

# Winmostar tutorial Quantum ESPRESSO First-Principles Molecular Dynamics V7.021

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# Contents

- I. Molecular modeling
- II. Periodic boundary condition
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#### **Environment setting**

See Quantum ESPRESSO install manual https://winmostar.com/jp/QE\_install\_manual\_en\_win.pdf to install Quantum ESPRESSO



## Molecular modeling

Model  $CH_4$  on the graphics.

Ι.





# II. Periodic boundary condition

Click Edit | Create/Edit Cell.
Click Create.
Click OK.





## III. Energy minimization 1

#### Click Solid | Quantum ESPRESSO | Keywords Setup.

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



## III. Energy minimization 2

- 1. Set Output Directory to Create, Preset to SCF.
- 2. Set Calculation to MD, Electron Dynamics to sd.
- 3. Click Set.
- 4. Click Solid | Quantum ESPRESS | Start Quantum ESPRESS.
- 5. Save the file.





# IV. Energy plots 1

1. After the calculation,

click Solid | Quantum ESPRESSO | Energy Plot(evp).

2. Select the default path.

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	Wi⊓most≀		Animation(pwout)					
			Electron Density					
			Lowdin Charge					
	1.0		Potential Energy Distribution					
	2 H		Band Structure					
			Density of States					
			Difference Density/Energy (esm1)					
			Animation(pos)					
			Energy Plot(evp)					



# IV. Energy plots 2

1. On the Energy Plot window,

check **ekinc** (imaginary kinetic energy of electrons) check **etot** (Electric potential energy of electrons) check **econt** (Total energy)

2. Click **Draw** to get the following graph.



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# V. Relaxation

- 1. Click Solid | Quantum ESPRESSO | Keywords Setup.
- Set Output Directory to Continue, Ion Dynamics to sd, Electron Dynamics to damp.
- 3. Click Set.
- 4. Click Solid | Quantum ESPRESSO | Start Quantum ESPRESSO.
- 5. After the calculation,

click Solid | Quantum ESPRESSO | Energy Plot(evp).

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						A	utomatically	y convert to	primitive cel			
									Set	Car	ncel	



## VI. MD of constant temperature

- 1. Click Solid | Quantum ESPRESSO | Keywords Setup.
- 2. Set lon Dynamics to verlet, Electron Dynamics to verlet.
- 3. Click Set.
- 4. After the calculation,

click | Solid Quantum ESPRESSO | Start Quantum ESPRESSO.

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## VII. Animation 1

- 1. After the calculation, click **Solid** | **Quantum ESPRESSO** | **Animation(pos)**.
- 2. Select the default path.

Solid Tools Tutorial Help								
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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						
		Fermi Surface						
		IR, Raman						
		Phonon Band Structure						
		Phonon Density of States						
⊨O		Dielectric Function						
		Difference Density/Energy (esm1)						
		Animation(pos)						
		Energy Plot(evp)						

2017/07/06



#### VII. Animation 2

#### Click (|>) to play the steps

