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Winmostar tutorial
Quantum ESPRESSO
Dielectric Function
V7.025

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Environment setting

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

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I. SCF & Dielectric Function

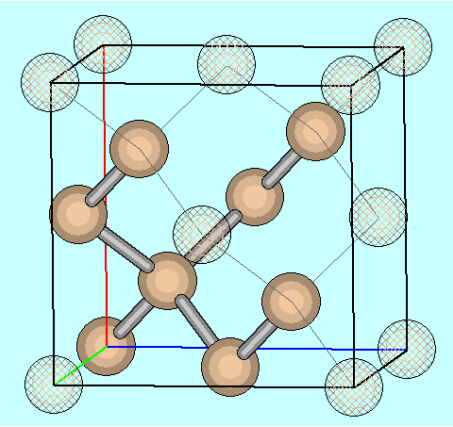
1. Click **File | Open**.
2. Select **si.cif.** (C:¥winmos7¥samples¥si.cif)

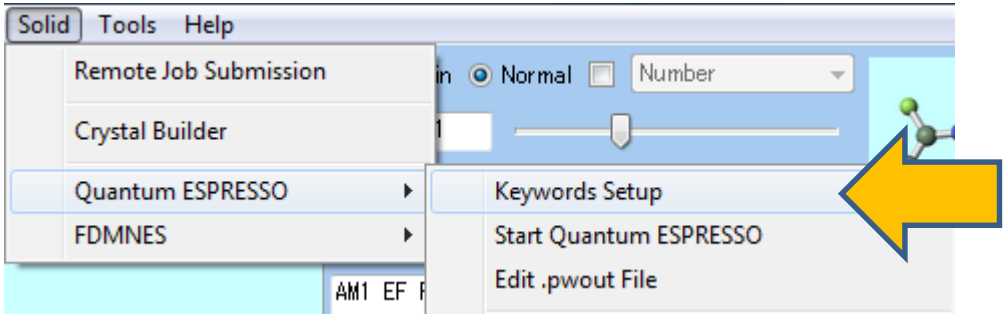
You can also make the same CIF file using Crystal Builder.
See crystal modeling tutorial and apply the following information.

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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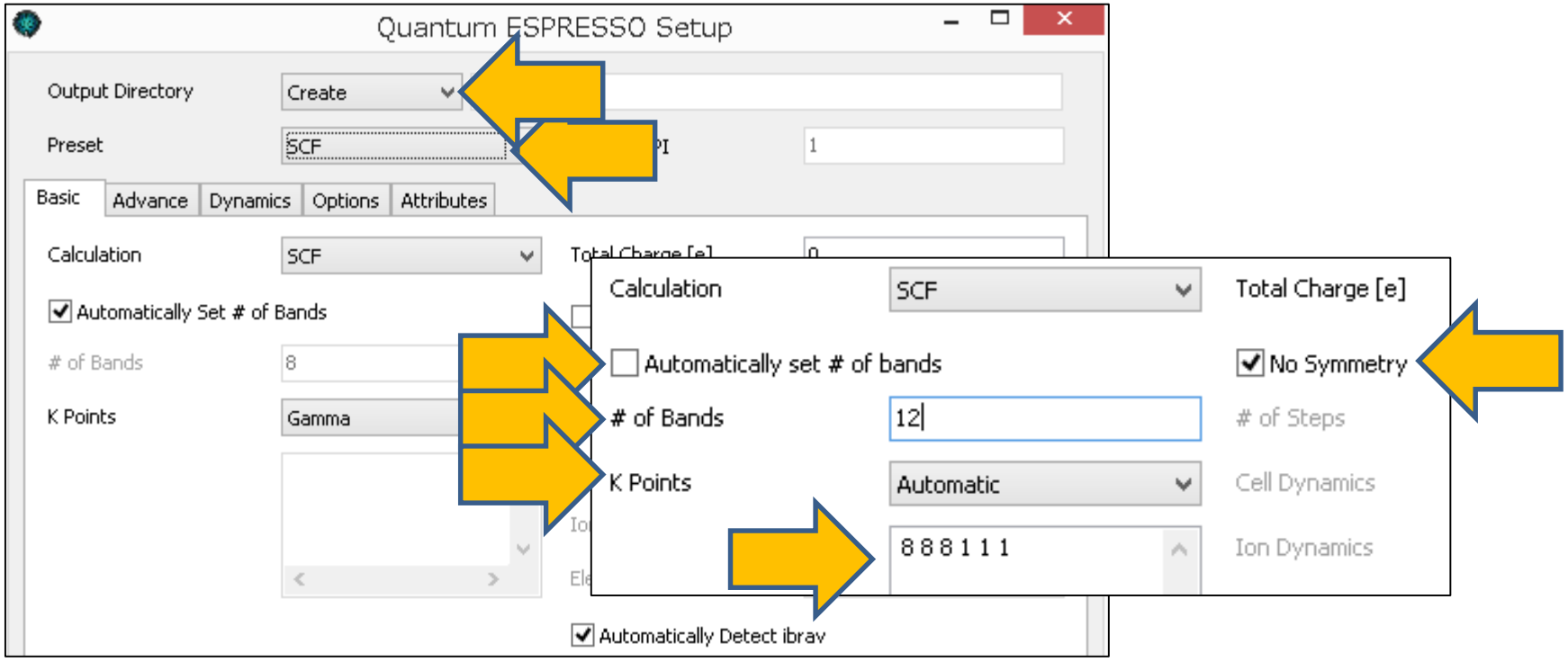
I. SCF & Dielectric Function

