

# Winmostar tutorial

## Quantum ESPRESSO

### Work function

V8.007

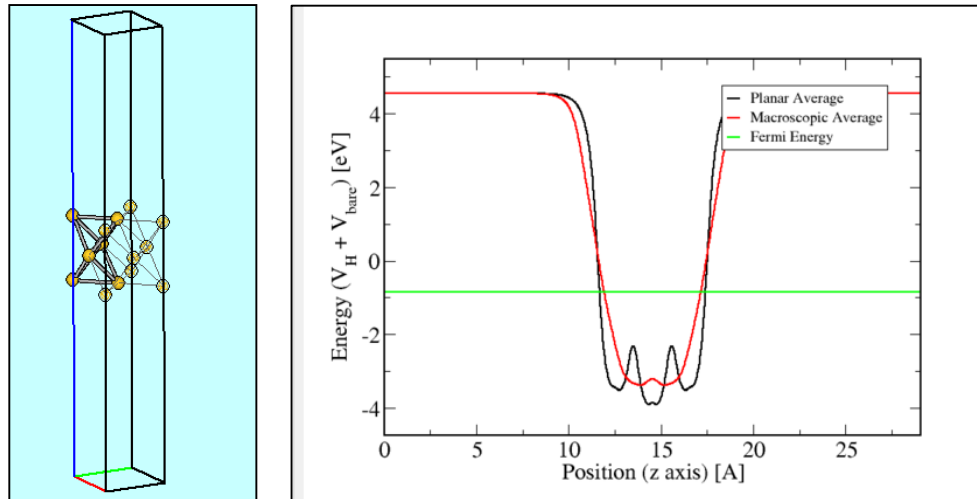
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# Summary

- 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).

# Configuration

① See Quantum ESPRESSO install manual

[https://winmostar.com/en/QE\\_install\\_manual\\_en\\_win.pdf](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.*

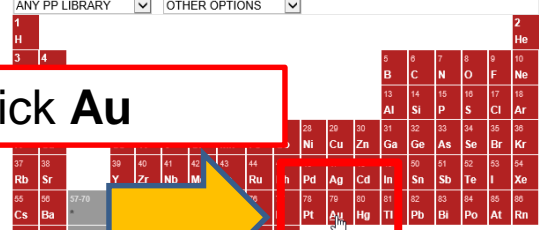
More information about **pseudopotentials in general**, the **naming convention** adopted for pseudopotential files, the **Unified Pseudopotential Format**, and on other pseudopotential databases, can be found via the links of the menu at the left.

*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:\winmos8\samples\au\_slab.cif**.

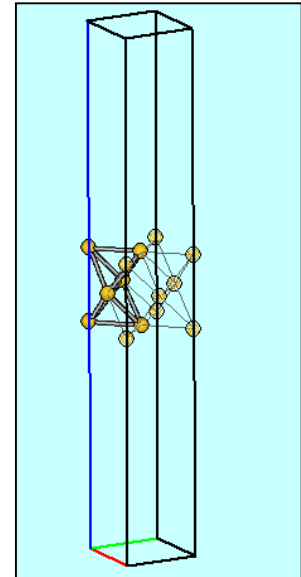
You can also make the same CIF file using **Crystal Builder**.  
See **crystal modeling tutorial** and apply the following information.

### To Make Au unit cell

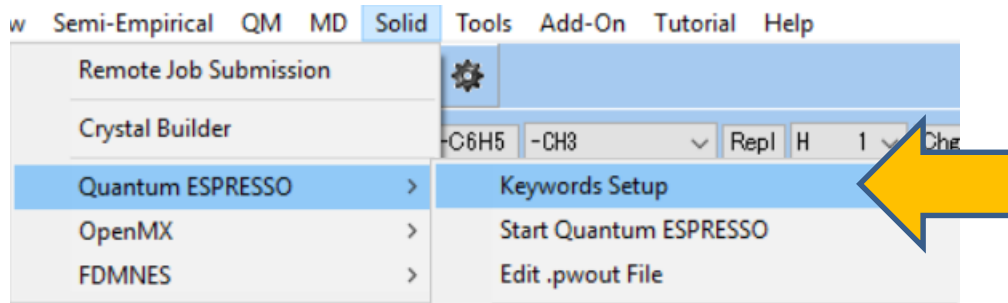
Crystal system : Cubic  
Space group : Fm-3m (225)  
Lattice constants : a=4.078830 Å  
Fractional coordinates : Au (0.0 0.0 0.0)

