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

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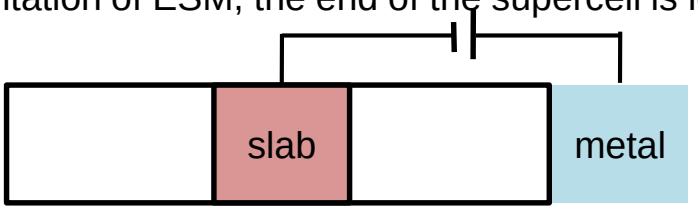
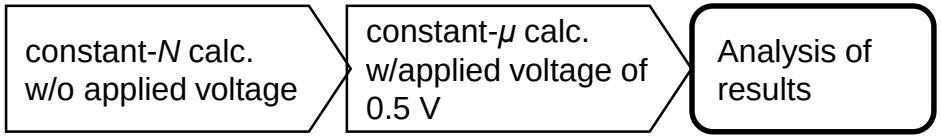
Summary

- 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.

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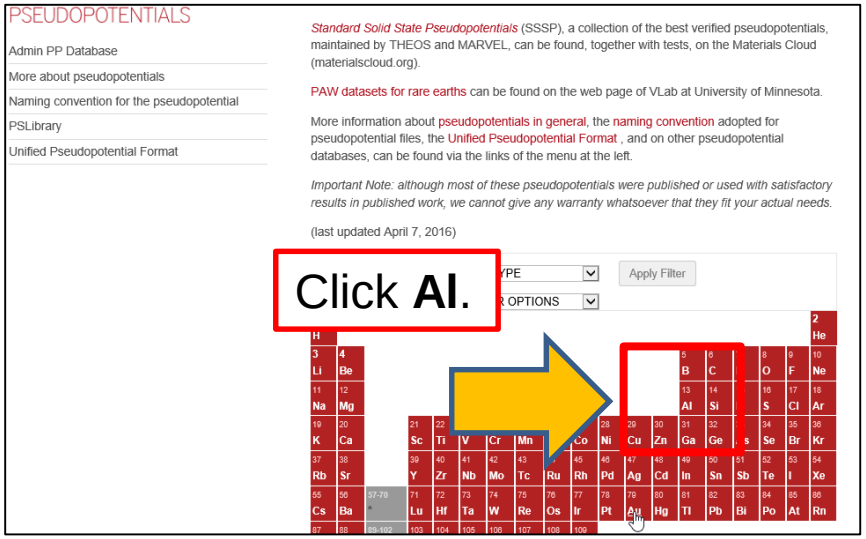
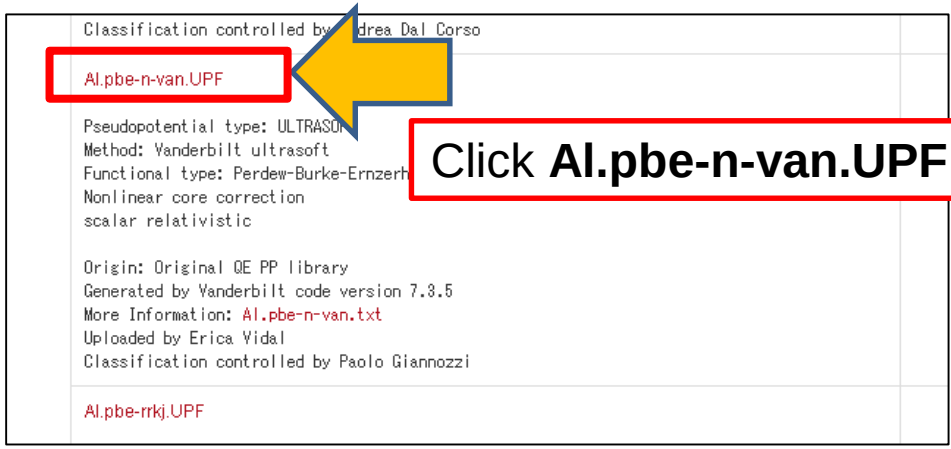
Configuration

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 ESPERSSO installation directory.
Then reopen Winmostar.
http://www.quantum-espresso.org/pseudopotentials/





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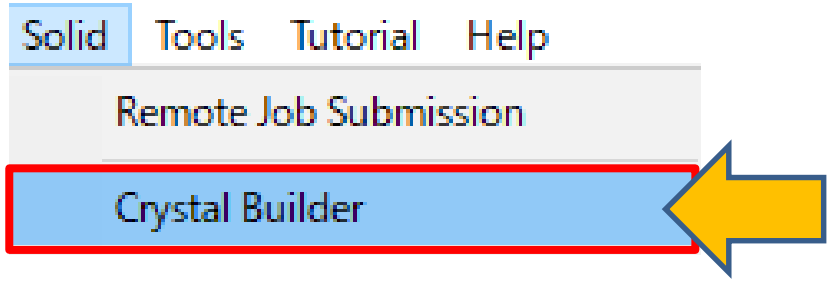
I. Slab model 1

Click **Solid** | **Crystal Builder**.



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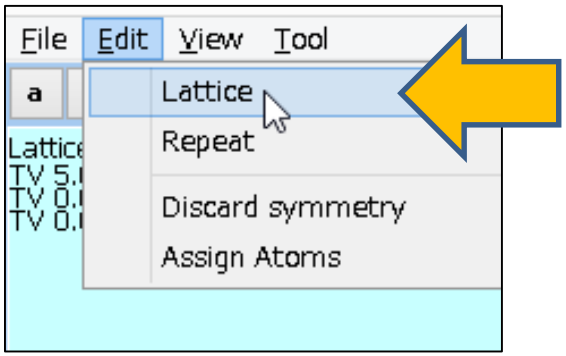
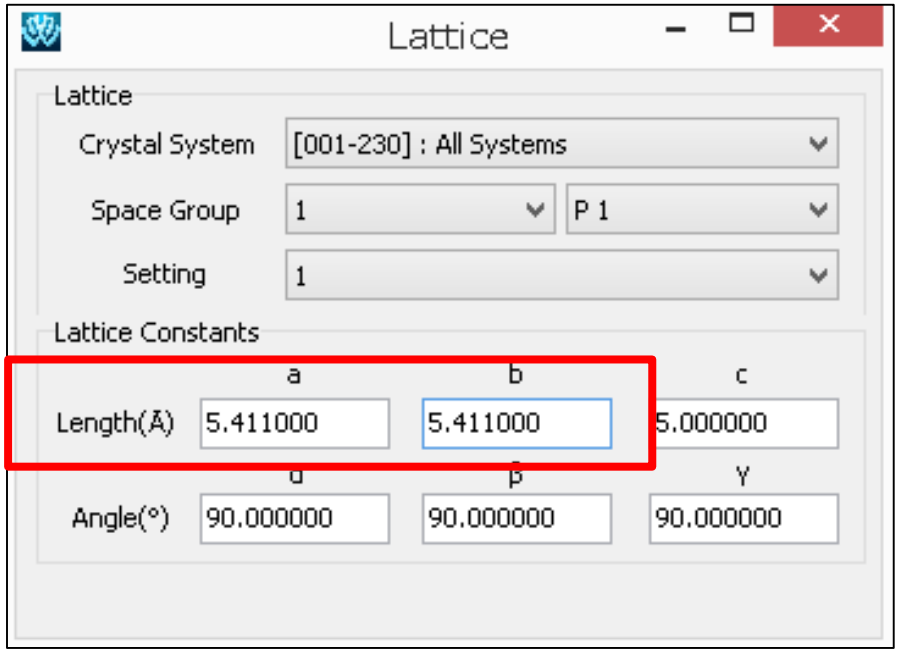
I. Slab model 2

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.





