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Winmostar tutorial
Quantum ESPRESSO
Relaxation
V8.007

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2018/01/15

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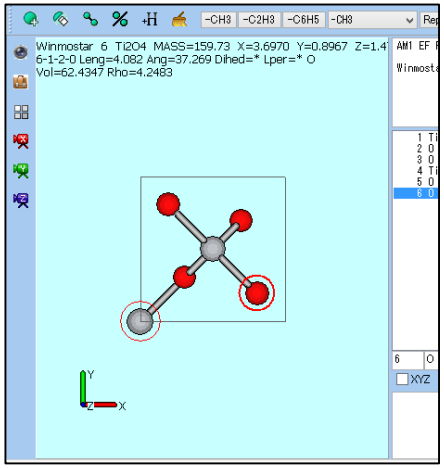
Summary

- In this tutorial, we will execute relaxation of a rutile type TiO 2 crystal. We will simultaneously optimize both cell and atomic nucleus location.



Notes:

- Method for obtaining k points, number of bands, type of pseudopotential, cutoff energy, and settings for smearing will all affect calculation results.
- Parameters of the DFT calculation during relaxation are adjusted by the initial structure. If the final structure differs significantly from the initial structure, we recommend executing relaxation procedures again with the optimized structure.

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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 pseudopotential files from the link below and allocate the files under the pseudo directory within QE install directory. Restart Winmostar. http://www.quantum-espresso.org/pseudopotentials/
   - For O atom: O.pw-mt_fhi.UPF
   - For Ti atom: Ti.pw-mt_fhi.UPF

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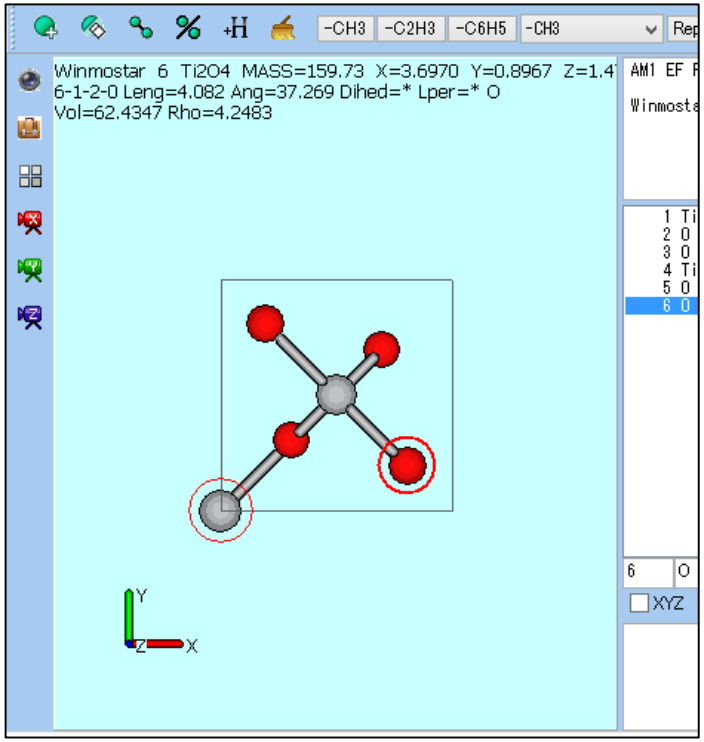
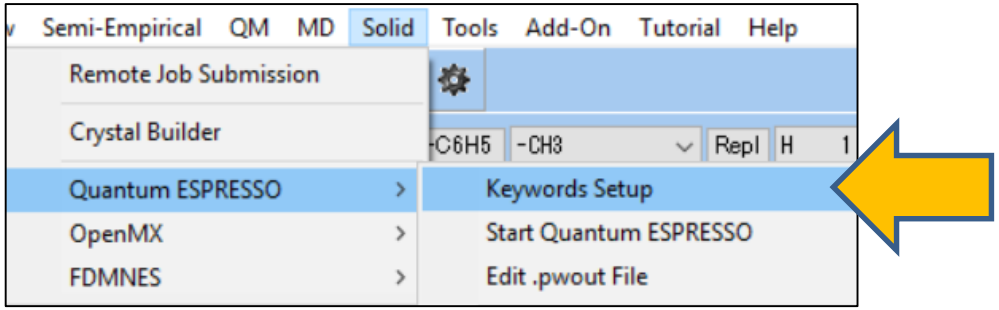
I. Molecular Modeling

1. Click **File | Open**.
2. Select **C:¥winmos8¥samples¥rutile_tio2.cif**.
3. Click **Solid | Quantum ESPRESSO | Keywords Setup**.





