

Winmostar tutorial

Quantum ESPRESSO

Work function

V7.021

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- I. SCF calculation
- II. Work function

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/>

PSEUDOPOTENTIALS

Admin PP Database
More about pseudopotentials
Naming convention for the pseudopotential
PSLibrary
Unified Pseudopotential Format

Standard Solid State Pseudopotentials (SSSP), a collection of the best verified pseudopotentials, maintained by THEOS and MARVEL, can be found, together with tests, on the Materials Cloud (materialscloud.org).

PAW datasets for rare earths can be found on the web page of VLab at University of Minnesota.

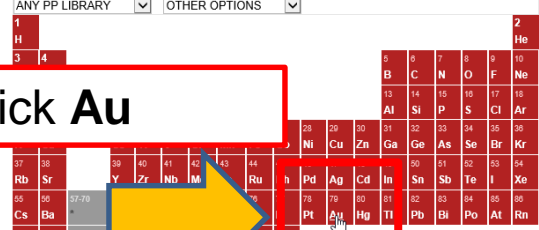
More information about pseudopotentials in general, the naming convention adopted for pseudopotential files, the Unified Pseudopotential Format, and on other pseudopotential databases, can be found via the links of the menu at the left.

Important Note: although most of these pseudopotentials were published or used with satisfactory results in published work, we cannot give any warranty whatsoever that they fit your actual needs.

(last updated April 7, 2016)

ANY FUNCTIONAL ANY TYPE

ANY PP LIBRARY OTHER OPTIONS



Click Au

Classification controlled by Andrea Dal Corso

Au.pbe-dn-rrkjus_psl.0.1.UPF

Pseudopotential type: ULTRASOFT
Method: Rappe Rabe Kaxiras Joannopoulos

Click Au.pbe-dn-rrkjus_psl.0.1.UPF

Author: Andrea Dal Corso
Generated using atomic code by A. Dal Corso v.5.0.2 svn rev. 9415
Uploaded by Erica Vidal
Classification controlled by Andrea Dal Corso

Au.pbe-ml_fhi.UPF

Pseudopotential type: NORMCONS
Method: Martins-Troullier

I. SCF calculation

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

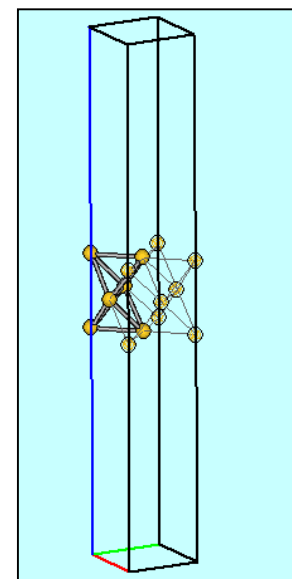
You can also make the same CIF file using **Crystal Builder**.
See **crystal modeling tutorial** and apply the following information.

To Make Au unit cell

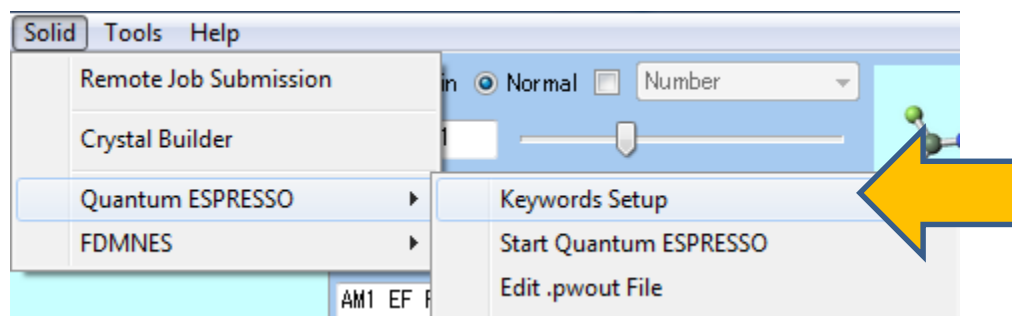
Crystal system : Cubic
Space group : Fm-3m (225)
Lattice constants : a=4.078830 Å
Fractional coordinates : Au (0.0 0.0 0.0)

