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Winmostar tutorial
Quantum ESPRESSO
Work function
V7.021

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Contents

I. SCF calculation
II. Work function

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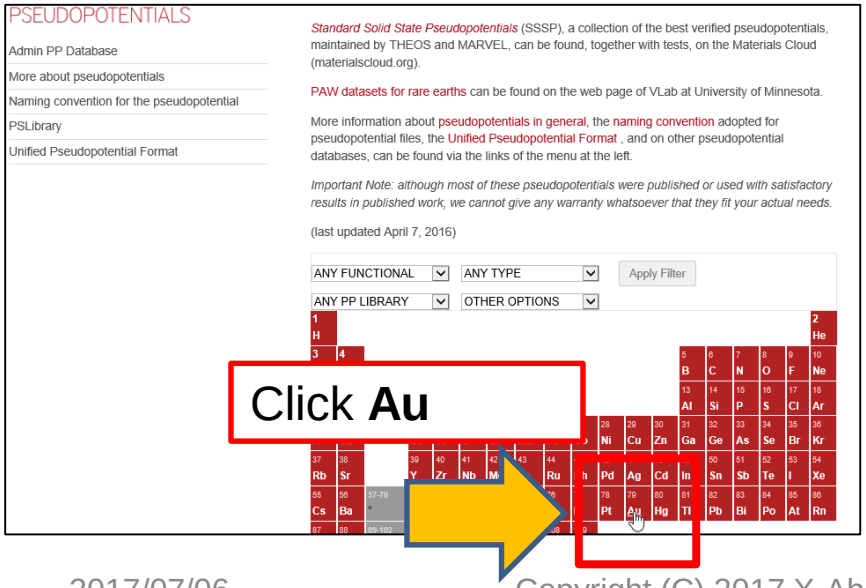
Environment setting

① See Quantum ESPRESSO install manual
https://winmostar.com/en/QE_install_manual_en_win.pdf
to install Quantum ESPRESSO.

② Download **Au.pbe-dn-rrkjus_psl.0.1.UPF** via the following URL.
Move it to the **pseudo** folder in the install folder of Quantum ESPRESSO and restart Winmostar.
http://www.quantum-espresso.org/pseudopotentials/



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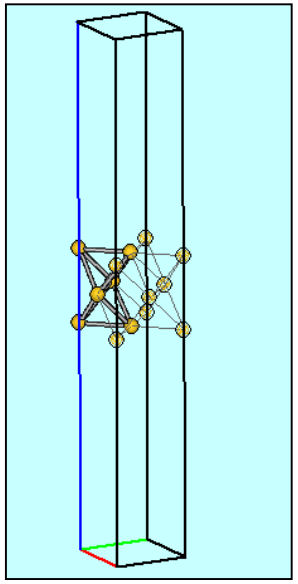
I. SCF calculation

1. Click **File | Open**.
2. Select **C:¥winmos7¥samples¥au_slab.cif**.

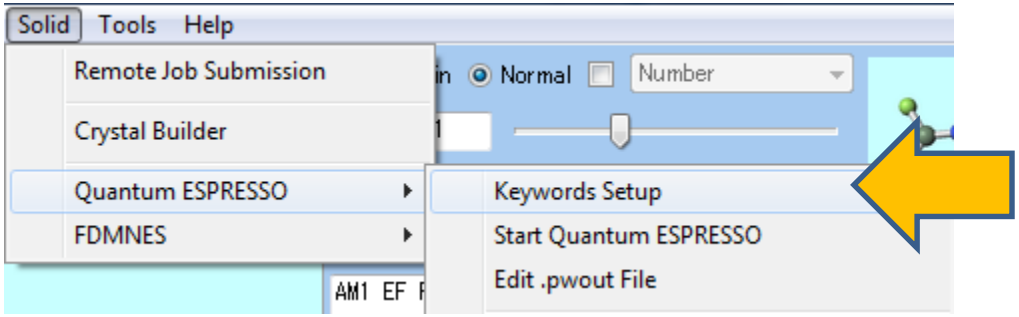


You can also make the same CIF file using **Crystal Builder**.
See **crystal modeling tutorial** and apply the following information.