1. Set **Output Directory** to **Create**, **Preset** to **SCF**.
2. Uncheck **Automatically set # of bands**, and set **# of Bands** to **12**.
3. Set **K Points** to **Automatic**, set "**8 8 8 1 1 1**"（space separated）below.
4. Check **No Symmetry**.



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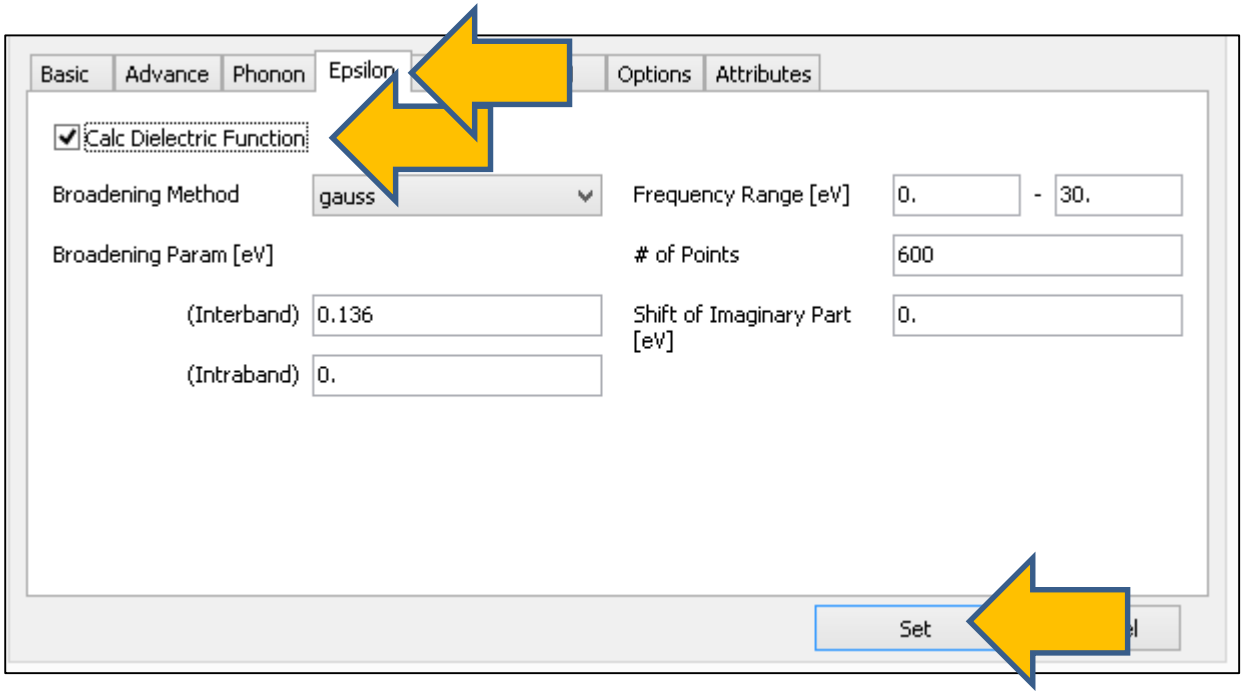
I. SCF & Dielectric Function