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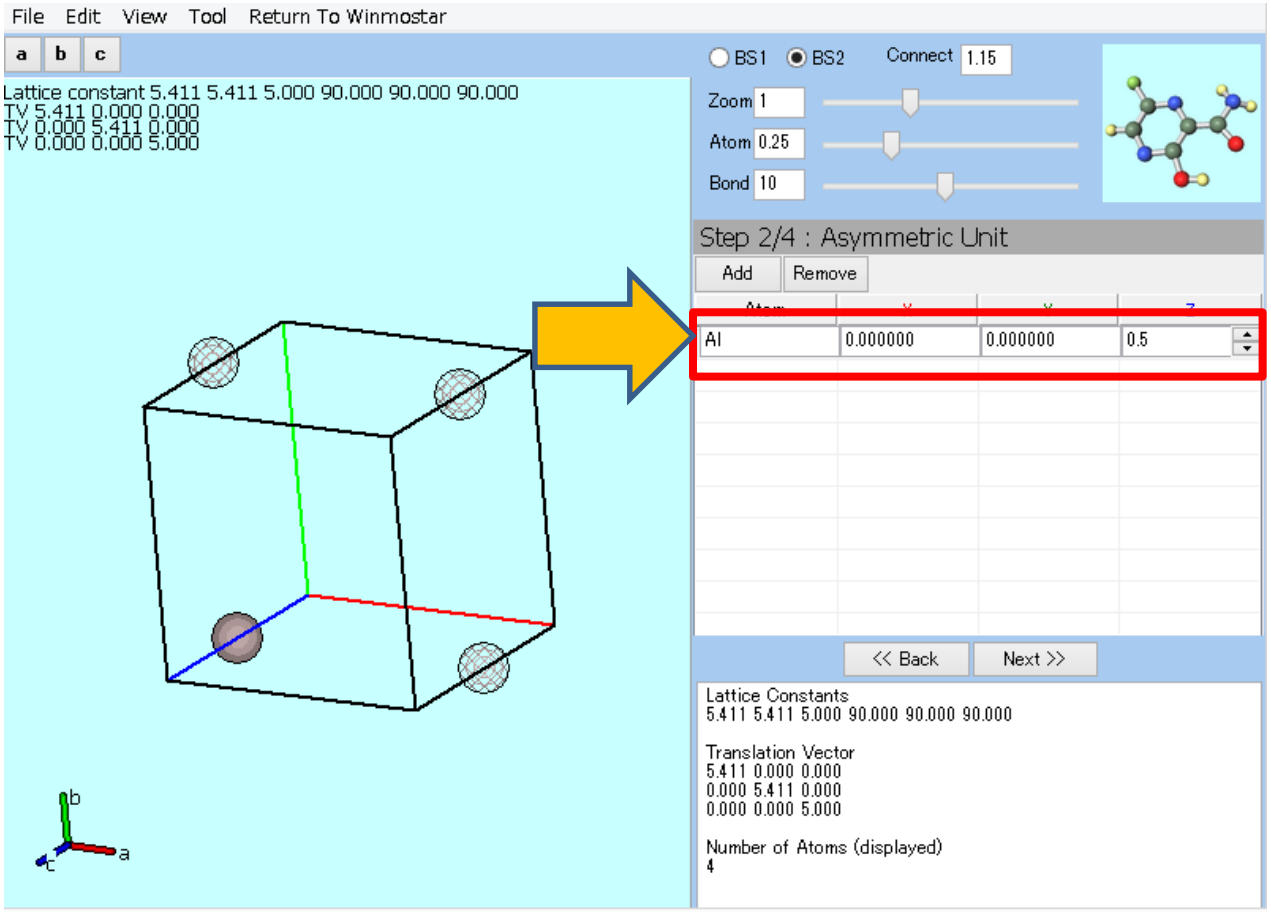
I. Slab model 3

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



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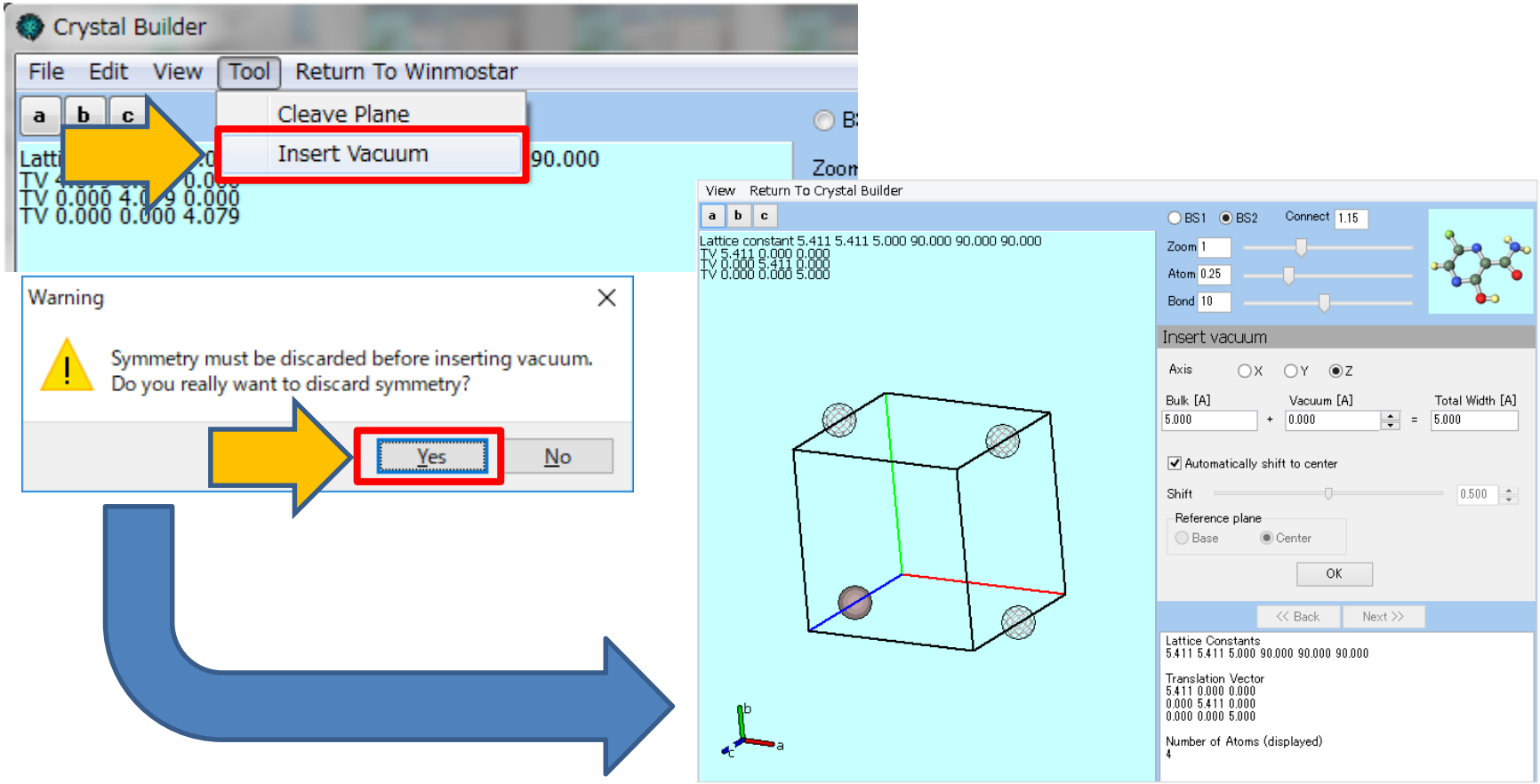
I. Slab model 4

