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Winmostar tutorial
Quantum ESPRESSO
Work function
V8.007

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2018/01/15

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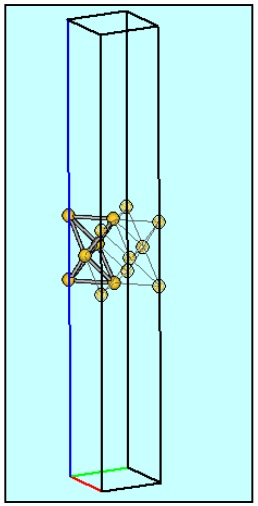
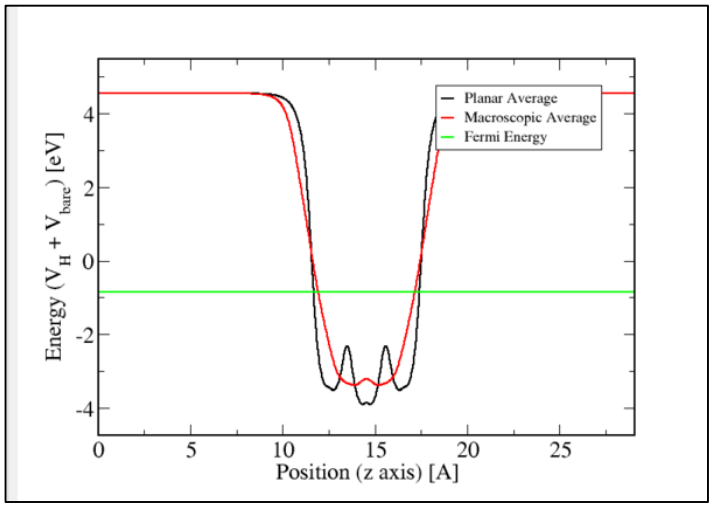
Summary

- In this tutorial we will calculate a work function of Au from the potential energy distribution in a slab model.





Notes:

- Method for obtaining k points, number of bands, type of pseudopotential, cutoff energy, and settings for smearing will all affect calculation results. In this tutorial, we use a setting with reduced precision for faster processing.
- Size of slab model and vacuum layer will also influence calculation results.
- Other than the method described in this tutorial, work function can also be estimated using the ESM method (contact us for more information).

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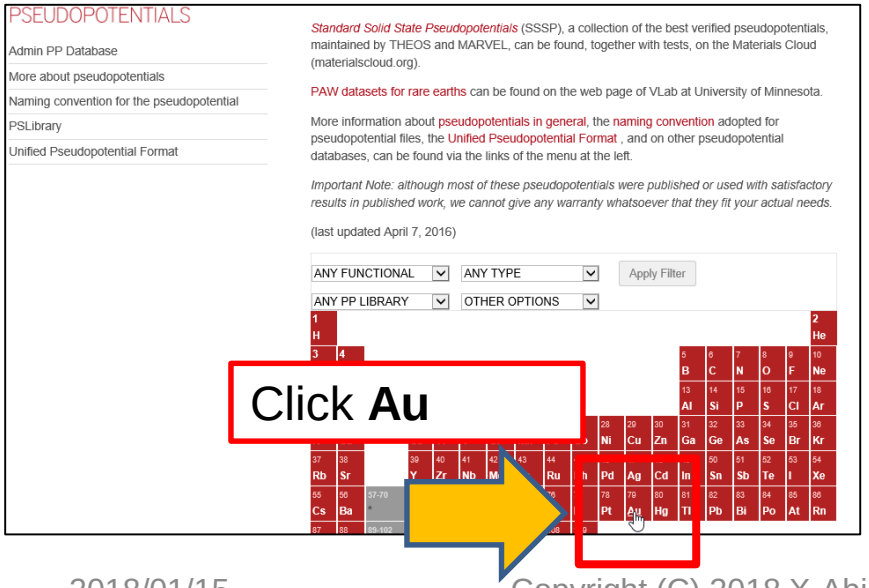
Configuration

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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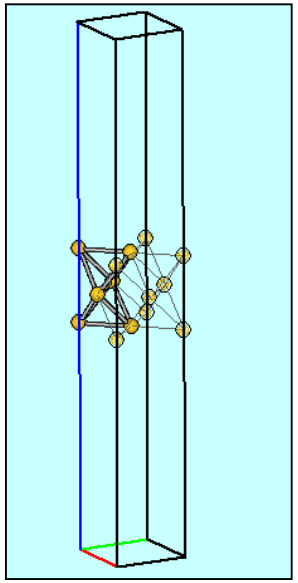
I. SCF calculation

