

Winmostar tutorial
Quantum ESPRESSO
Effective Screening Medium (ESM)
V8.007

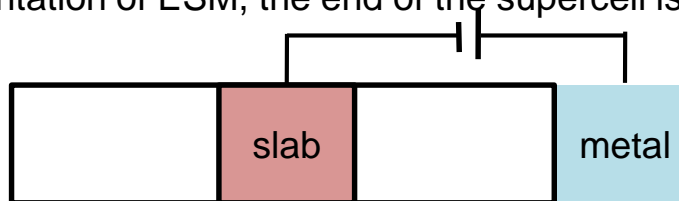
X-Ability Co., Ltd.
question@winmostar.com

2018/01/15

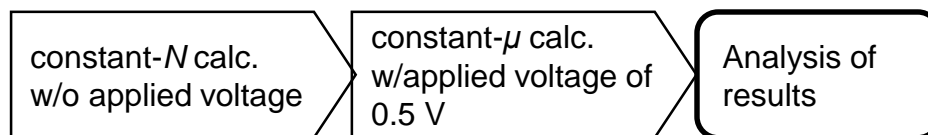
Summary

- In this tutorial we will perform ESM method calculation that will treat Al monoatomic slab as electrodes. Here, we use the boundary conditions representing the Vacuum-slab-metal (bc3) (see below).

Note: Due to QE's implementation of ESM, the end of the supercell is located at the center of the figure shown below.



First, we will perform a constant- N calculation without applied voltage. Secondly, we will perform a constant- μ calculation with an applied voltage of 0.5 V. After implementation, we will confirm that a potential difference of 0.5 V is generated between slab and virtual electrodes (metal).



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.
- The size of systems will affect calculation results.

Configuration

1. See Quantum ESPRESSO install manual

https://winmostar.com/en/QE_install_manual_en_win.pdf

2. Via the following URL, download **Al.pbe-n-van.UPF** and move it into Pseudo folder in Quantum ESPRESSO installation directory. Then reopen 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)

Click **AI.**

TYPE Apply Filter
OPTIONS

Classification controlled by Andrea Dal Corso

Al.pbe-n-van.UPF

Pseudopotential type: ULTRASOFT
Method: Vanderbilt ultrasoft
Functional type: Perdew-Burke-Ernzerhof
Nonlinear core correction
scalar relativistic

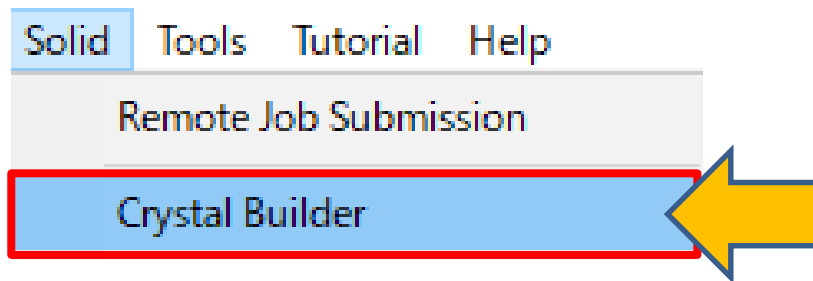
Origin: Original QE PP library
Generated by Vanderbilt code version 7.3.5
More Information: [Al.pbe-n-van.txt](#)
Uploaded by Erica Vidal
Classification controlled by Paolo Giannozzi

Click Al.pbe-n-van.UPF.

Al.pbe-rrkj.UPF

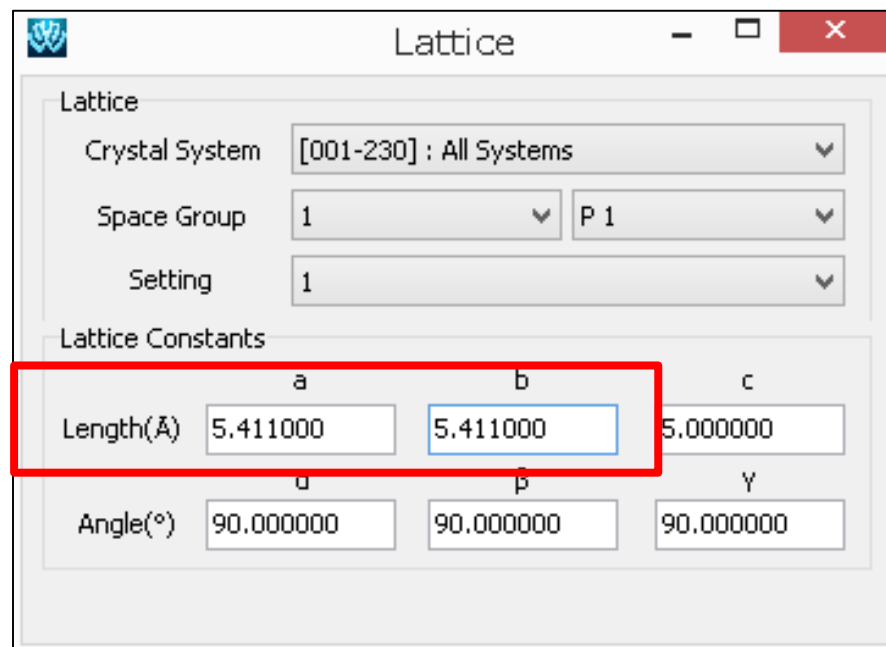
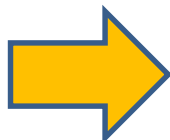
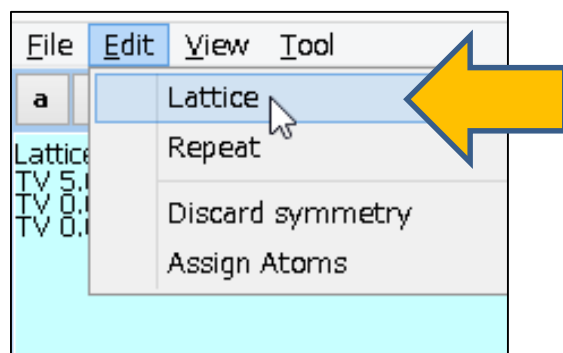
I. Slab model 1