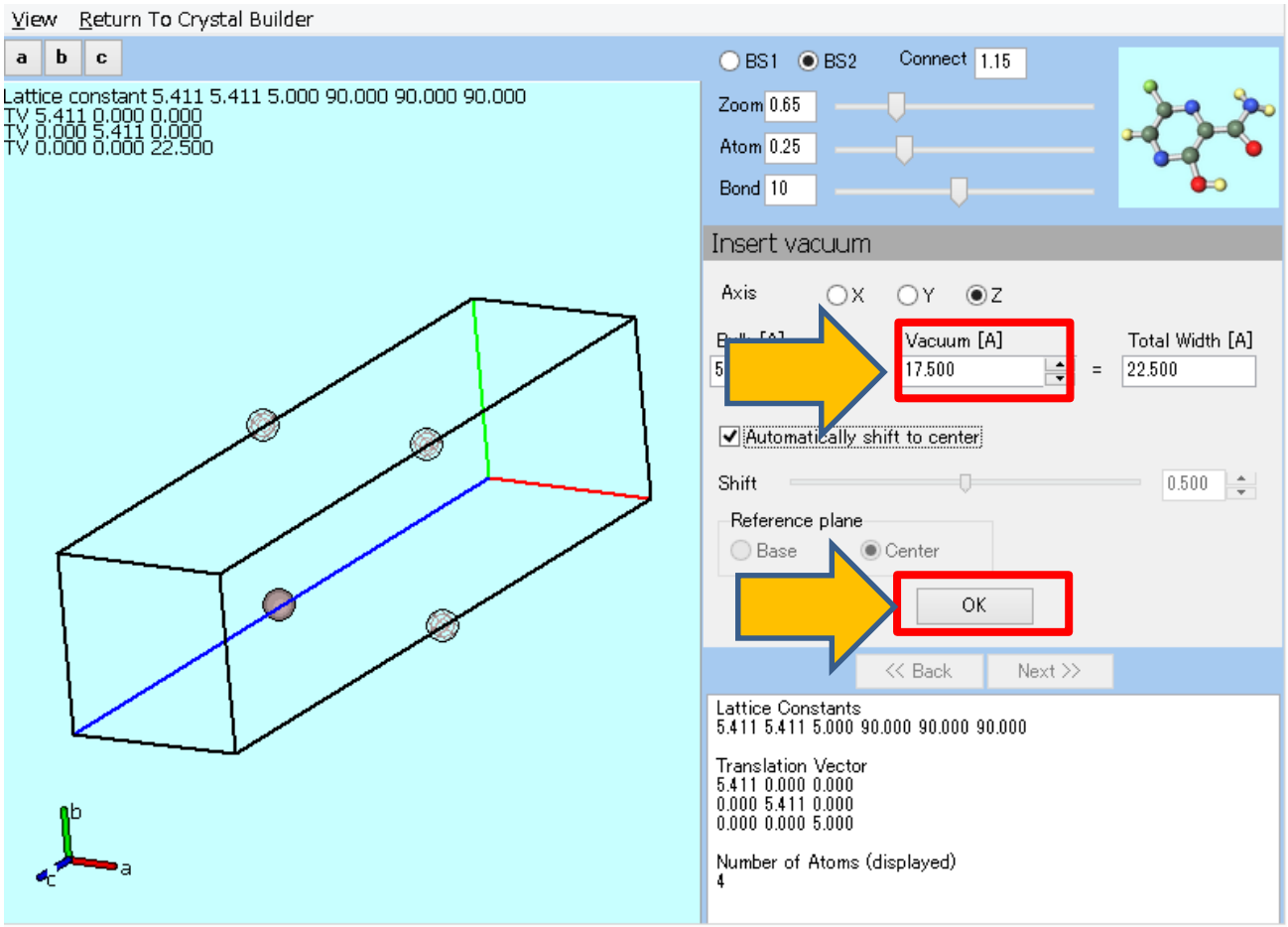
1. Click **Tool** | **Insert Vacuum**.
2. Click Yes.

（**Insert vacuum mode** will start.）



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.



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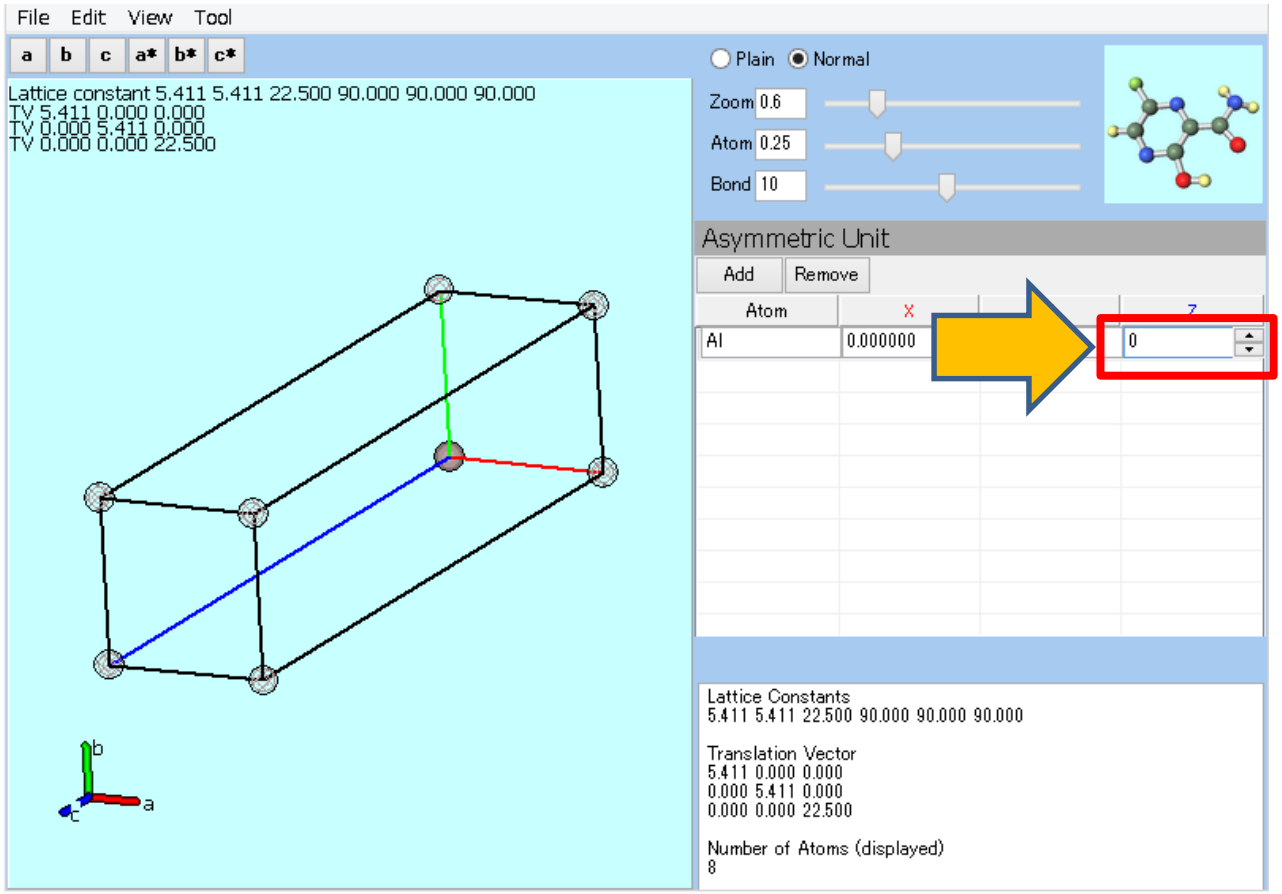
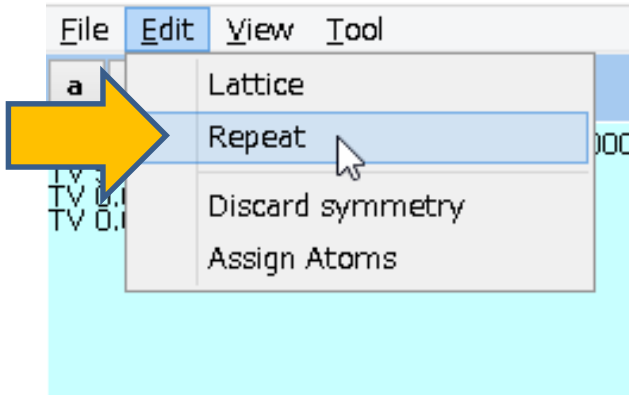
I. Slab model 6