To Make Slab

Thickness of vacuum layer 25 Å

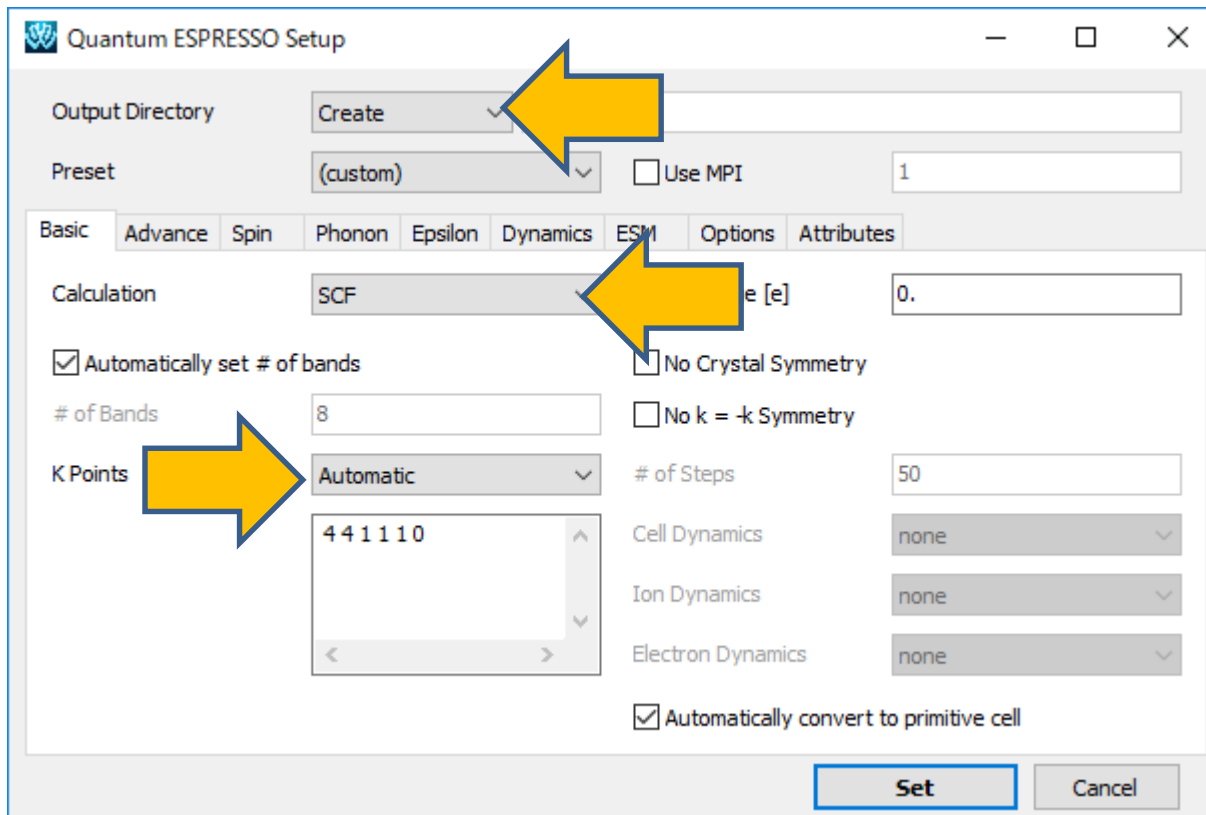


2. Click **Solid | Quantum ESPRESSO | Keywords Setup**.



