

#### Winmostar tutorial Quantum ESPRESSO Phonon V7.025

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#### Contents

- I. IR, Raman spectrum
- II. Phonon dispersion dispersion curve-DOS



#### **Environment setting**

See Quantum ESPRESSO install manual <a href="https://winmostar.com/en/QE\_install\_manual\_en\_win.pdf">https://winmostar.com/en/QE\_install\_manual\_en\_win.pdf</a>



# 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	l Tools Help	_	
	Remote Job Submission	in 🤇	Normal 🔲 Number 🚽
	Crystal Builder		
	Quantum ESPRESSO		Keywords Setup
	FDMNES •		Start Quantum ESPRESSO
_	AM1 EF		Edit .pwout File



1. Set Output Directory to Create, Preset to SCF.

2. Set K Points to Automatic, "4 4 4 1 1 1" (space separated) below.

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K Points	Gamma 🗸	# of Steps	50	K Points	Automatic
	^	Cell Dynamics Ion Dynamics	none		444111
	< >	Electron Dynamics	none		< >
		<ul> <li>Automatically Deter</li> </ul>	ct ibrav		
			Set	Cancel	



## IR, Raman spectrum

- On Phonon tab, check Run Phonon Calculation as Postprocess, Calc Macroscopic Dielectric Constant, Calc Non-resonant Raman, set Acoustic Sum Rule to simple.
- 2. Click Set.





- 1. Click Solid | Quantum ESPRESSO | Start Quantum ESPRESSO.
- 2. Save as **si\_vib.pwin**.

So	lid Tools Tutorial Help			
	Remote Job Submission			
	Crystal Builder			
	Quantum ESPRESSO	>	Keywords Setup	
	OpenMX	>	Start Quantum ESPRESSO	



1. Click Solid | Quantum ESPRESSO | IR, Raman.

Ι.

2. Select the QE working directory and output file which are suggested by default.





IR/Raman spectrum visualization window will appear.

- 1. Select the peak of the spectrum on the left side of the window.
- 2. Click **Anim** to visualize the vibration as an animation.

IR/Raman Spectrum	
Quit       Save Excel       DispIF        1       Y-Level        0.5       498.9       1/cm v       0.0000       647.8562       Ra         Anim.       Vector       copy       ScalF       1.000 v       edit       Width        20       X-min 0       X-max       4200 v       X-Rev. v       I         0       0.000       0.000       4000       3500       3000       2500       2000       1500       1000         499       0.000       647.856       493       0.000       647.856       493       0.000       647.856         493       0.000       647.856       493       0.000       647.856       493       0.000       647.856	Iman       Iman         IR       Rev.         500       (1/cm) 0



I.

## IR, Raman spectrum

Dielectric constant has been calculated with IR and Raman spectrum. Open **ph.out** in **si\_vib\_qe\_data** folder where **si\_vib.pwin** was saved.

289 290 End of self-consistent calculation∉ 291 292 Convergence has been achieved 🚽 293 294 Number of a in the star = 14 295 List of q in the star:↔ 296 0.000000000 0.000000000 0.000000000 297 298 Dielectric constant in cartesian axis 🗧 299 13.959743499 -0.0000000000.000000000) -0.00000000013.959743499 -0.000000000) 0.000000000 -0.00000000013,959743499 )↔ 302 303 304 Effective charges (d Force / dE) in cartesian axis∉ 305 306 SI 🗸 atom 307 -0.078690.00000 -0.00000) Εx 308 Eу -0.07869 0.00000 -0.00000) 309 -0.00000 Ez 0.00000 -0.07869) 310 atom 2 SI 🗸 311 Εx -0.078690.00000 0.00000) 312 Eу 0.00000 -0.078690.00000) 313 Fz 0.00000 0.00000 -0.07869) 314 315 Diagonalizing the dynamical matrix↔ 316 317 q = ( 0.000000000 0.000000000 0.000000000) 🗸 318 0.1.0

2017/8/8



- 1. Re-open the initial structure of Si crystal.
- 2. Click Solid | Quantum ESPRESSO | Keywords Setup.





- 1. Set Output Directory to Create, Preset to SCF.
- 2. Set K Points to Automatic, "4 4 4 1 1 1" (space separated) below.

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Output Directory Preset Basic Advance Dynar	Create	и	1	Preset Basic Advance Dyn	(custom) V namics Options Attributes
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✓ Automatically Set # of Bands	of Bands	No Symmetry		✓ Automatically Set # # of Bands	t of Bands
K Points	Gamma 🗸	# of Steps	50	K Points	Automatic
	^	Cell Dynamics Ion Dynamics	none		444111
	< >	Electron Dynamics	none		< >
		✓ Automatically Determination	ct ibrav		
			Set	Cancel	



- 1. On Phonon tab, check Run Phonon Calculation as Postprocess, Calc Phonon Dispersion.
- 2. Click Set.

Basic	Advance	Phonon	mics E	SM	Options	Attributes				
<b>√</b> Ru	n Phonon C	alculation as Postp	rocess							
Threst	hold	1e-12			🖌 Calc	Phonon Disper	sion			
Ca	lc Macrosco	pic Dielectric Const	ant		K Points	(Dispersion)	4	4	4	
Ca	lc Non-reso	nant Raman								
Acous	tic Sum Rule	e no		~						
							Set			
							200			



Click Solid | Quantum ESPRESSO | Start Quantum ESPRESSO.
 Save as si\_disp.pwin.

Solid	Tools Tutorial Help				
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	Crystal Builder				
	Quantum ESPRESSO	>	Keywords Setup		
	OpenMX	>	Start Quantum ESPRESSO	$\boldsymbol{<}$	



#### 1. Click | Quantum ESPRESSO | Phonon Band Structure.

2. Select QE working directory which is suggested by default.

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



- 1. Set ASR to Simple.
- 2. Set **K Points** as shown below.





#### Click **Draw** to draw phonon dispersion.





#### 1. Click Solid | Quantum ESPRESSO | Phonon Density of States.

2. Select a working directory of QE. Here, the suggested directory by default should be selected.

Solid	Tools	Tutorial	Help		
F	Remote Jo	ob Submis	sion		
C	Crystal Bu	ilder			
0	Quantum	ESPRESS	C	>	Keywords Setup
(	OpenMX			>	Start Quantum ESPRESSO
F	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



#### Set **ASR** to **simple**.

80	Phonon DOS		- □ ×
Path:	Phonon DOS C:¥Users¥sakamaki¥Desktop¥work¥wm¥trunk¥release32¥samples¥si_disp_qe_data	Phonon DOS ASR K Points	simple 16 16 16 16 16 16 16 16 16 16 16 16 16
		Excel	Draw Close



Click **Draw** to draw phonon density of states.