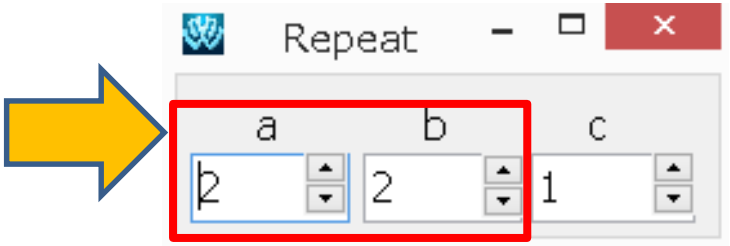
Change fractional z coordinate of **Al** to **0**.



I. Slab model 7

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





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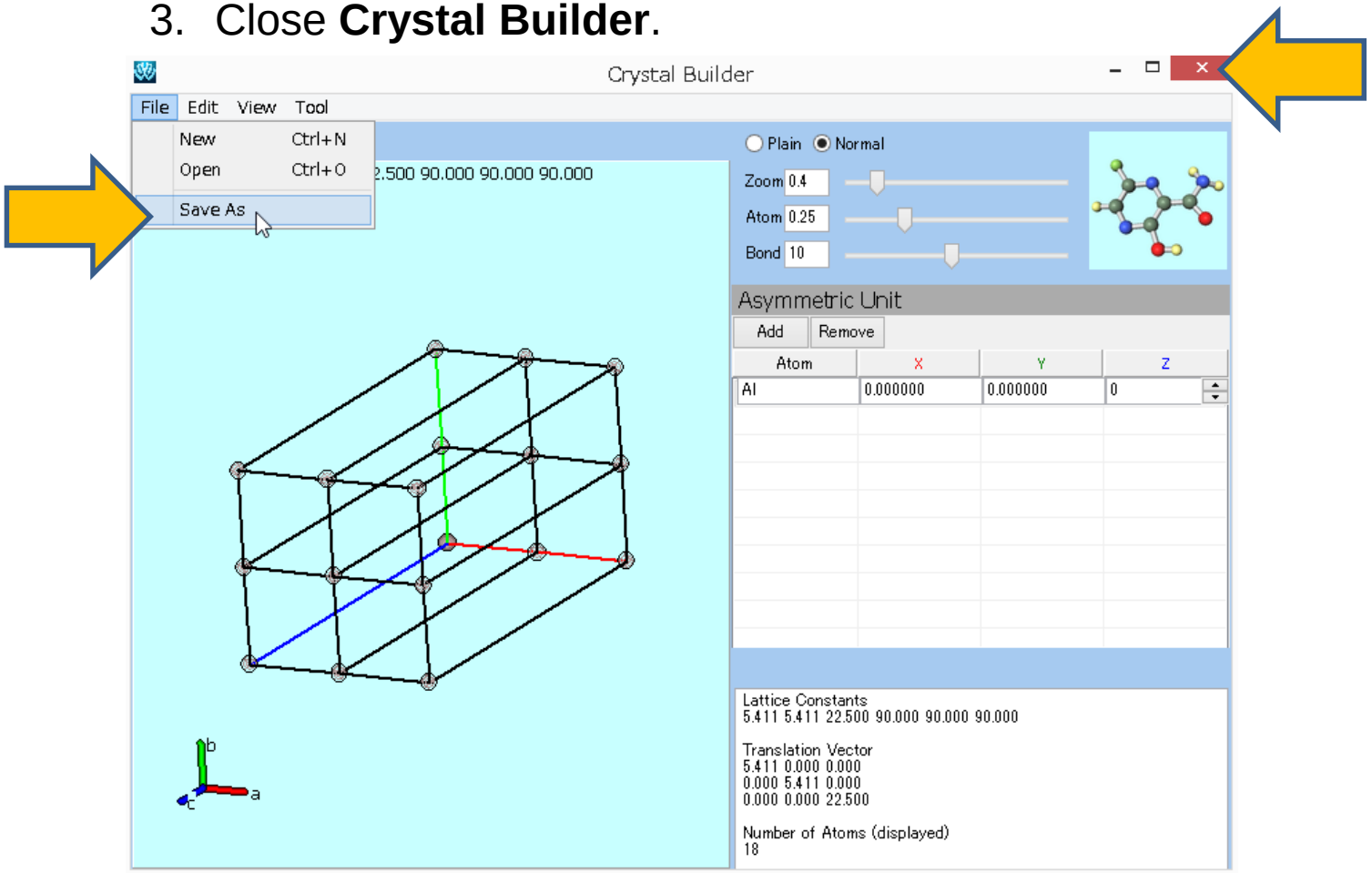
I. Slab model 7

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



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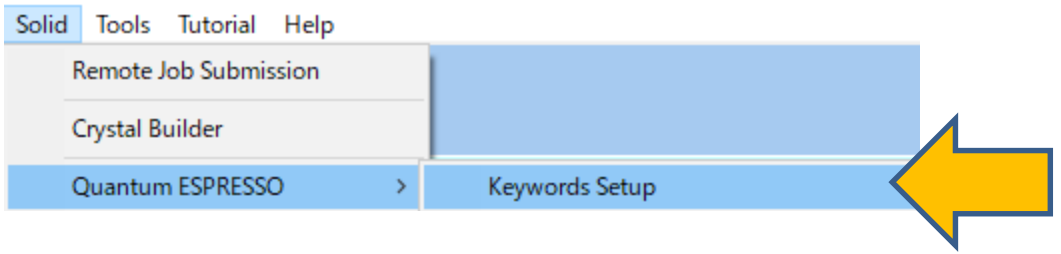
II. Constant-*N* 1

