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Winmostar tutorial
Quantum ESPRESSO
Dielectric Function
V8.007

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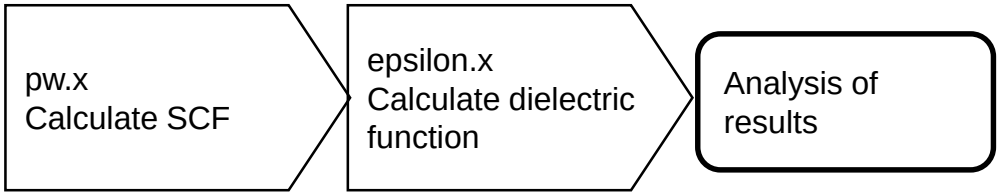
Summary

In this tutorial we will acquire the dielectric function of Si crystal.



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.

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Configuration

See Quantum ESPRESSO install manual
https://winmostar.com/en/QE_install_manual_en_win.pdf

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I. SCF & Dielectric Function

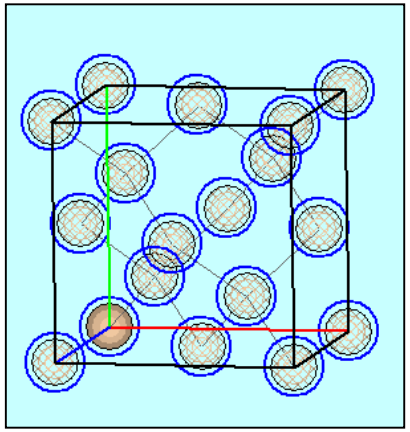
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos8¥samples¥si.cif)

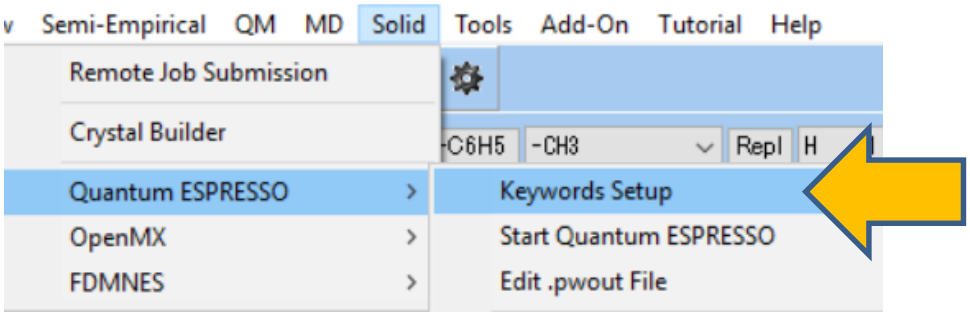
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

To make Si unit cell

Crystal system: Cubic
Space group : Fm-3m (227)
Lattice constants : a=5.4309 Å
Fractional coordinates: Si (0.0 0.0 0.0)

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





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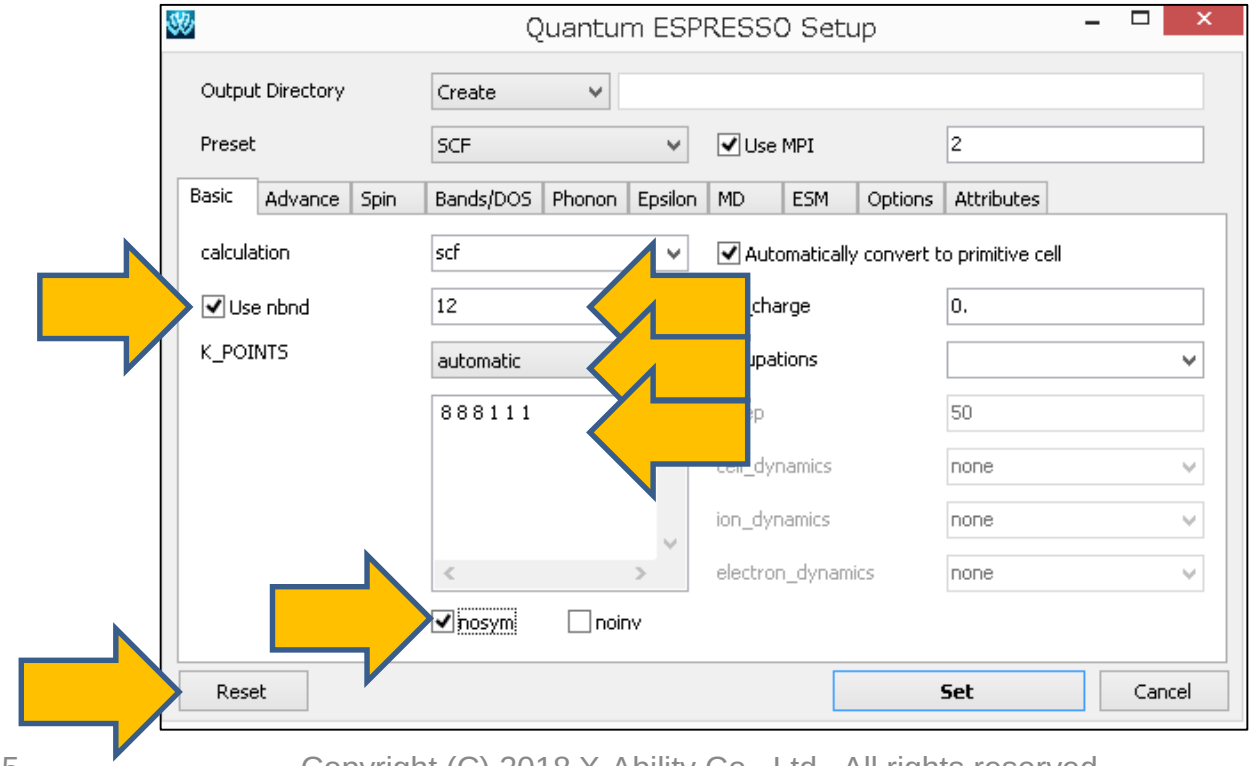
I. SCF & Dielectric Function