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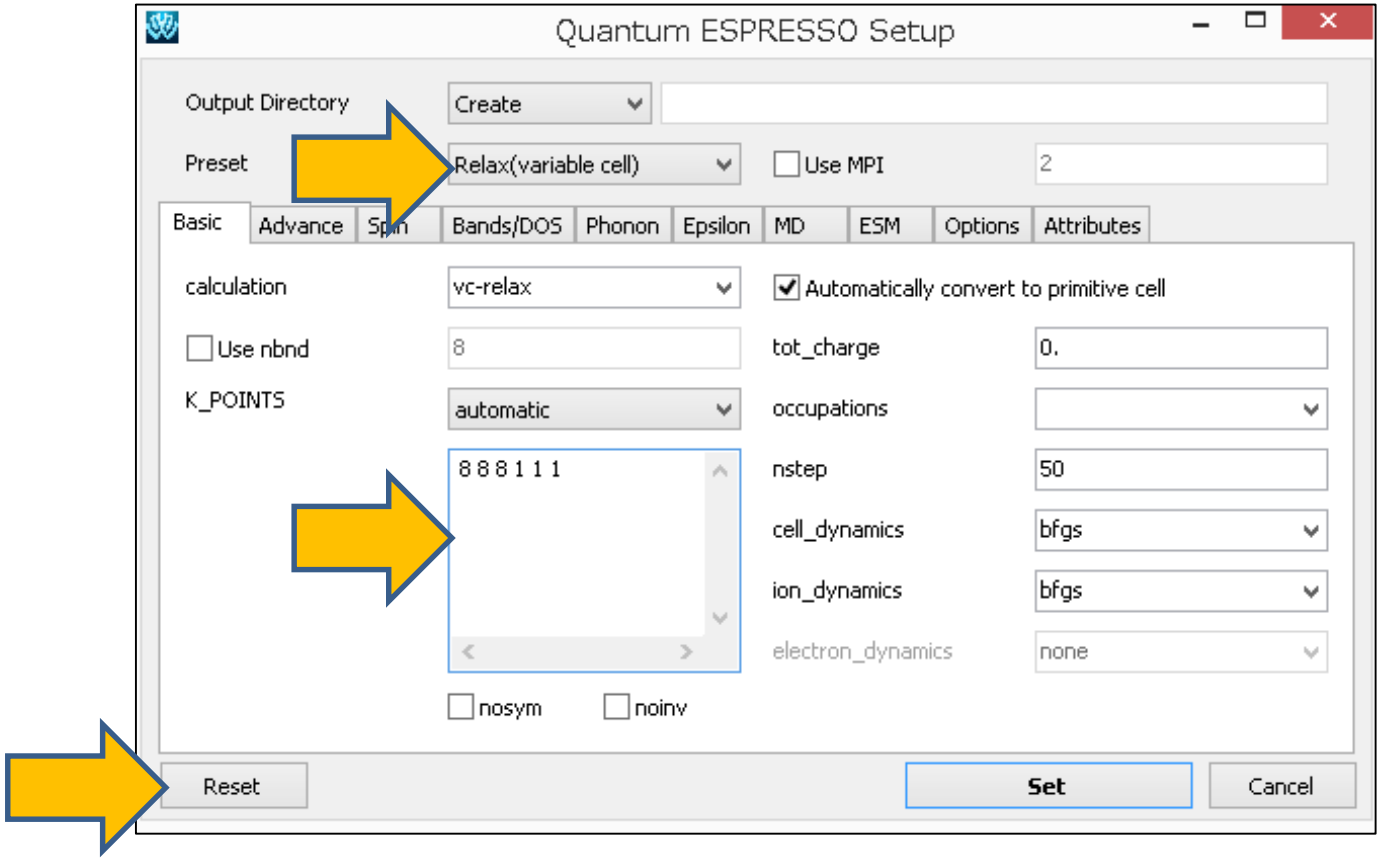
II. Relaxation

1. Click **Reset**. Set **Preset** to “**Relax(variable cell)**.”
2. Set **K_POINTS** to “**automatic**” and enter “**8 8 8 1 1 1**” (space separated) in the text box below.