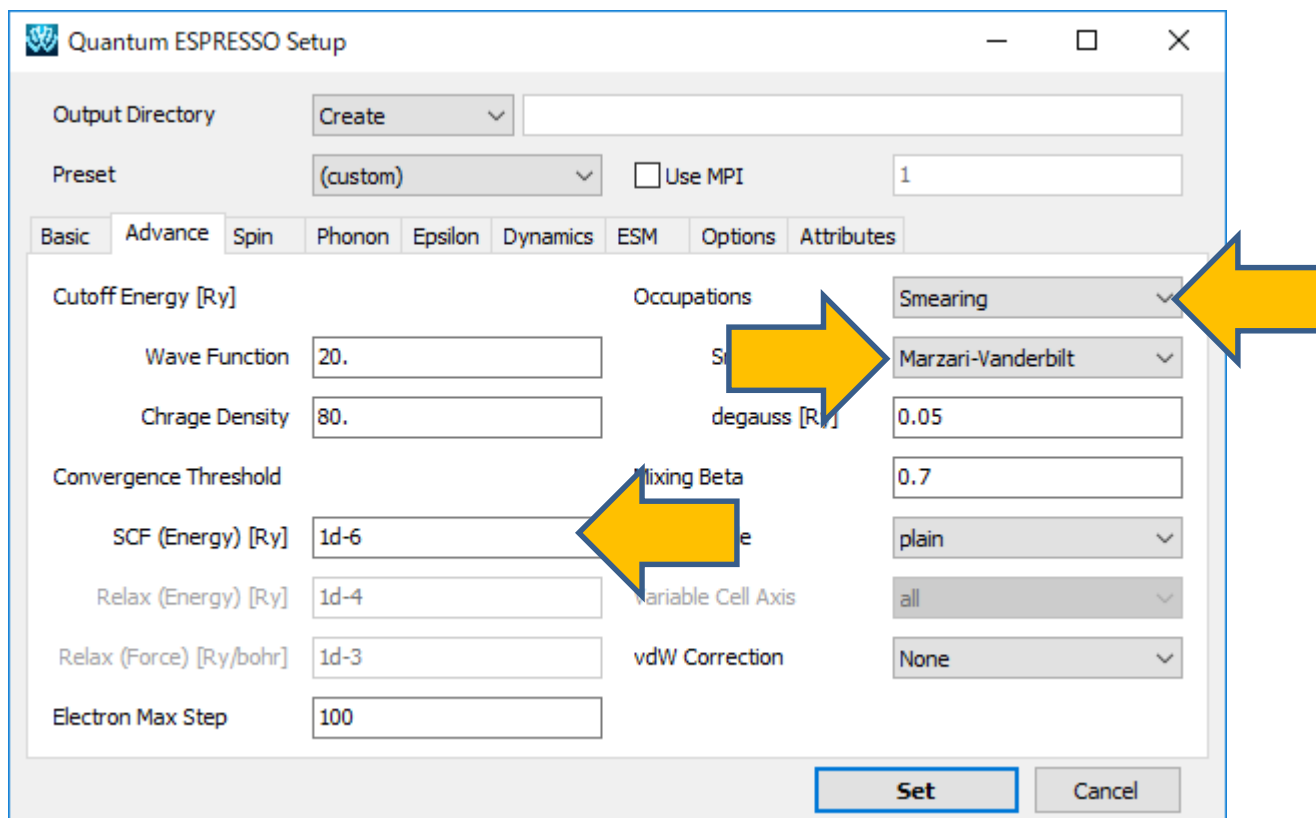
I. SCF calculation

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.