1. First click **Reset**.
2. Check **Use nbnd**, and enter “**12**” in the text box.
3. Set **K_POINTS** to **automatic** and enter “**8 8 8 1 1 1**” (space separated) in the box below.
4. Check **nosym**.



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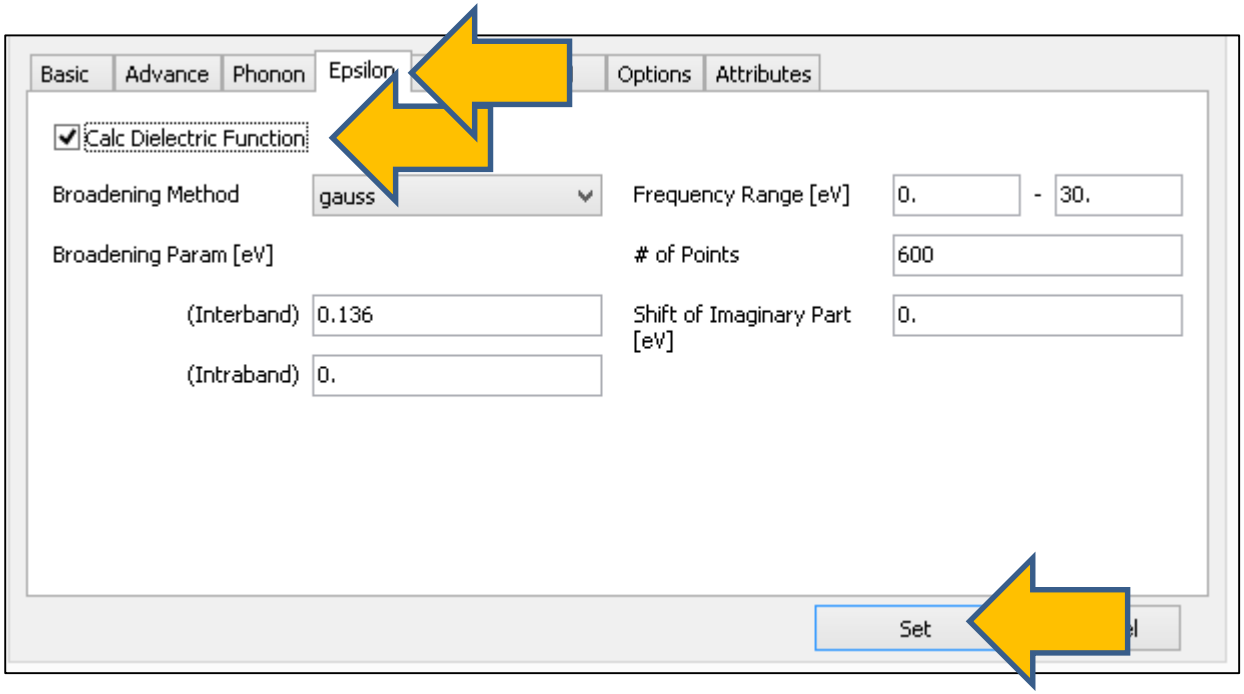
I. SCF & Dielectric Function