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



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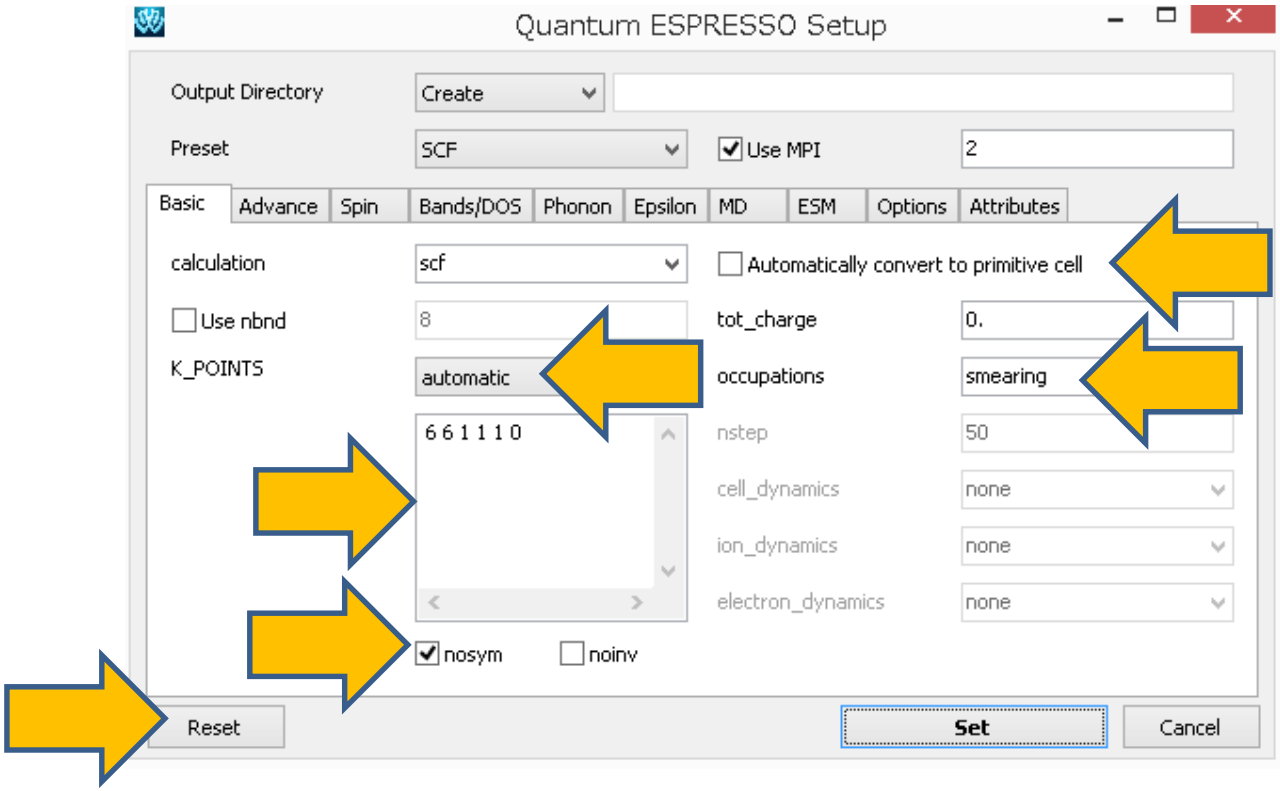
II. Constant-*N* 2

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**.



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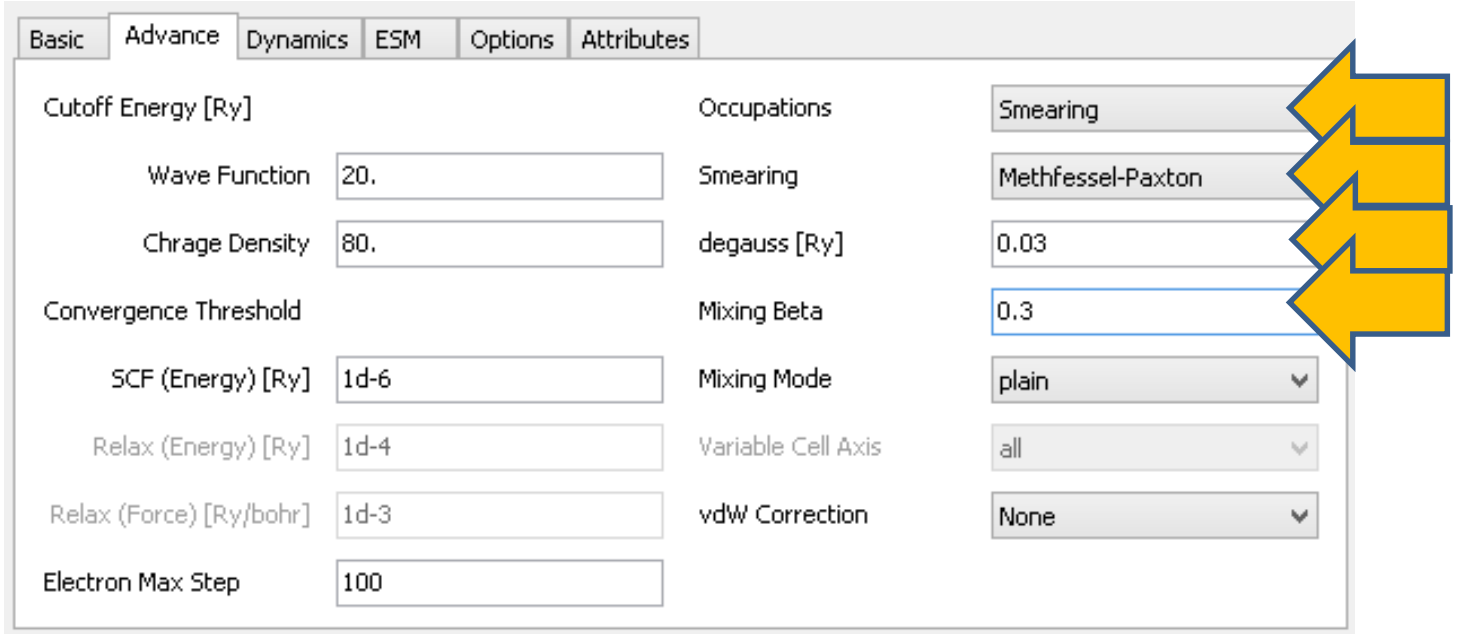
II. Constant-*N* 3

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



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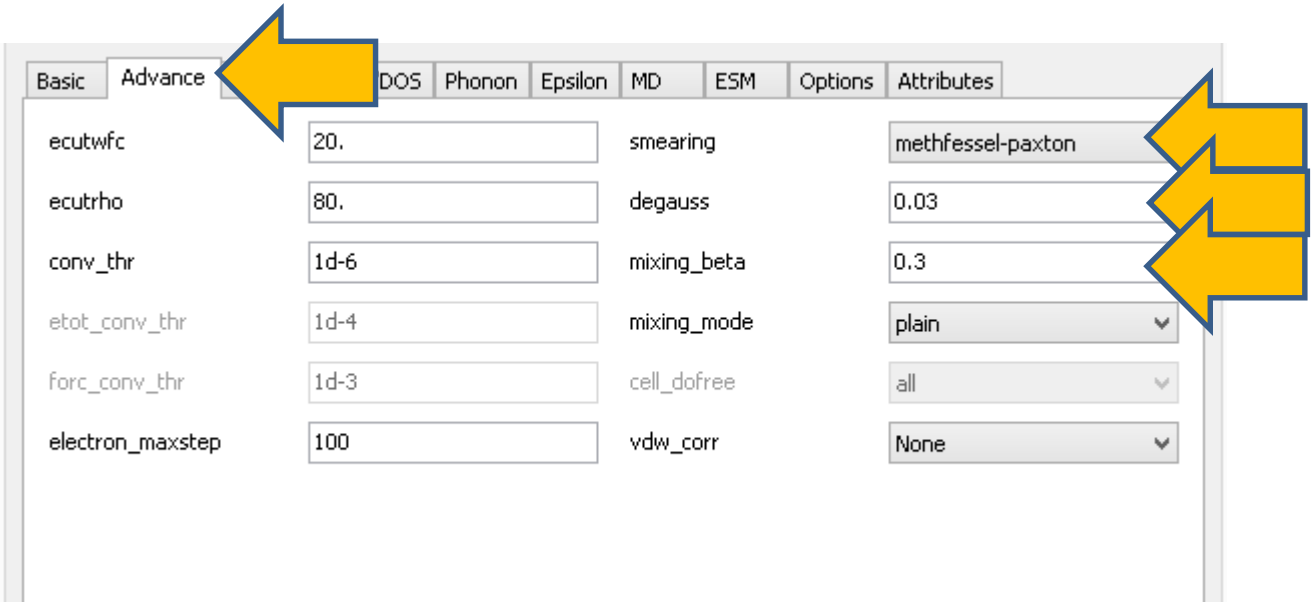
II. Constant-*N* 3