### To Make Slab

Thickness of vacuum layer 25 Å

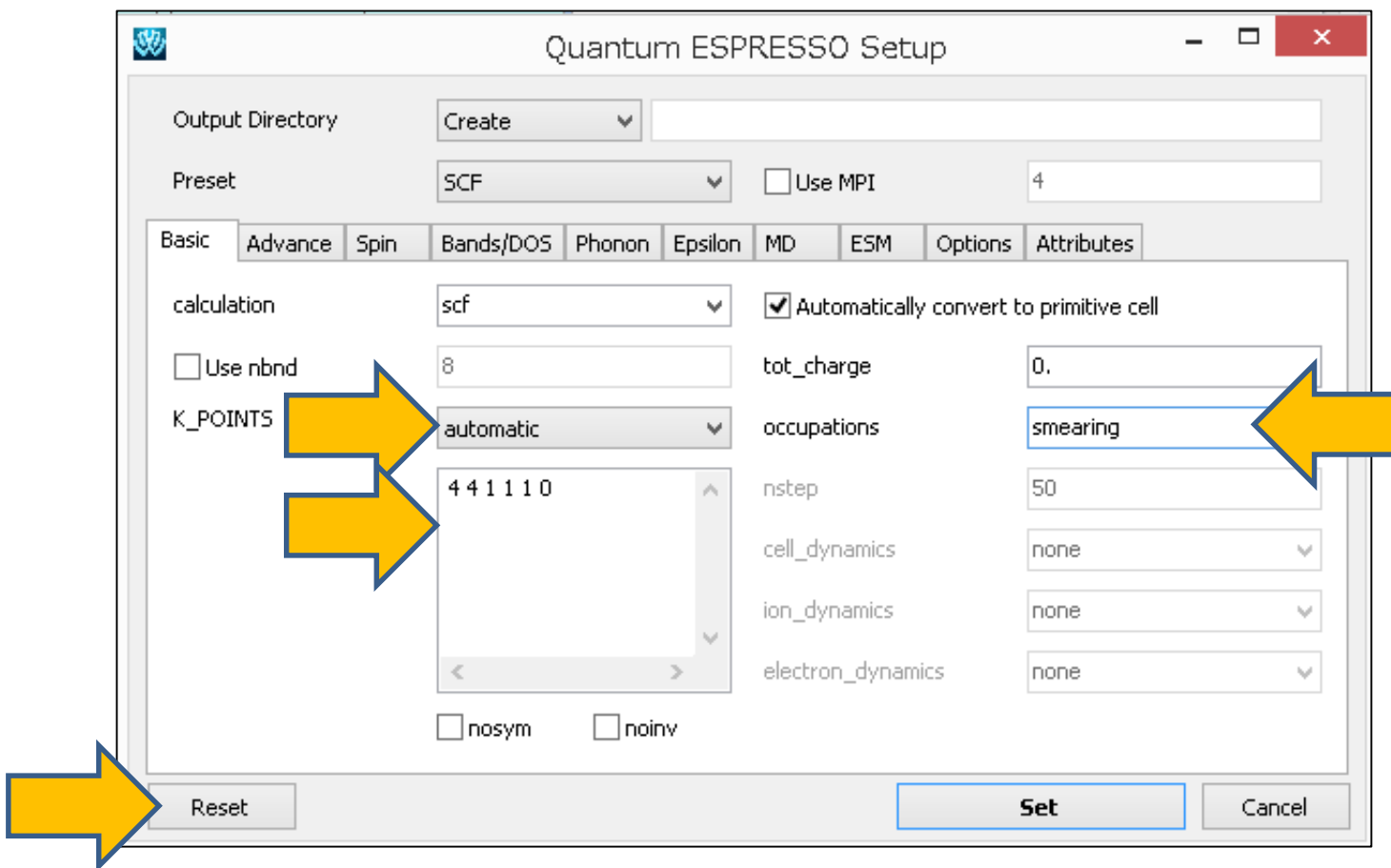


2. Click **Solid | Quantum ESPRESSO | Keywords Setup**.



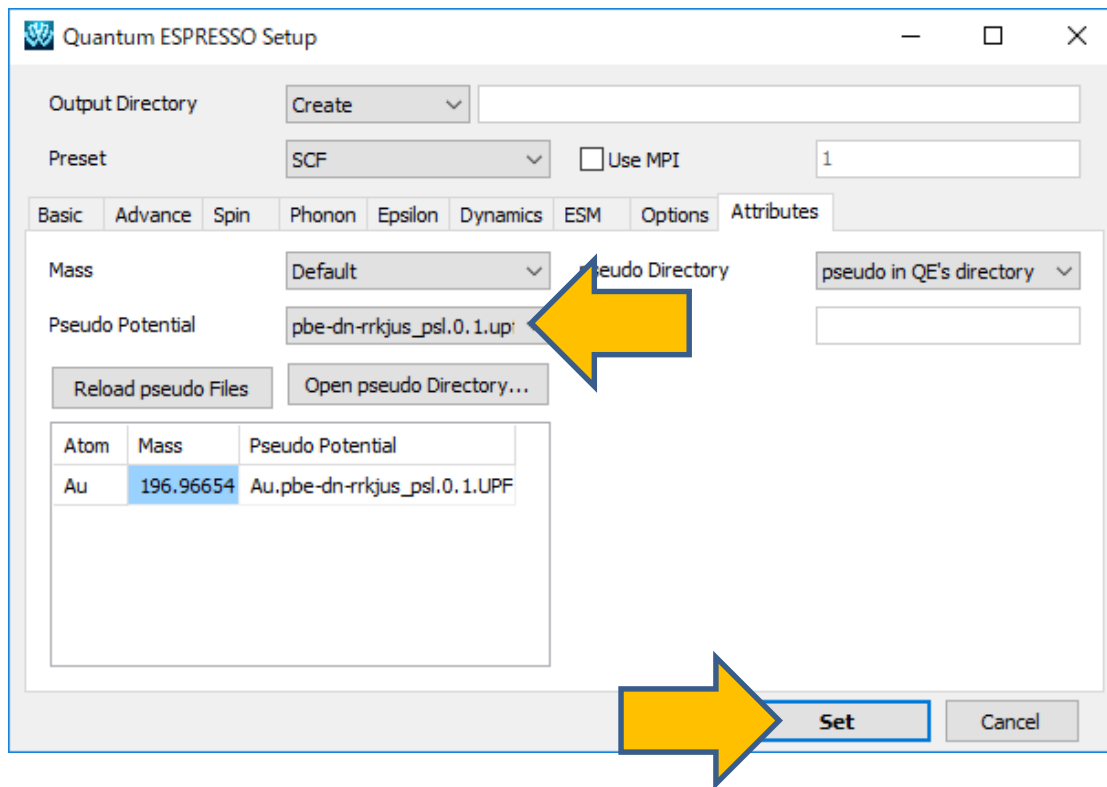