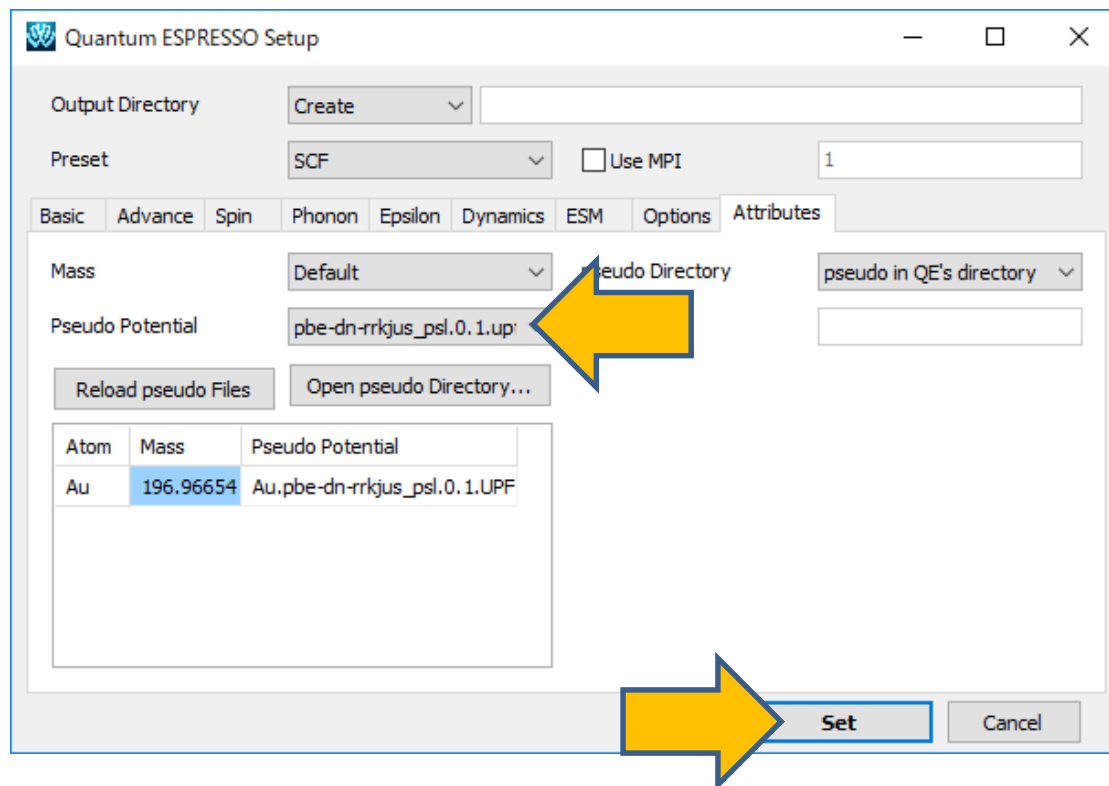
I. SCF calculation

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



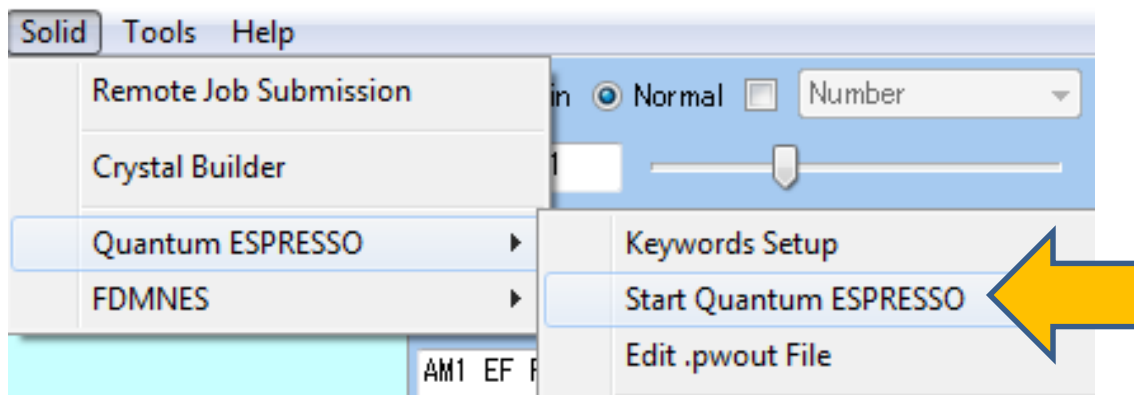
I. SCF calculation

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**.



I. SCF calculation

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



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.