1. Click **File | Open**.
2. Select **C:¥winmos8¥samples¥au_slab.cif**.

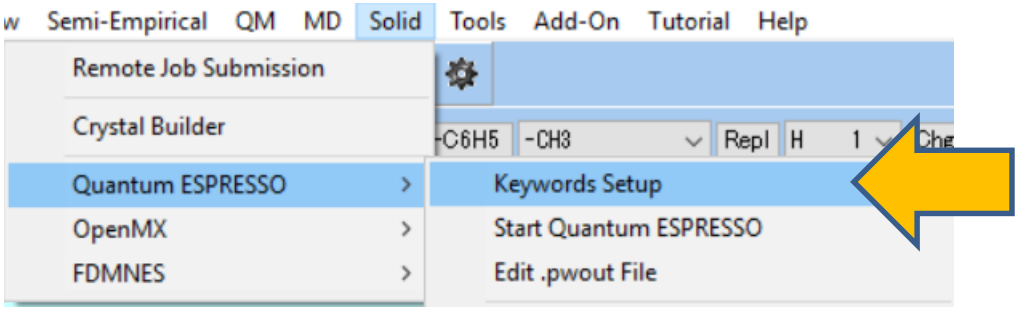


You can also make the same CIF file using **Crystal Builder**.
See **crystal modeling tutorial** and apply the following information.

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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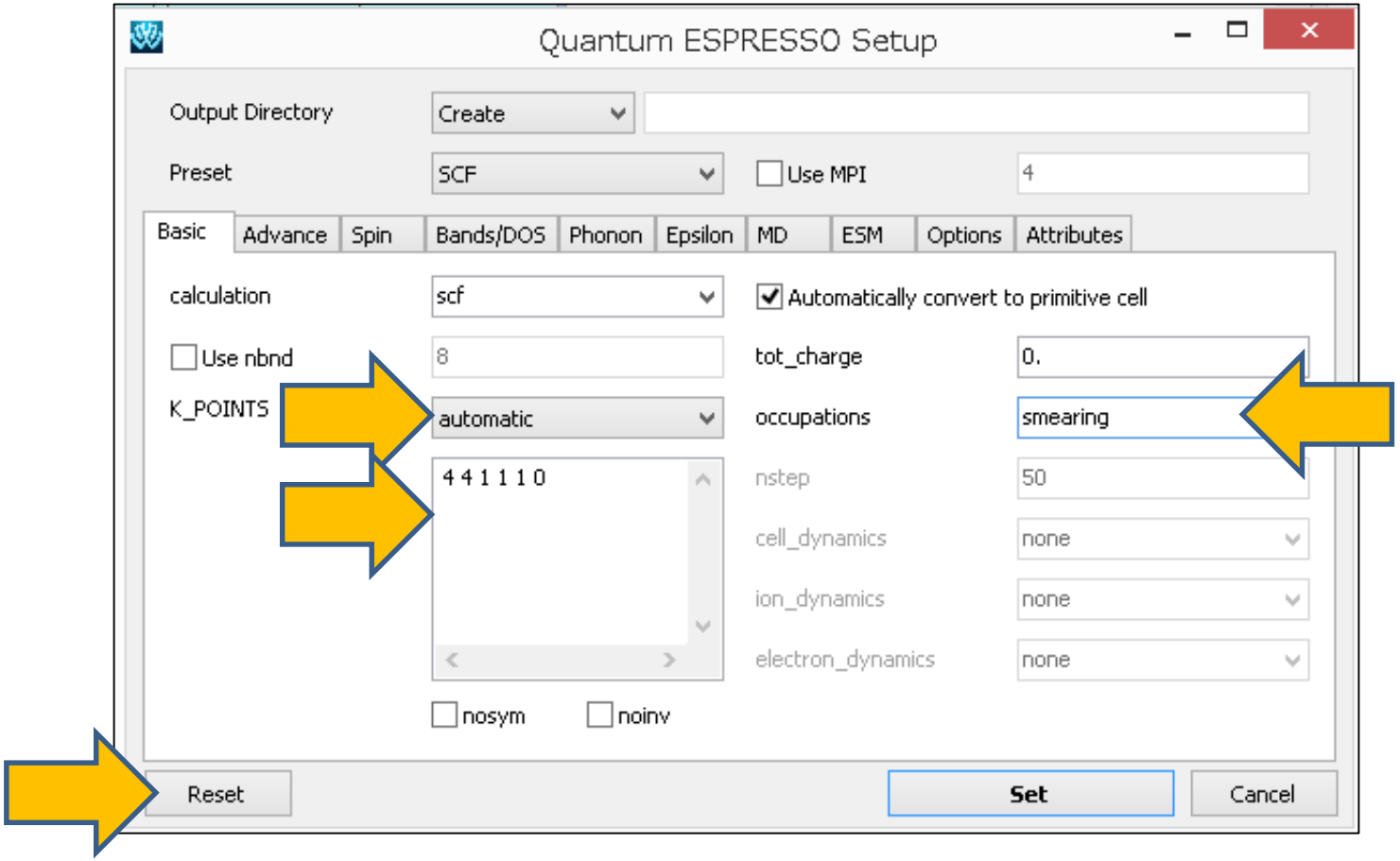
I. SCF Calculation

First, click **Reset**. Next set **K_POINTS** to “**automatic**” and enter “**4 4 1 1 1 0**” (space separated) in the text box below. Set **occupations** to “**smearing**.”