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



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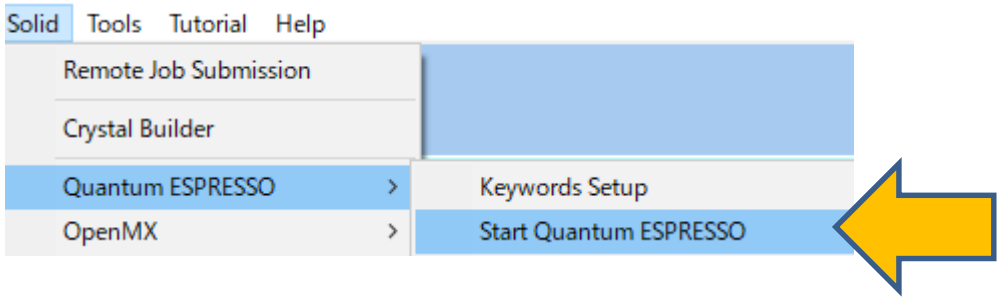
I. SCF & Dielectric Function

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



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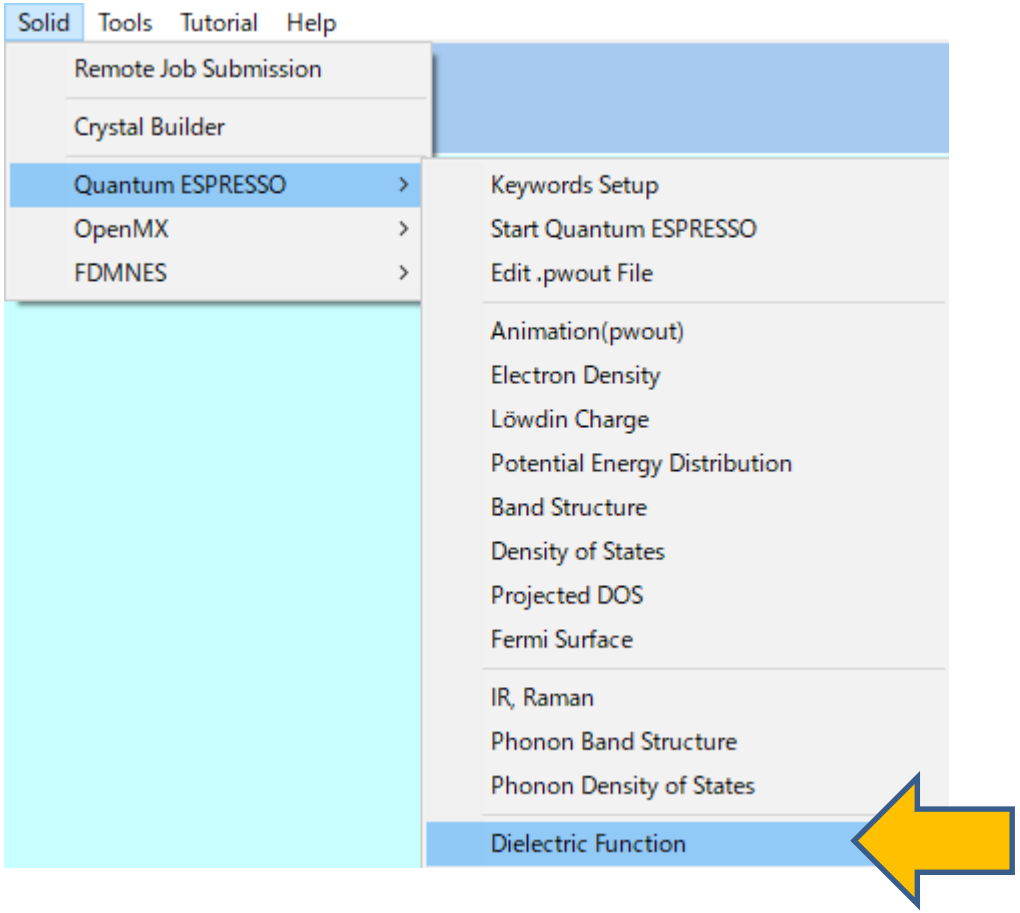
II. Visualization

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



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II. Visualization

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