Click **Solid | Crystal Builder**.



I. Slab model 2

1. On crystal builder, click **Edit | Lattice**.
2. Set **Space Group** to **P1**, **a** to **5.411**, **b** to **5.411**.
3. Close Lattice window.



I. Slab model 3

Change atom from **C** to **Al**, set the coordinate to “**0 0 0.5**”.

The screenshot shows the X-Ability software interface. On the left, a 3D unit cell is displayed with axes labeled a, b, and c. A yellow arrow points from the unit cell to the atom definition table on the right. The table is titled "Step 2/4 : Asymmetric Unit" and has columns for Atom, x, y, and z. The first row is highlighted with a red box and contains the following data:

Atom	x	y	z
Al	0.000000	0.000000	0.5

Below the table, the "Lattice Constants" and "Translation Vector" are displayed:

```
Lattice Constants
5.411 5.411 5.000 90.000 90.000 90.000

Translation Vector
5.411 0.000 0.000
0.000 5.411 0.000
0.000 0.000 5.000

Number of Atoms (displayed)
4
```

I. Slab model 4

1. Click **Tool | Insert Vacuum**.
2. Click Yes.
(**Insert vacuum mode** will start.)

Crystal Builder

File Edit View **Tool** Return To Winmostar

a b c

Cleave Plane

Insert Vacuum

Lattice constant 90.000

Zoom

Warning

! Symmetry must be discarded before inserting vacuum.
Do you really want to discard symmetry?

Yes No

View Return To Crystal Builder

a b c

Lattice constant 5.411 5.411 5.000 90.000 90.000 90.000

TV 5.411 0.000 0.000

TV 0.000 5.411 0.000

TV 0.000 0.000 5.000

BS1 BS2 Connect 1.15

Zoom 1

Atom 0.25

Bond 10

Insert vacuum

Axis X Y Z

Bulk [A] Vacuum [A] Total Width [A]

5.000 + 0.000 = 5.000

Automatically shift to center

Shift 0.500

Reference plane

Base Center

OK

<< Back Next >>

Lattice Constants
5.411 5.411 5.000 90.000 90.000 90.000

Translation Vector
5.411 0.000 0.000
0.000 5.411 0.000
0.000 0.000 5.000

Number of Atoms (displayed)
4

I. Slab model 5

1. Set **Vacuum** to **17.5** to define the thickness of vacuum layer.
2. Click **OK** to switch manual mode of crystal builder.

View Return To Crystal Builder

a b c

Lattice constant 5.411 5.411 5.000 90.000 90.000 90.000
 TV 5.411 0.000 0.000
 TV 0.000 5.411 0.000
 TV 0.000 0.000 22.500

BS1 BS2 Connect 1.15

Zoom 0.65

Atom 0.25

Bond 10

Insert vacuum

Axis X Y Z

Build [Å] Vacuum [A] Total Width [A]
 5 17.500 = 22.500

Automatically shift to center

Shift 0.500

Reference plane Base Center

OK

<< Back Next >>

Lattice Constants
 5.411 5.411 5.000 90.000 90.000 90.000

Translation Vector
 5.411 0.000 0.000
 0.000 5.411 0.000
 0.000 0.000 5.000

Number of Atoms (displayed)
 4

I. Slab model 6

Change fractional z coordinate of **Al** to **0**.

File Edit View Tool

a b c a* b* c*

Lattice constant 5.411 5.411 22.500 90.000 90.000 90.000
 TV 5.411 0.000 0.000
 TV 0.000 5.411 0.000
 TV 0.000 0.000 22.500

Plain Normal

Zoom 0.6

Atom 0.25

Bond 10

Asymmetric Unit

Add Remove

Atom	x	y	z
Al	0.000000		0

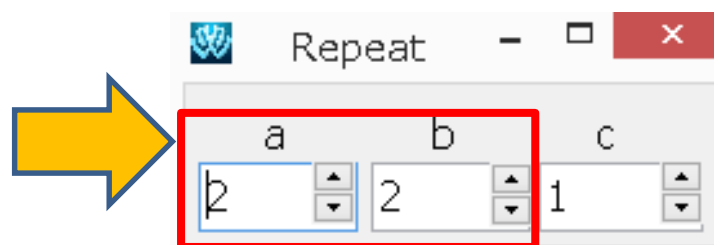
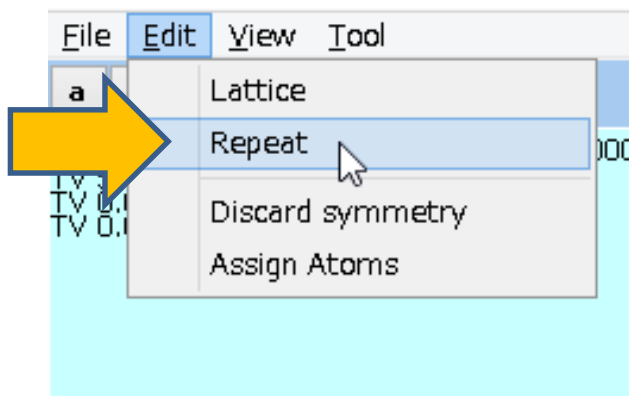
Lattice Constants
5.411 5.411 22.500 90.000 90.000 90.000