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



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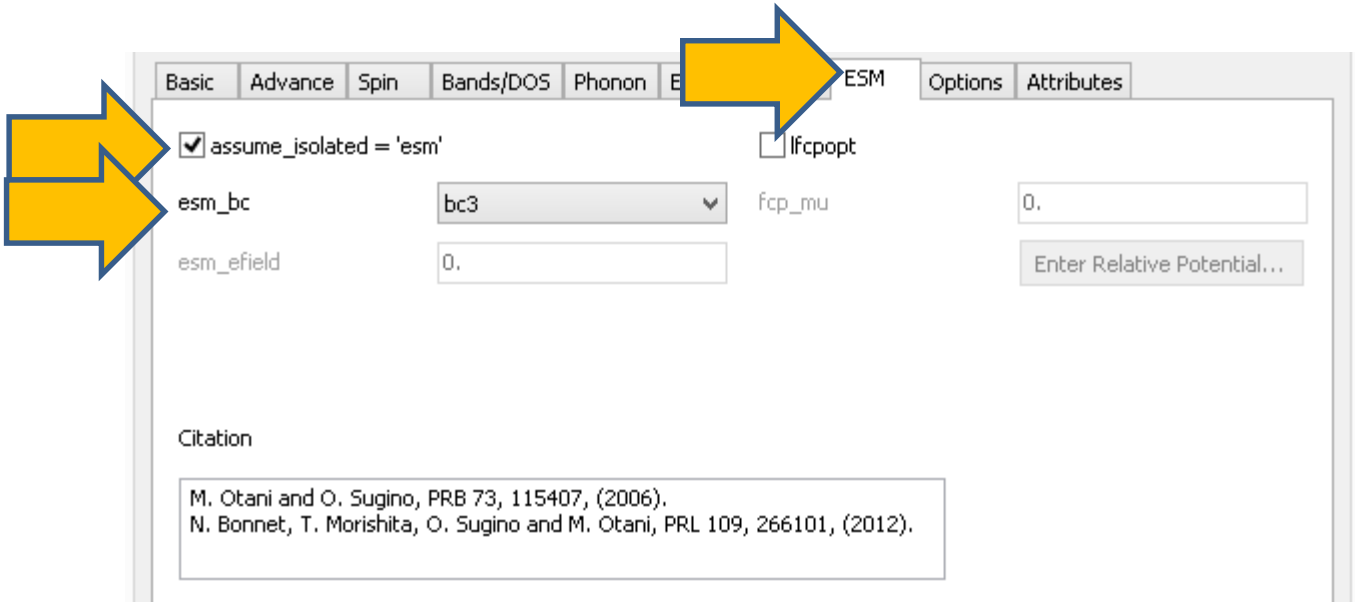
II. Constant-*N* 4

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



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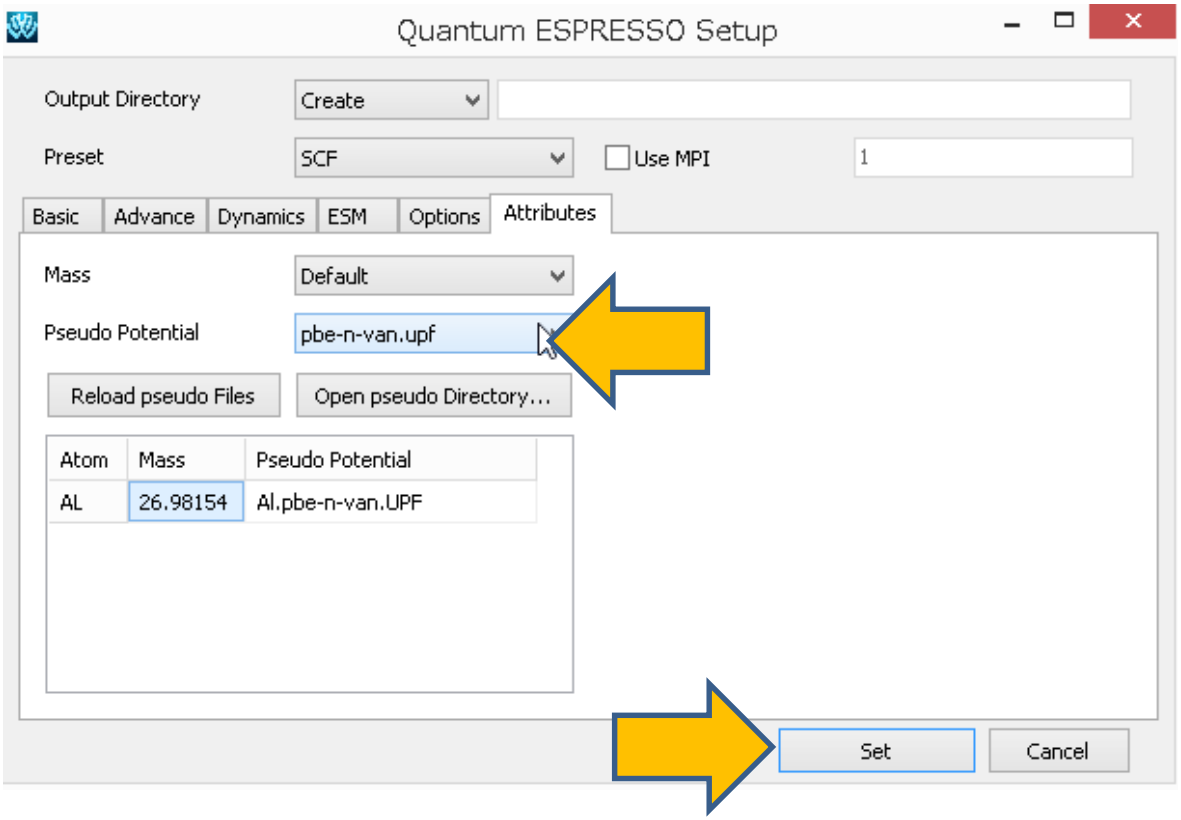
II. Constant-*N* 5

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**.