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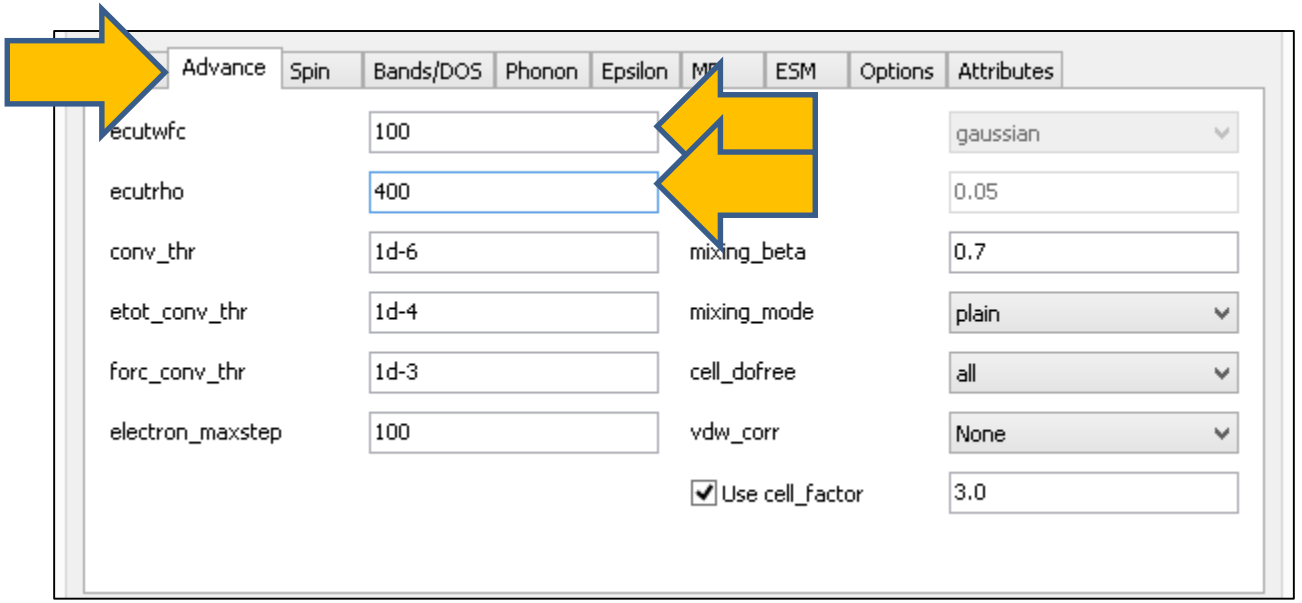
II. Relaxation

In the **Advance** tab, set “**ecutwfc**” to “**100**”, and “**ecutrho**” to “**400**.”



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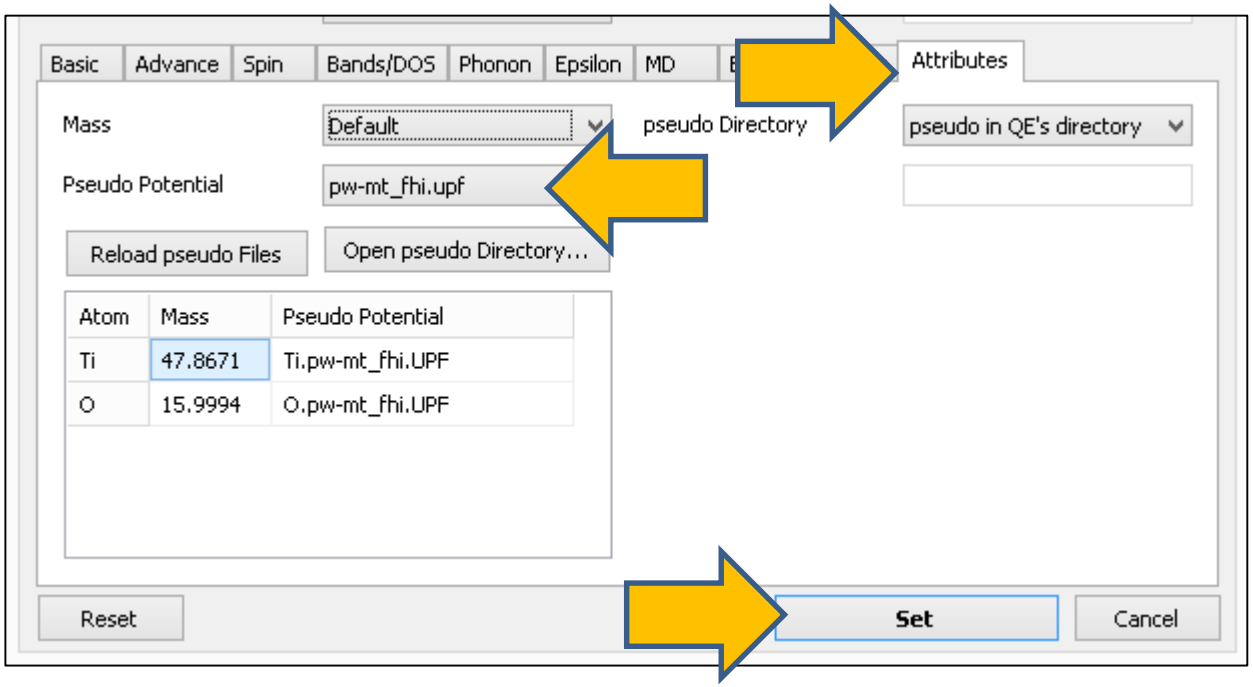
II. Relaxation