Translation Vector
5.411 0.000 0.000
0.000 5.411 0.000
0.000 0.000 22.500

Number of Atoms (displayed)
8

I. Slab model 7

1. Click **Edit | Repeat**.
2. Set **a** and **b** to **2**.
3. Close **Repeat**.



I. Slab model 7

1. Click **File | Save As**.
2. Save as **al_slab.cif**.
3. Close **Crystal Builder**.

Crystal Builder

File Edit View Tool

- New Ctrl+N
- Open Ctrl+O
- Save As

2.500 90.000 90.000 90.000

Plain Normal

Zoom 0.4

Atom 0.25

Bond 10

Asymmetric Unit

Atom	X	Y	Z
Al	0.000000	0.000000	0

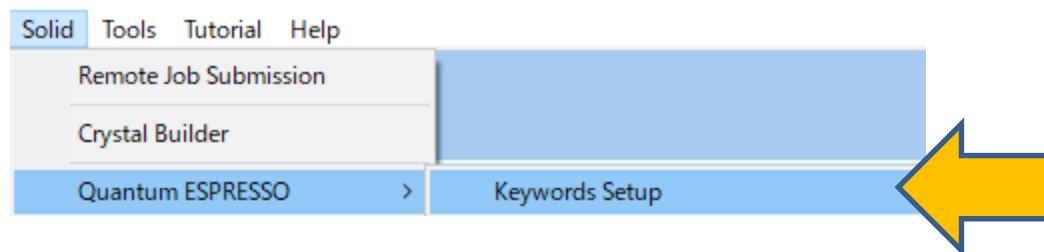
Lattice Constants
5.411 5.411 22.500 90.000 90.000 90.000