To Make Au unit cell
Crystal system: Cubic
Space group : Fm-3m (225)
Lattice constants : a=4.078830 Å
Fractional coordinates: Au (0.0 0.0 0.0)

To Make Slab
Thickness of vacuum layer 25 Å

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



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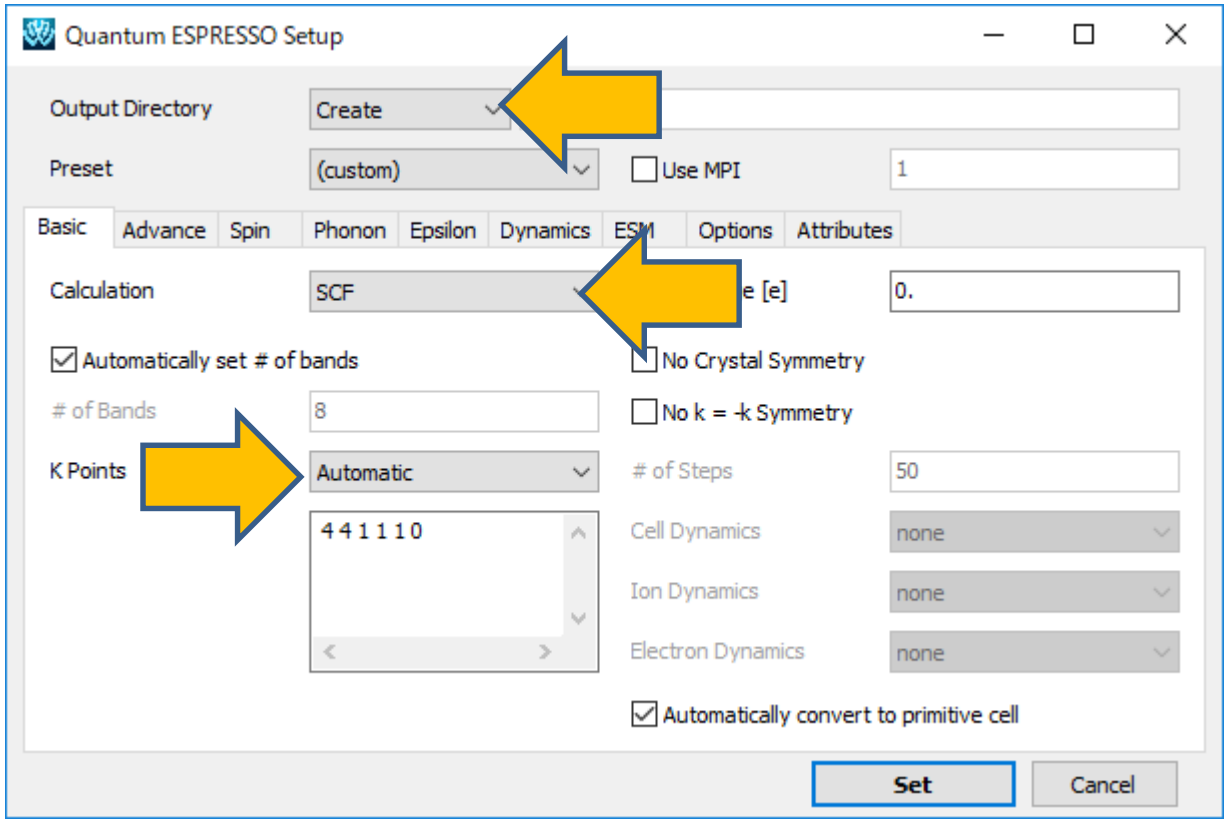
I. SCF calculation

1. Set **Output Directory** to **Create**.
2. Set **Preset** to **SCF**.
3. At **Basic** tab, Set **K Points** to **Automatic** and enter **4 4 1 1 1 0** in the text area.



