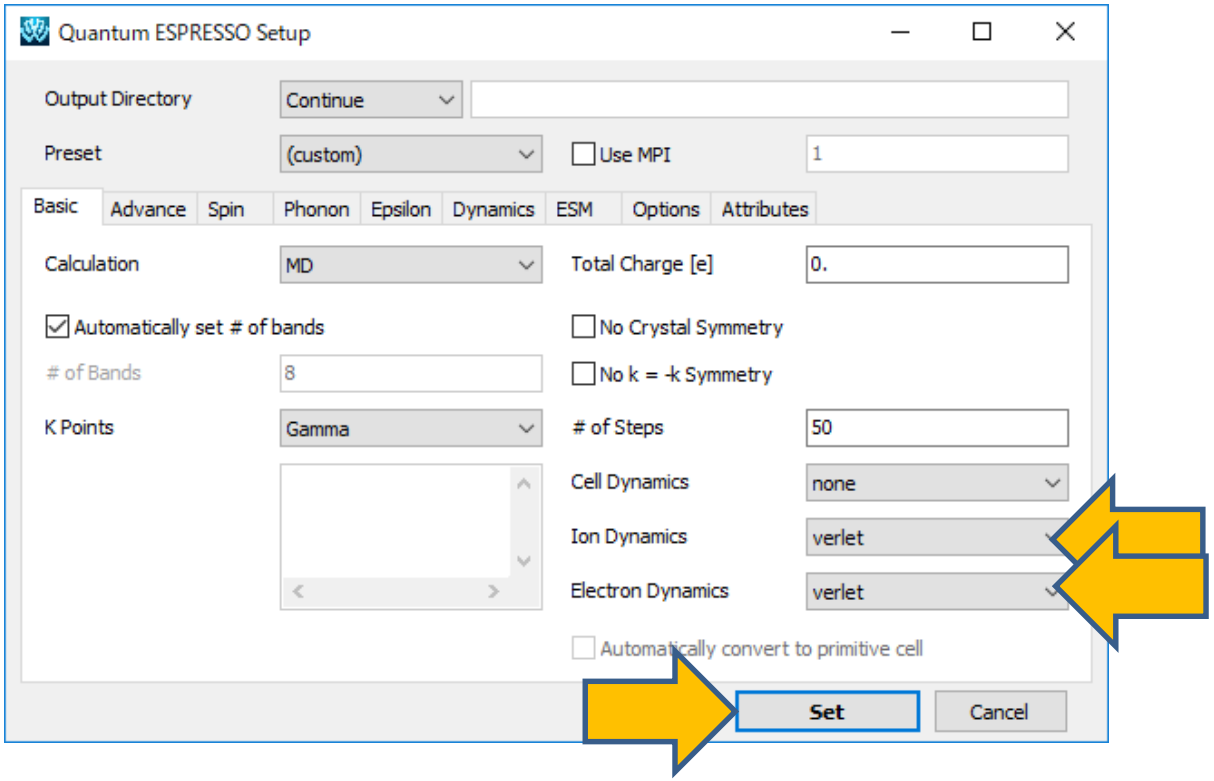
1. Click **Solid** | **Quantum ESPRESSO** | **Keywords Setup**.
2. Set **Output Directory** to **Continue,**
   Ion Dynamics to **sd**, **Electron Dynamics** to **damp**.
3. Click **Set**.
4. Click **Solid** | **Quantum ESPRESSO** | **Start Quantum ESPRESSO**.
5. After the calculation,
   click **Solid** | **Quantum ESPRESSO** | **Energy Plot(evp)**.



X-Ability
クロスアビリティ

VI. MD of constant temperature

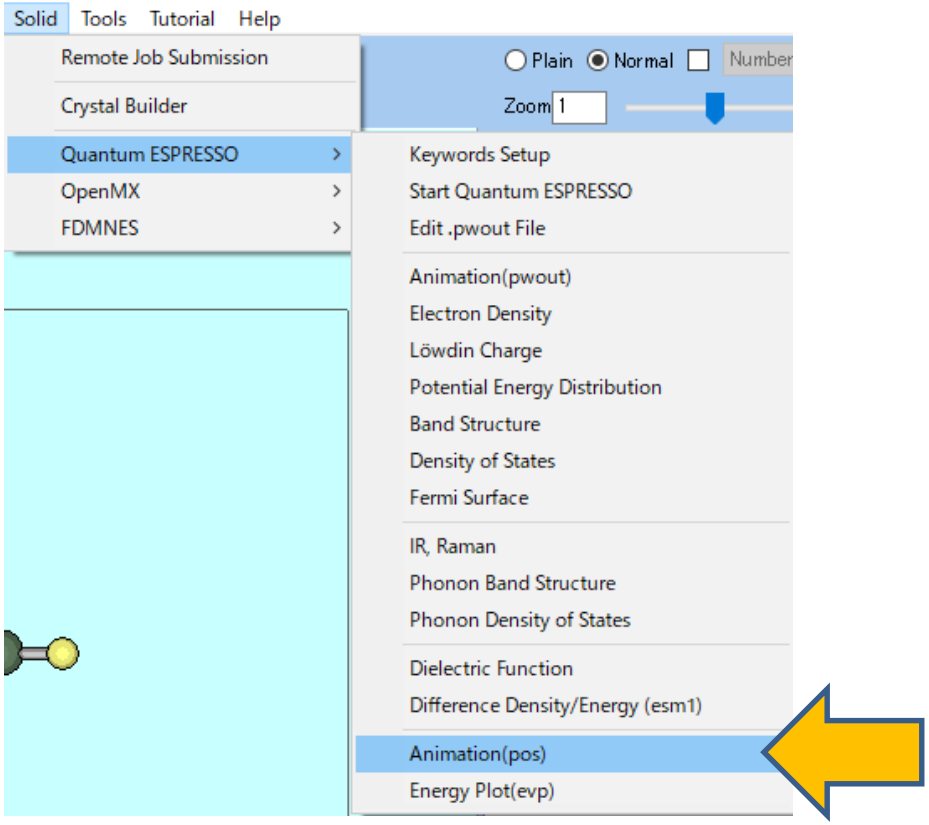
1. Click **Solid** | **Quantum ESPRESSO | Keywords Setup**.
2. Set **Ion Dynamics** to **verlet**, **Electron Dynamics** to **verlet**.
3. Click **Set**.
4. After the calculation,
   click | **Solid Quantum ESPRESSO** | **Start Quantum ESPRESSO**.



X-Ability
クロスアビリティ

VII. Animation 1

1. After the calculation,
   click **Solid | Quantum ESPRESSO | Animation(pos)**.
2. Select the default path.



X-Ability
クロスアビリティ

VII. Animation 2

Click (|>) to play the steps