Translation Vector
5.411 0.000 0.000
0.000 5.411 0.000
0.000 0.000 22.500

Number of Atoms (displayed)
18

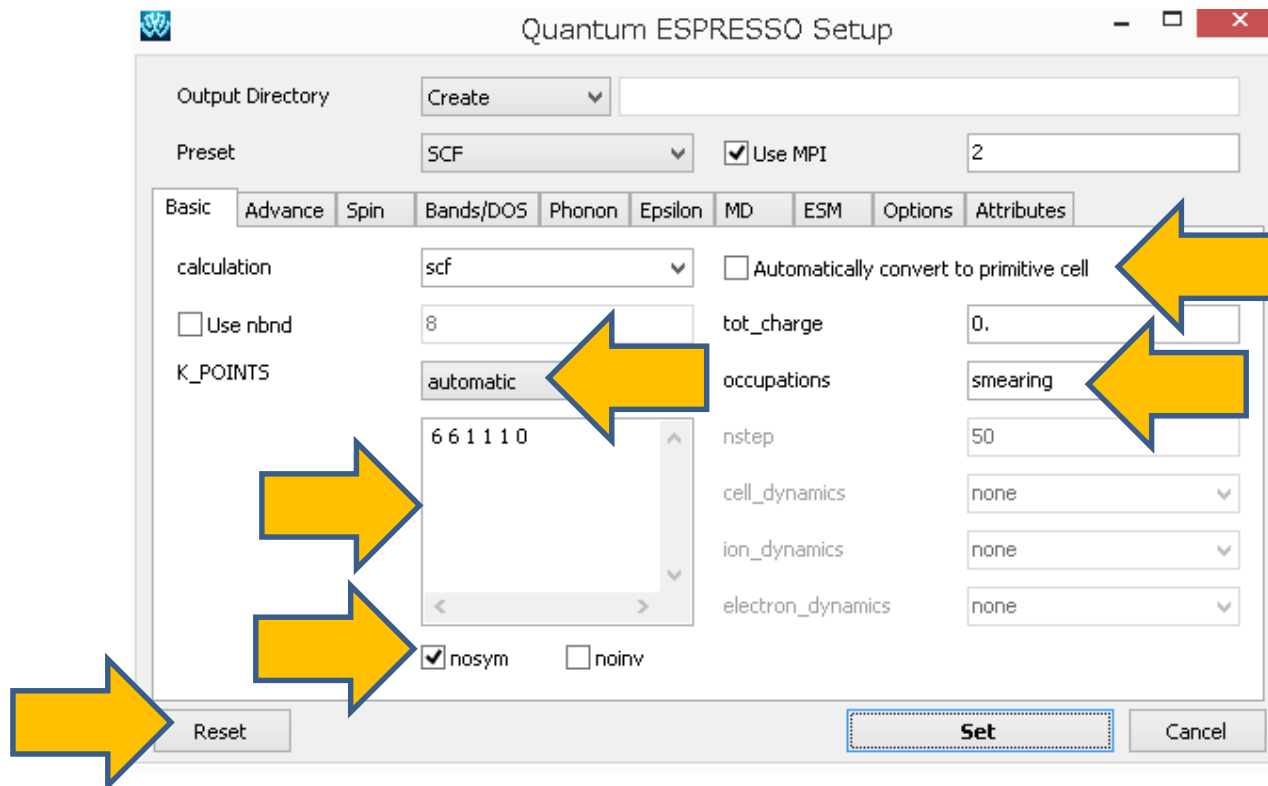
II. Constant- N 1

1. Click **File | Open**.
2. Open **al_slab.cif**.
3. Click **Solid | Quantum ESPRESSO | Keywords Setup**.



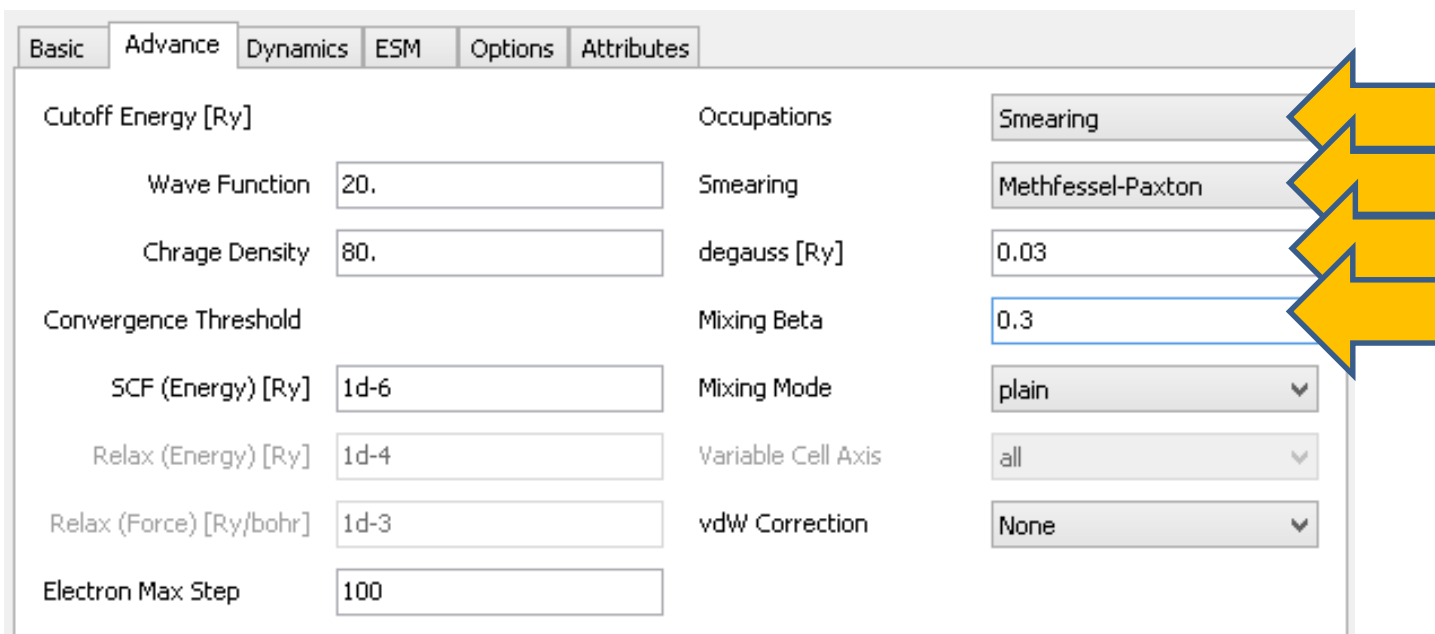
II. Constant- N^2

Click **Reset**. In the **Basic** tab set **K_POINTS** to **automatic** and enter **6 6 1 1 1 0** (space separated) in the text box below. Check **nosym** and uncheck **Automatically Convert to Primitive Cell**, then set **occupations** to **smearing**.



II. Constant-N 3

1. Click **Advance** tab
2. Set **Occupations** to **Smearing**.
3. Set **Smearing** to **Methfessel-Paxton**, **degauss** to **0.03**, **Mixing Beta** to **0.3**.



Basic		Advance	Dynamics	ESM	Options	Attributes
Cutoff Energy [Ry]		Occupations		Smearing		
Wave Function	20.	Smearing		Methfessel-Paxton		
Charge Density	80.	degauss [Ry]		0.03		
Convergence Threshold		Mixing Beta		0.3		
SCF (Energy) [Ry]	1d-6	Mixing Mode		plain		
Relax (Energy) [Ry]	1d-4	Variable Cell Axis		all		
Relax (Force) [Ry/bohr]	1d-3	vdW Correction		None		
Electron Max Step	100					