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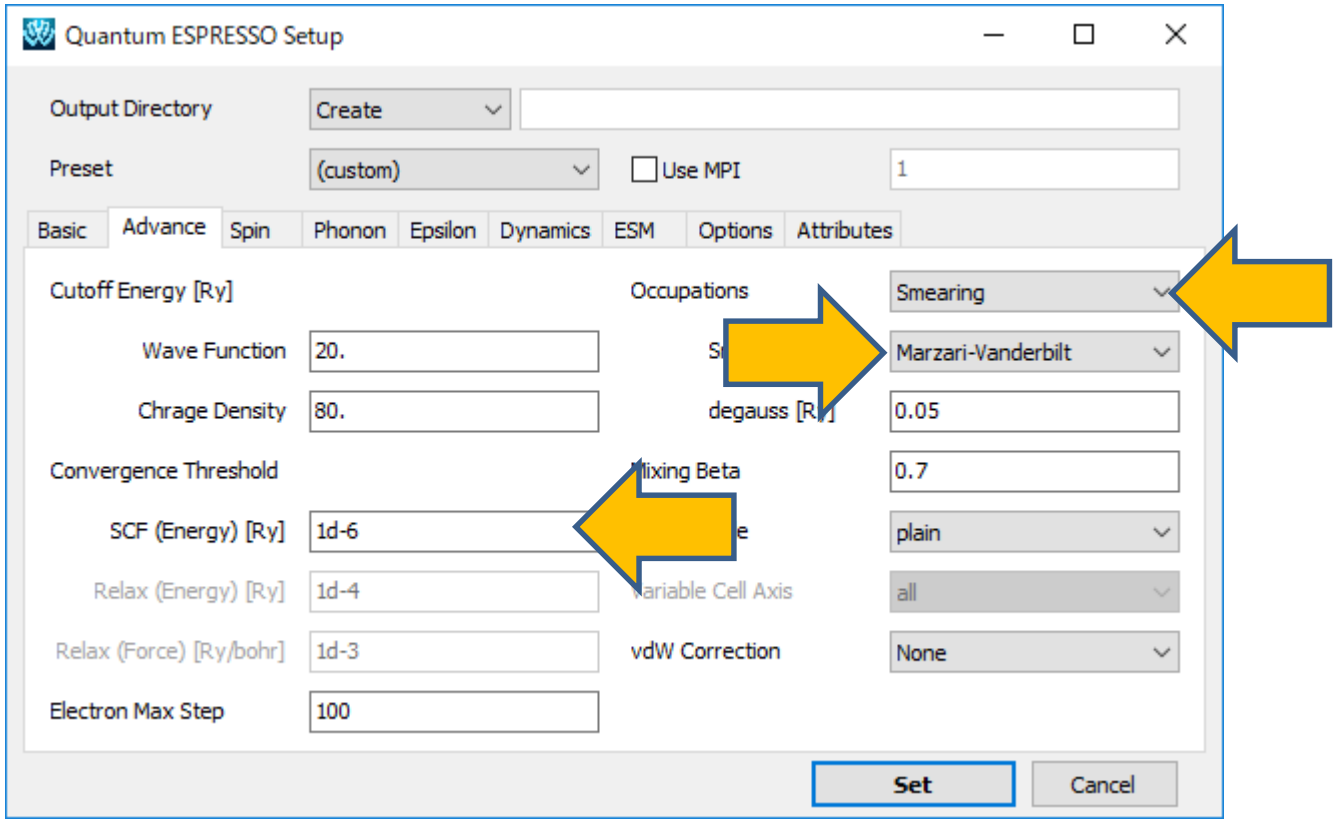
I. SCF calculation

1. Click **Advance** tab.
2. Set **Occupations** to **Smearing**.
3. Set **Smearing** to **Marzari-Vanderbilt**.
4. Set **SCF (Energy)** to **1d-6**.