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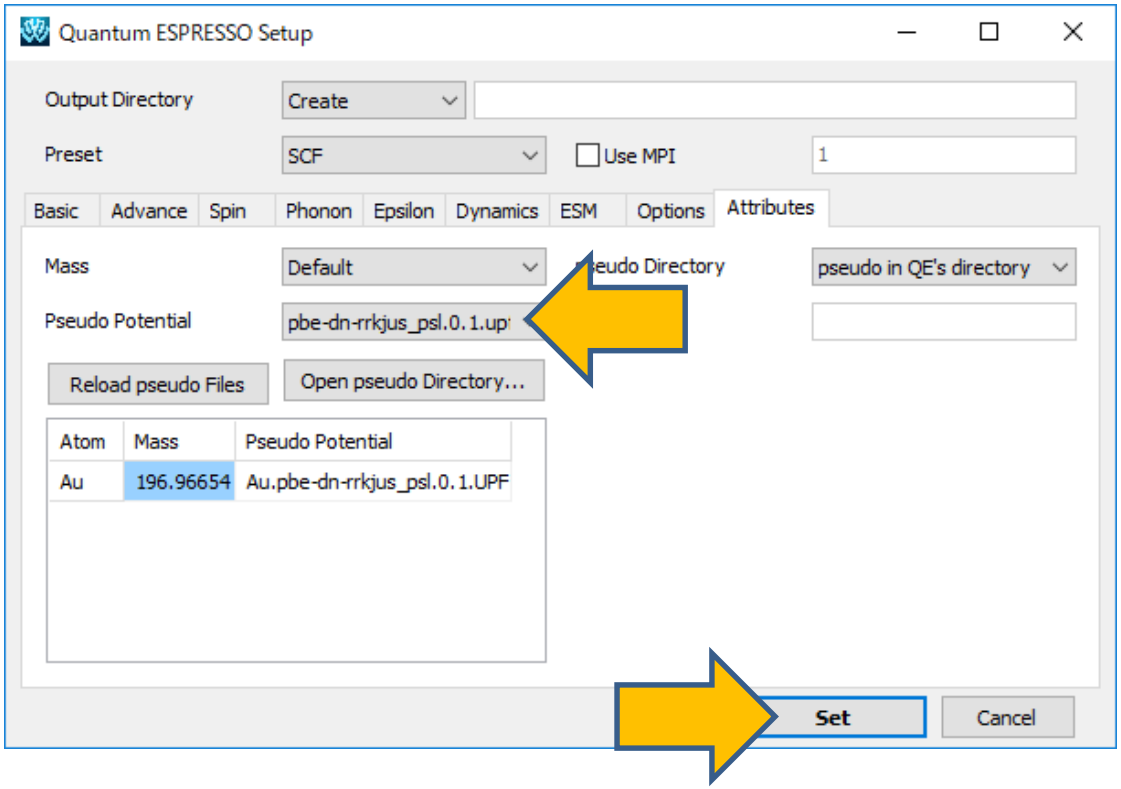
I. SCF calculation

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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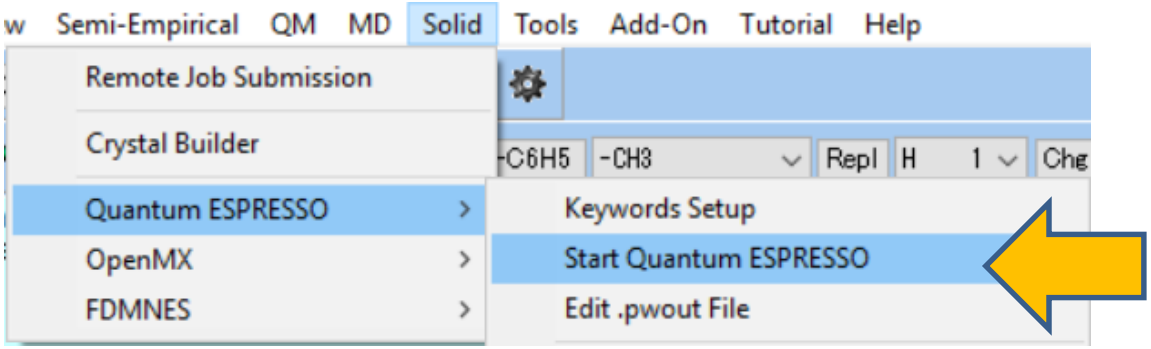
I. SCF calculation

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.
   Click **Draw** on the new window to display potential energy distribution.
   The predicted value of work function will be displayed at the bottom.