II. Constant- N 3

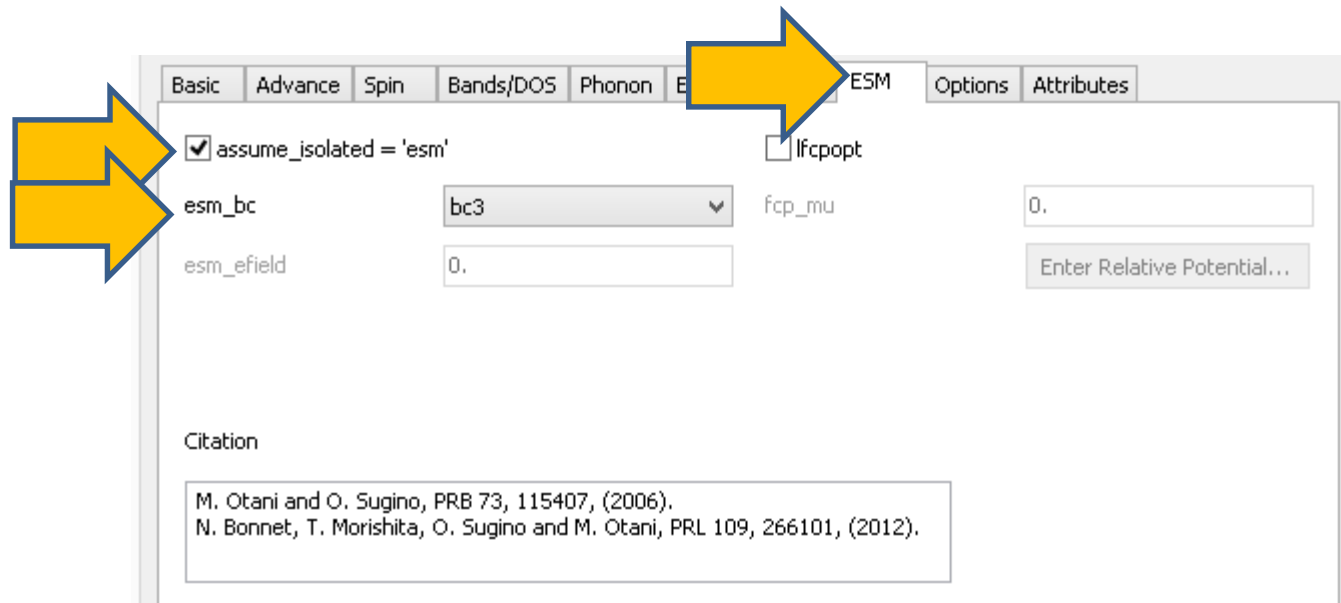
In the **Advance** tab, set **Smearing** to **Methfessel-Paxton**, **degauss** to **0.03**, and **Mixing Beta** to **0.3**.

The screenshot shows a software interface with a tabbed menu at the top. The 'Advance' tab is selected and highlighted with a yellow arrow. Below the tabs, there are several input fields and dropdown menus. Three yellow arrows point to the 'smearing' dropdown (set to 'methfessel-paxton'), the 'degauss' input field (set to '0.03'), and the 'mixing_beta' input field (set to '0.3').

Parameter	Value	Parameter	Value
ecutwfc	20.	smearing	methfessel-paxton
ecutrho	80.	degauss	0.03
conv_thr	1d-6	mixing_beta	0.3
etot_conv_thr	1d-4	mixing_mode	plain
forc_conv_thr	1d-3	cell_dofree	all
electron_maxstep	100	vdw_corr	None

II. Constant- N 4

In the **ESM** tab, check **assume_isolated = 'esm'** and set **esm_bc** to **bc3**.