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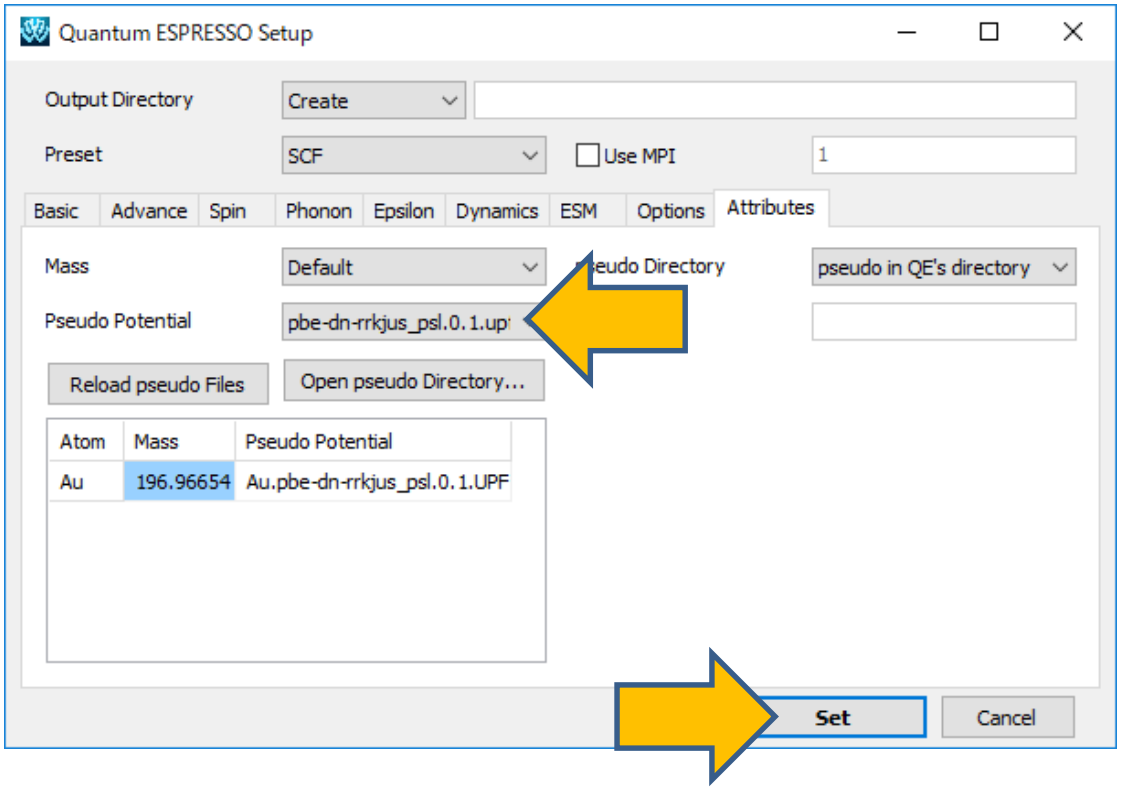
I. SCF calculation

1. Click **Attributes** tab.
2. Set Pseudo Potential to **pbe-dn-rrkjus_psl.0.1.UPF**.
   - If you do not have **pbe-dn-rrkjus_psl.0.1.UPF**, follow the instruction in page. 4.
   - Move Pseudo file to pseudo folder and click **Reload pseudo Files**.
3. Click **Set**.



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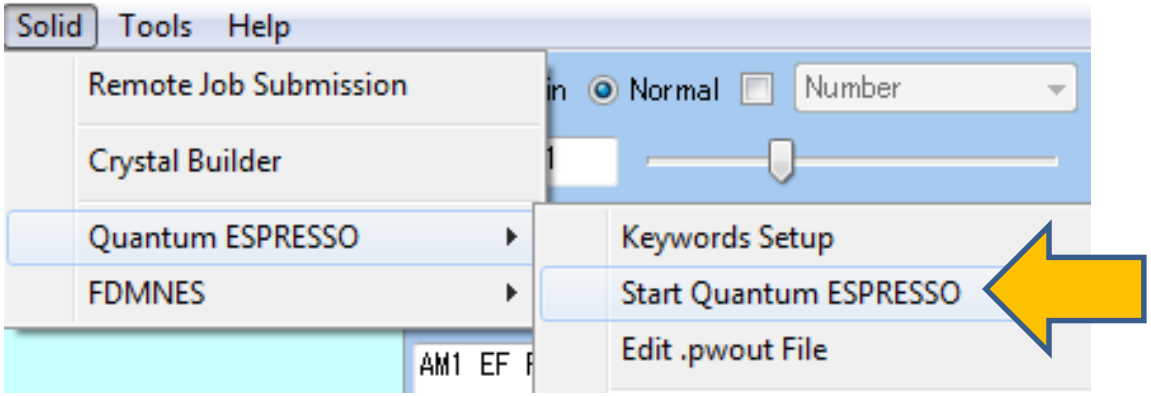
I. SCF calculation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Click **Yes** and save the file.
3. Save as **au_slab.pwin**.



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II. Work function

1. After the calculation,
   click **Solid | Quantum ESPRESSO | Potential Energy Distribution**.
2. Select the folder and the pwout file by default.
   Potential energy distribution window will appear.
   The predicted value of work function will be displayed at the bottom.