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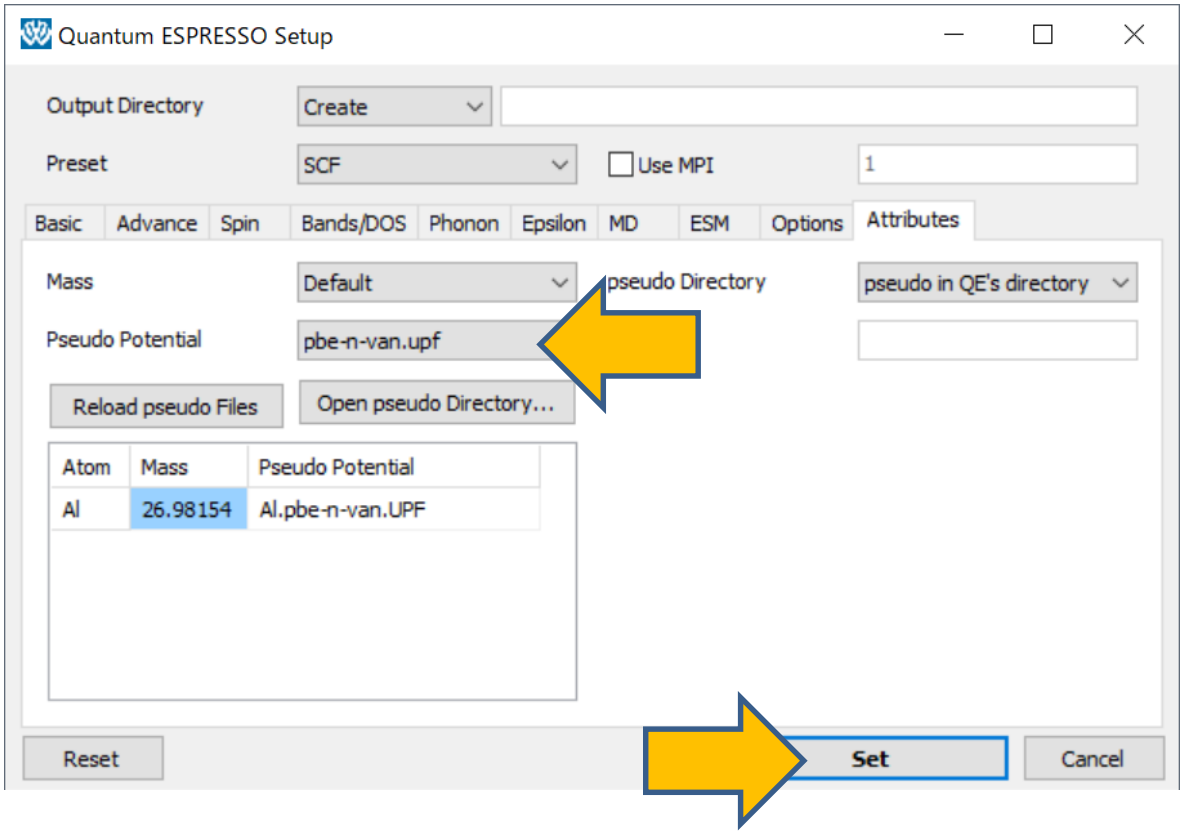
II. Constant-*N* 5

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**.



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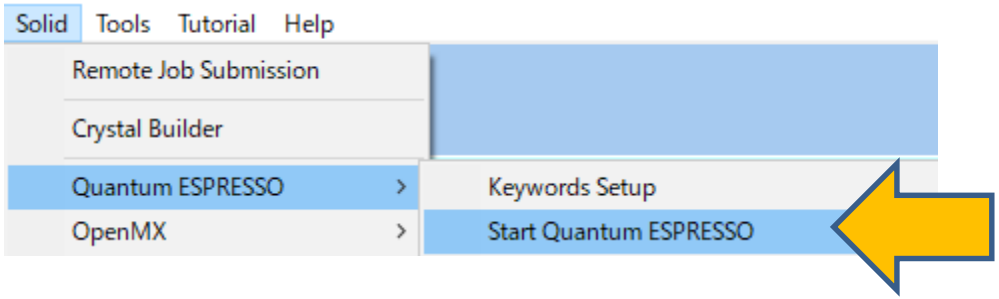
II. Constant-*N* 6

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



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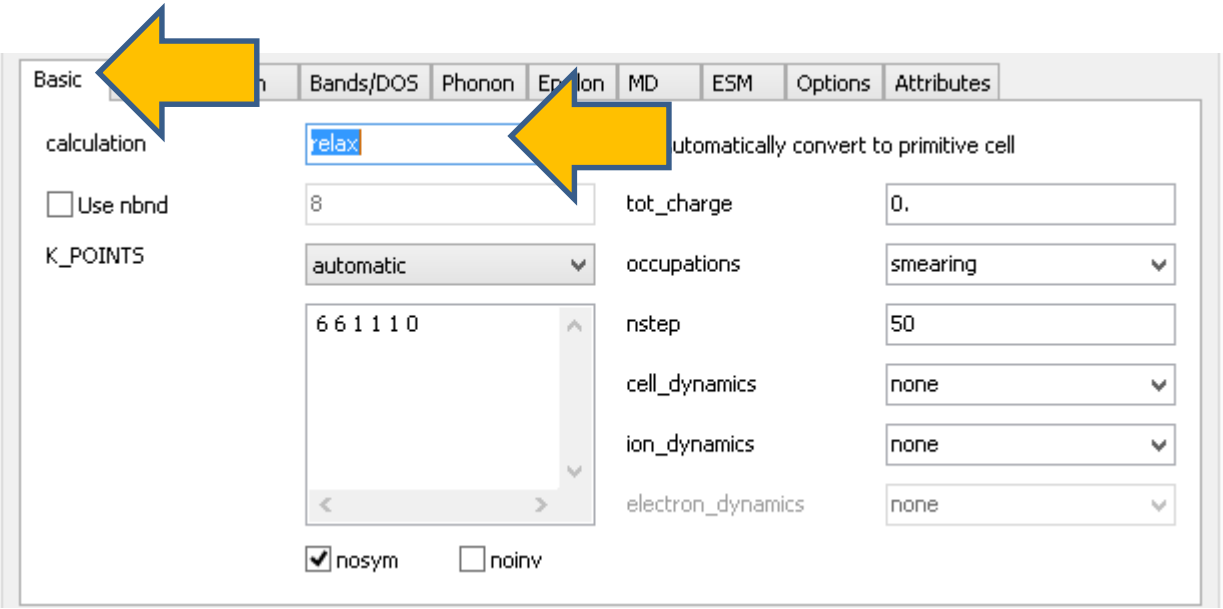
III. Applied voltage 0.5 V, Constant-μ 1

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



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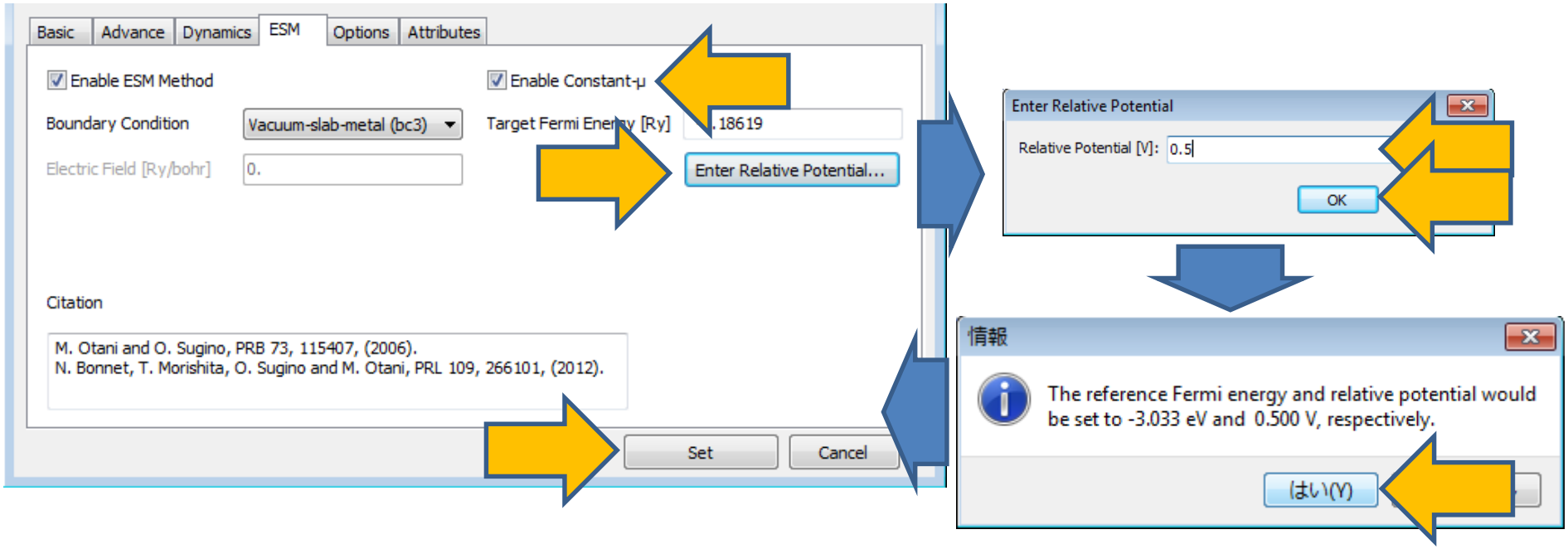
III. Applied voltage 0.5 V, Constant-*μ* 2

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**.