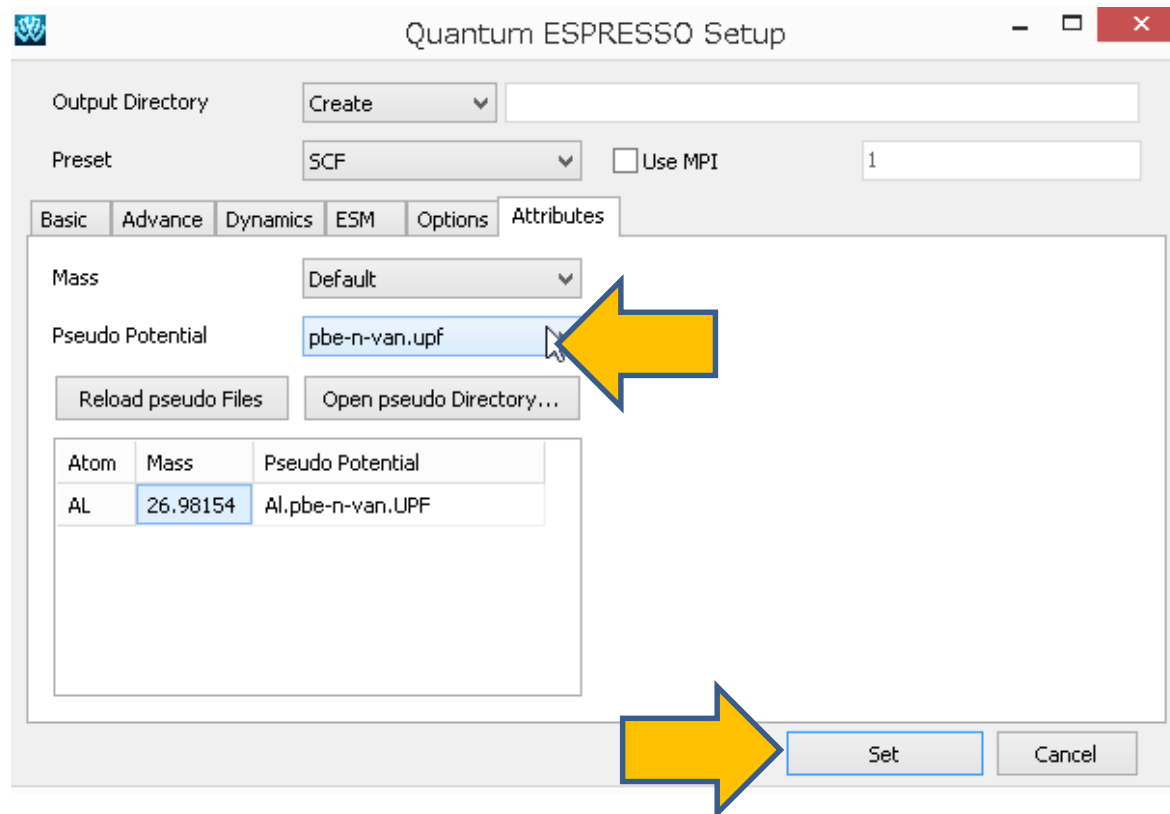


II. Constant- N 5

1. On **Attributes** tab, set **Pseudo Potential** to **pbe-n-van.upf**.

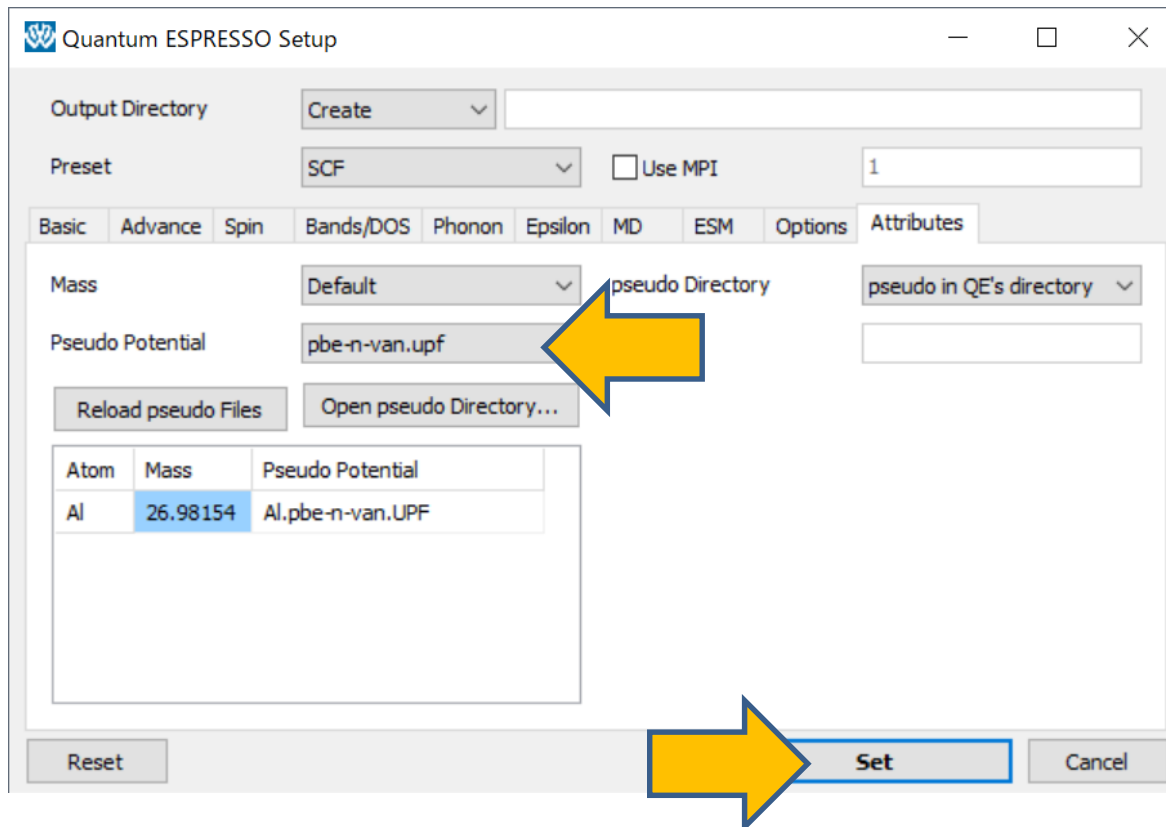
* If pbe-n-van.upf is not found, follow the procedure in Page 3 and place a pseudo file in the pseudo folder. Then click **Reload pseudo Files**.

2. Click **Set**.



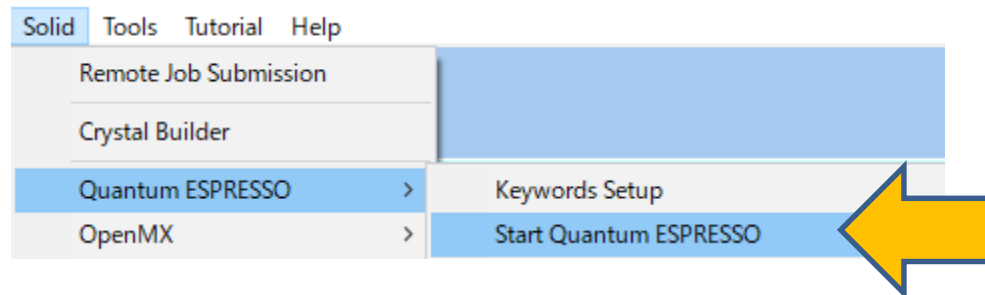
II. Constant- N 5

1. On **Attributes** tab, set **Pseudo Potential** to **pbe-n-van.upf**.
* If pbe-n-van.upf is not found, follow the procedure in Page 3 and place a pseudo file in the pseudo folder. Then click **Reload pseudo Files**.
2. Click **Set**.