1. On **Epsilon** tab, check **Calc Dielectric Function**.
2. Click **Set**.



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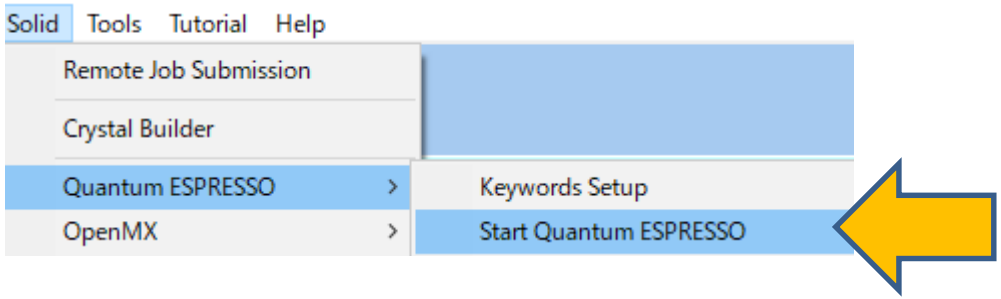
I. SCF & Dielectric Function

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



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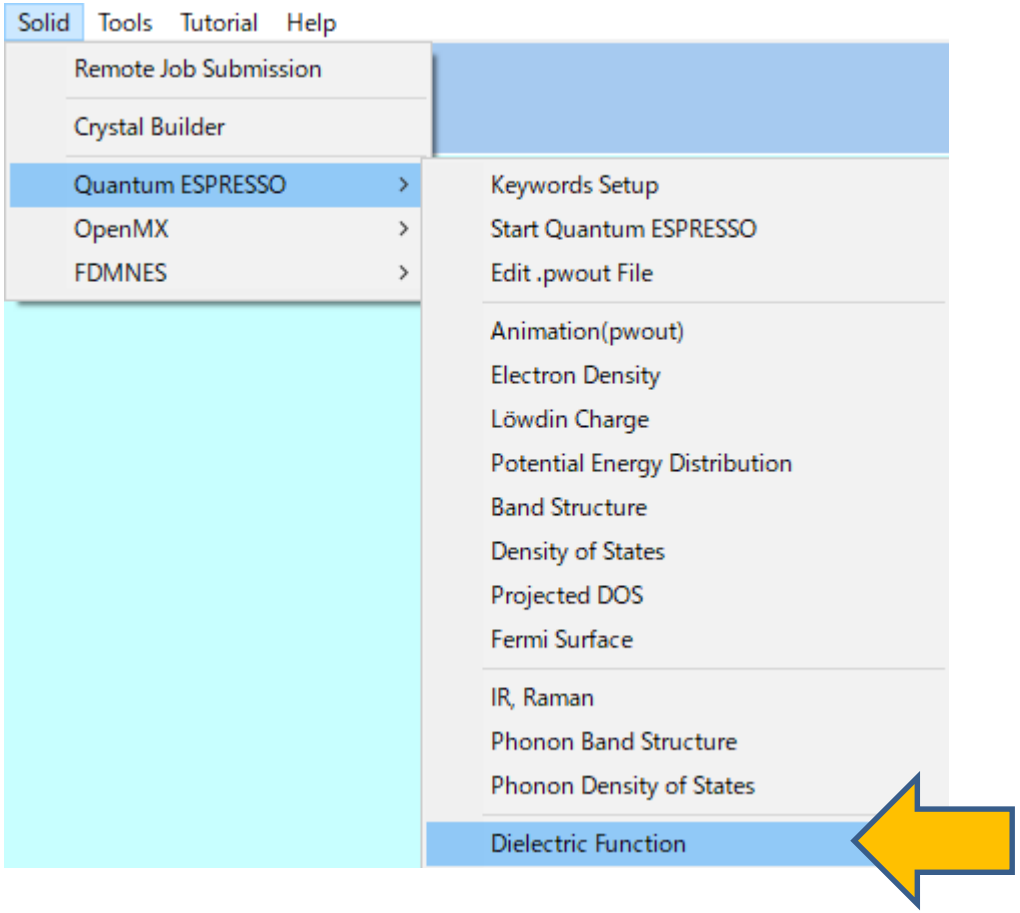
II. Visualization

1. Click **Solid** | **Quantum ESPRESSO** | **Dielectric Function**.
2. Select a working directory for Quantum ESPRESSO.



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II. Visualization

Click **Draw** button to draw dielectric function graph.