1. In the **Attributes** tab, set "**Pseudo Potential**" to "**pw-mt_fhi.upf**" and click **Set**.
2. If "**pw-mt.fhi.upf**" is unavailable, check that all settings are as according to the "Configuration" page in this tutorial.



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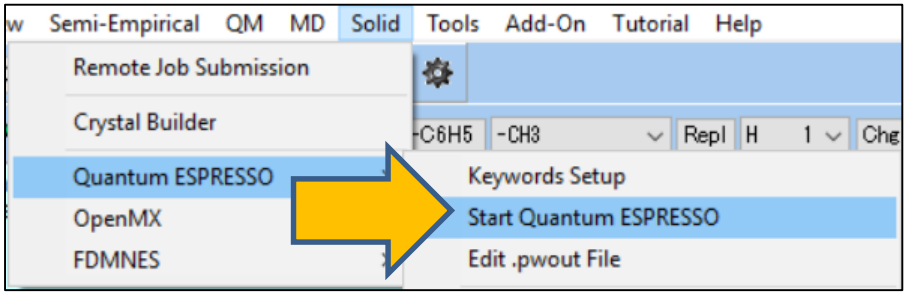
II. Relaxation

1. Click **Solid | Quantum ESPRESSO | Start Quantum ESPRESSO**.
2. Click **Yes** and save the file.
3. Calculation will begin (Approximately 2 mins with 2 cores).



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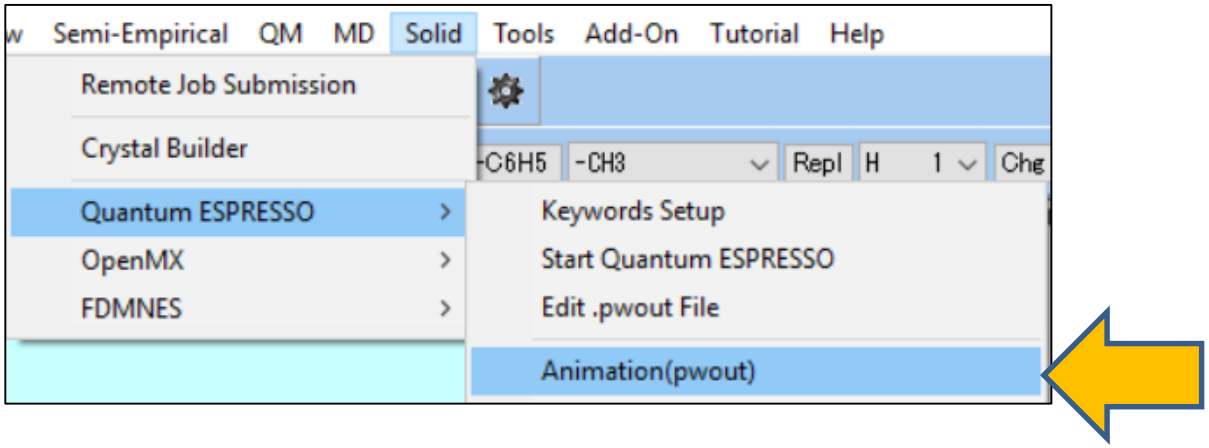
III. Visualization of Relaxation Steps

1. After the relaxation, click **Solid | Quantum ESPRESSO | Animation(pwout)**.
2. Select the file suggested by default.



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III. Visualization of Relaxation Steps

1. Animation window will appear.
2. Click the |> button (PLAY) to watch the relaxation steps.

During the optimization of the structure, parameters of the DFT calculation are not updated and only the final step has updated parameters using the optimized structure. Because SCF calculation is executed with the above conditions, the energy of the final step may deviate from previous values. This deviation can be reduced to some extent by increasing the cutoff energy.