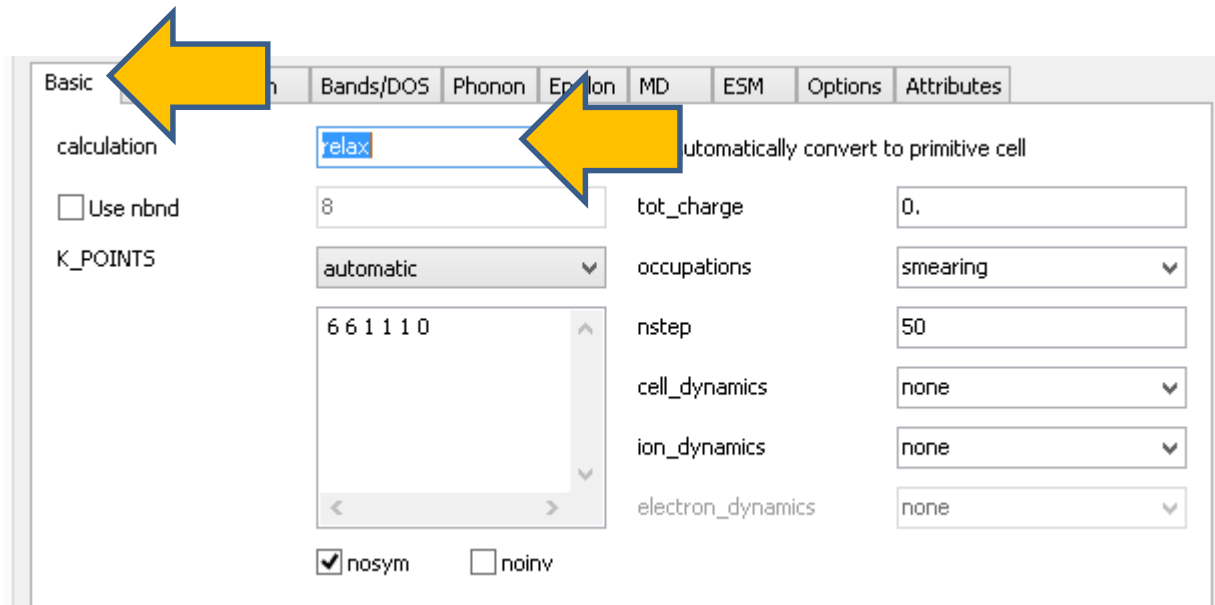
II. Constant- N 6

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Save as **al_slab_v0.pwin**.



III. Applied voltage 0.5 V, Constant- μ 1

1. After the calculation, click **Solid | Quantum ESPRESSO | Keywords Setup**.
2. On **Basic** tab, set **Calculation** to **Relax**.



III. Applied voltage 0.5 V, Constant- μ 2

1. On **ESM** tab, check **Enable Constant- μ** .
2. Click **Enter Relative Potential...**
3. Open **al_slab_v0.pwout**, set **Relative Potential** to **0.5 [V]**, then click **OK**.
4. Click **Yes**, then click **Set**.

The image shows a sequence of three windows from the X-Ability software interface, illustrating the steps to set a relative potential of 0.5 V. The first window is the 'ESM' tab of the main settings panel. It has several tabs: 'Basic', 'Advance', 'Dynamics', 'ESM', 'Options', and 'Attributes'. In the 'ESM' section, the 'Enable ESM Method' checkbox is checked. The 'Boundary Condition' is set to 'Vacuum-slab-metal (bc3)'. The 'Electric Field [Ry/bohr]' is set to '0'. The 'Target Fermi Energy [Ry]' is set to '-3.03319'. The 'Enable Constant- μ ' checkbox is checked. A yellow arrow points to this checkbox. Below the 'Target Fermi Energy' field is a button labeled 'Enter Relative Potential...'. A yellow arrow points to this button. At the bottom of the window are 'Set' and 'Cancel' buttons. A yellow arrow points to the 'Set' button. A blue arrow points from the 'Enter Relative Potential...' button to the second window. The second window is a dialog box titled 'Enter Relative Potential'. It has a text input field for 'Relative Potential [V]' with the value '0.5' entered. A yellow arrow points to this input field. Below the input field is an 'OK' button. A yellow arrow points to this button. A blue arrow points from the 'OK' button to the third window. The third window is an information dialog box titled '情報' (Information). It contains an information icon and the text: 'The reference Fermi energy and relative potential would be set to -3.033 eV and 0.500 V, respectively.' Below the text is a button labeled 'はい(Y)' (Yes). A yellow arrow points to this button.