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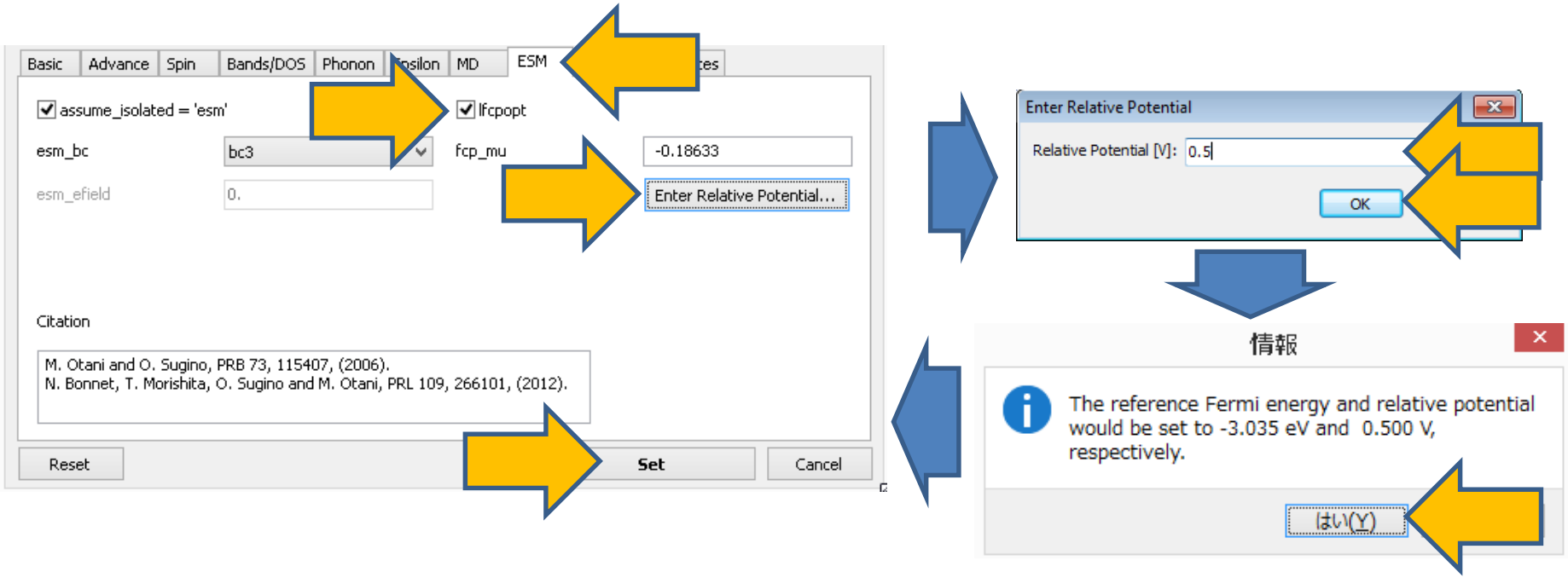
III. Applied voltage 0.5 V, Constant-μ 2

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**.



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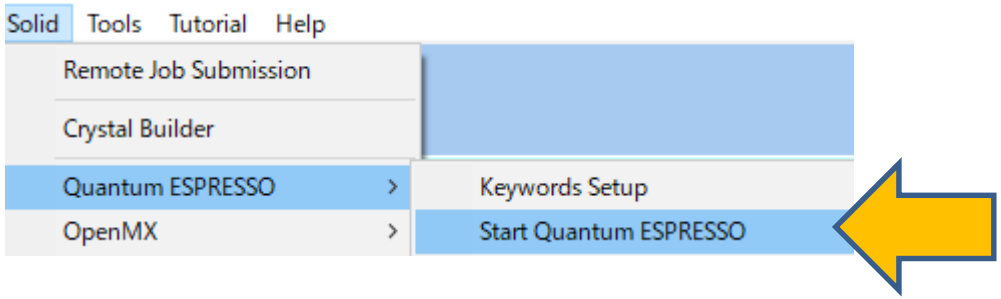
III. Applied voltage 0.5 V, Constant-μ 3

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



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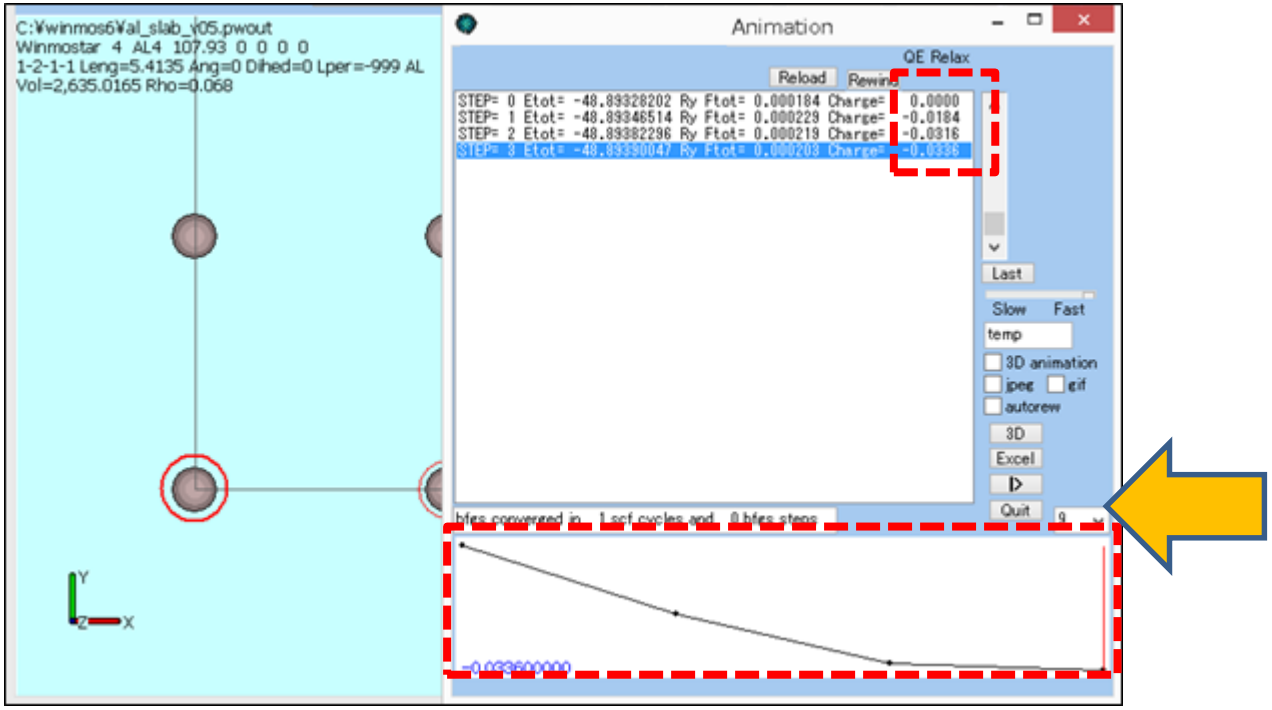
III. Applied voltage 0.5 V, Constant-μ 4

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.



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IV. Confirmation of ESM calculation

1. Click **Solid** | **Quantum ESPRESSO** | **Difference Denstiy/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.