

Winmostar tutorial Quantum ESPRESSO Dielectric Function V7.025

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I. SCF & Dielectric FunctionII. Visualization



Environment setting

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



SCF & Dielectric Function

1. Click File | Open.

2. Select si.cif. (C:\u00e4winmos7\u00e4samples\u00e4si.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.



Solid Tools Help						
	Remote Job Submission		Normal 🔲 Number 🗸			
	Crystal Builder					
	Quantum ESPRESSO		Keywords Setup			
	FDMNES •		Start Quantum ESPRESSO			
_	AM1 EF I		Edit .pwout File			



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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SCF & Dielectric Function

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

Basic Advance Phonon	Epsilon	Options Attributes	
Calc Dielectric Function		_	
Broadening Method	gauss 🗸 🗸	Frequency Range [eV]	0 30.
Broadening Param [eV]		# of Points	600
(Interband)	0.136	Shift of Imaginary Part	0,
(Intraband)	0.		
			Set



SCF & Dielectric Function

Click Solid | Quantum ESPRESSO | Start Quantum ESPRESSO.
Save as si_eps.pwin.

Solid	d Tools Tutorial Help			
	Remote Job Submission			
	Crystal Builder			
	Quantum ESPRESSO	>	Keywords Setup	
	OpenMX	>	Start Quantum ESPRESSO	



II. Visualization

1. Click Solid | Quantum ESPRESSO | Dielectric Function.

2. Select Quantum ESPRESSO working directory.

Solid Tools Tutorial Help		
Remote Job Submission		
Crystal Builder		
Quantum ESPRESSO	>	Keywords Setup
OpenMX	>	Start Quantum ESPRESSO
FDMNES	>	Edit .pwout File
		Animation(pwout)
		Electron Density
		Löwdin Charge
		Potential Energy Distribution
		Band Structure
		Density of States
		Projected DOS
		Fermi Surface
		IR, Raman
		Phonon Band Structure
		Phonon Density of States
		Dielectric Function

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II. Visualization

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



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