III. Applied voltage 0.5 V, Constant- μ 2

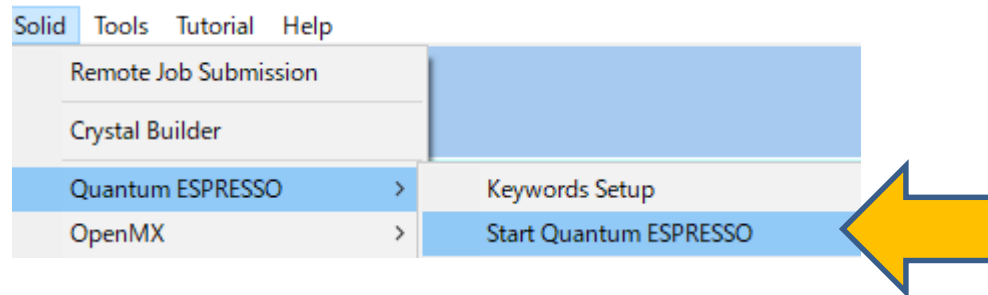
1. In the **ESM** tab check **lfcopt** then click **Enter Relative Potential...** button.
2. Open **al_slab_v0.pwout**, set **Relative Potential** to **0.5 [V]**, then click **OK**.
3. Click **Yes**, then click **Set**.

The image illustrates the process of setting the relative potential in the ESM tab. It consists of three sequential screenshots:

- First Screenshot:** The ESM tab is active. The **lfcopt** checkbox is checked. The **Enter Relative Potential...** button is highlighted with a yellow arrow. Other parameters like **esm_bc** (bc3) and **fcp_mu** (-0.18633) are visible.
- Second Screenshot:** The **Enter Relative Potential** dialog box is open. The **Relative Potential [V]** field is set to **0.5**. The **OK** button is highlighted with a yellow arrow.
- Third Screenshot:** An information dialog box titled **情報** (Information) is displayed. It contains the text: "The reference Fermi energy and relative potential would be set to -3.035 eV and 0.500 V, respectively." The **はい(Y)** (Yes) button is highlighted with a yellow arrow.

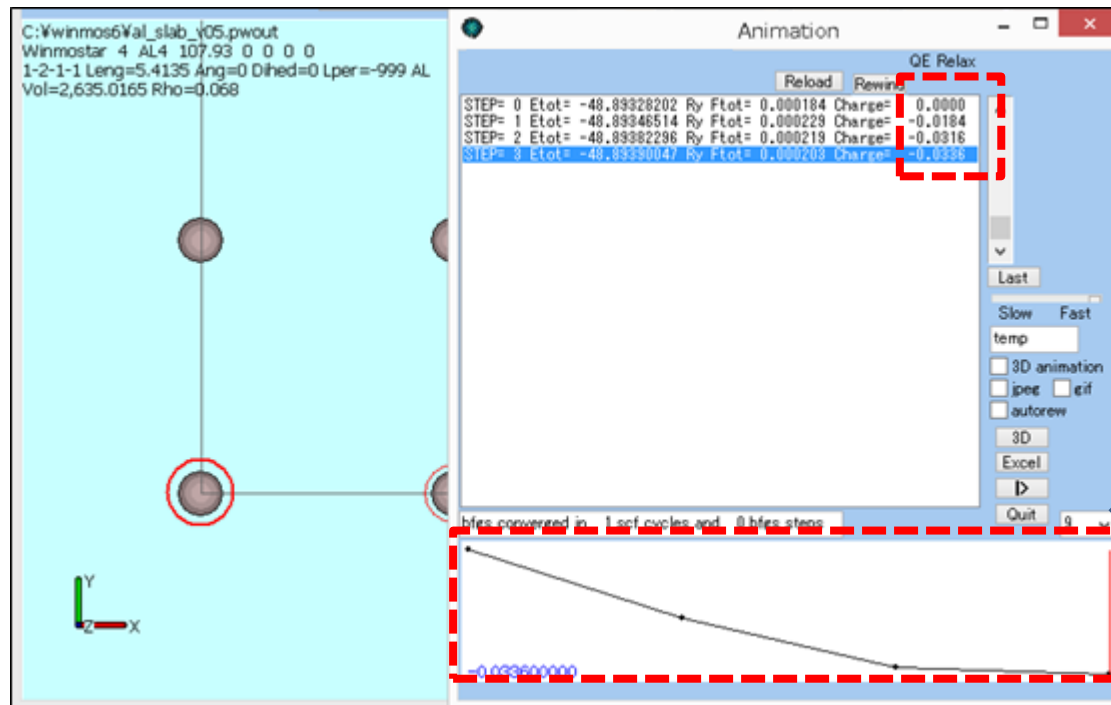
III. Applied voltage 0.5 V, Constant- μ 3

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Save as **al_slab_v05.pwin**.



III. Applied voltage 0.5 V, Constant- μ 4

1. After the calculation, click **Solid | Quantum ESPRESSO | Animation (pwout)**.
2. Open **al_slab_v05.pwout**.
3. Column **9** in the animations window shows **Total Charge** values. Set the pulldown to **9** to draw the graph of total charge.



IV. Confirmation of ESM calculation

1. Click **Solid | Quantum ESPRESSO | Difference Density/Energy (esm1)**.
2. Open esm1 file of reference. (`al_slab_v0_qe_data/wm.esm1`)
3. Open esm1 file of 0.5 V (`al_slab_v05_qe_data/wm.esm1`)
4. Click **Draw** to visualize the distribution of difference density and difference energy.
z=0 (the location of the slab) is the center of this graph.