# I. SCF Calculation

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**.”



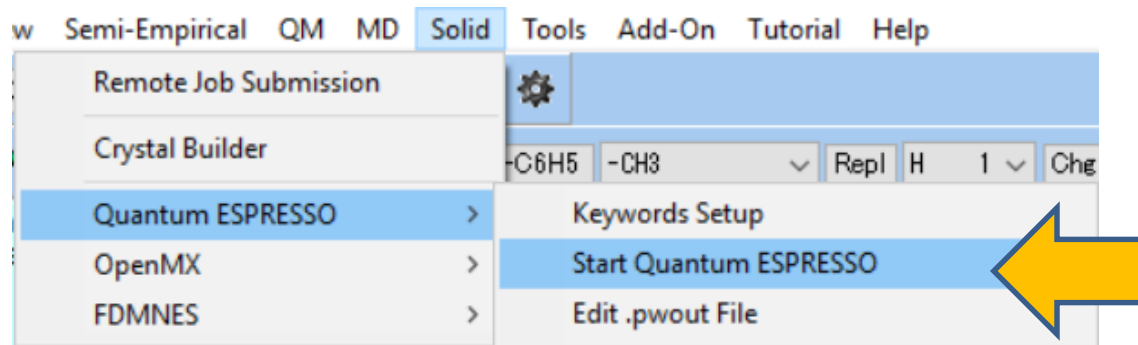
# I. SCF calculation

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

