

This Quantum Espresso exercise is adopted from ICMEd Summer School course module.

## DFT Module Walkthrough

1. Log into nanoHUB and search for Quantum Espresso. Launch the tool.
2. The initial screen looks like this. Make sure “Si diamond” is selected under Premade atomic structure.

1 Input → 2 Simulate

Input Geometry | Energy Expression | Phonons | Band Structure/DOS | Advanced Options

Create the model

Premade atomistic structure: Si diamond

Atomic Coordinates: Fractional

Structure type: cubic F (fcc)

Title of Run: Silicon band structure

Atomic Structure:

```
2
Silicon diamond structure
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
```

Cell Vectors (A):

```
-2.715 2.715 0.000
-2.715 0.000 2.715
0.000 2.715 2.715
```

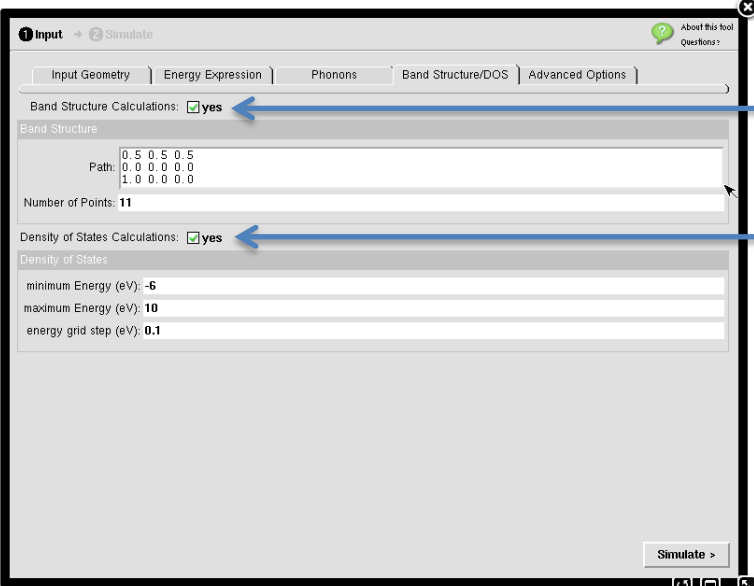
Lattice Parameter "a" (A): 5.43

Ratio Lattice Parameters "c/a" (A): 1

Simulate >

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3. For this assignment, you do not need to calculate the band structure or the density of states. Click on the “Band Structure/DOS tab and unclick the check marks for these calculations.



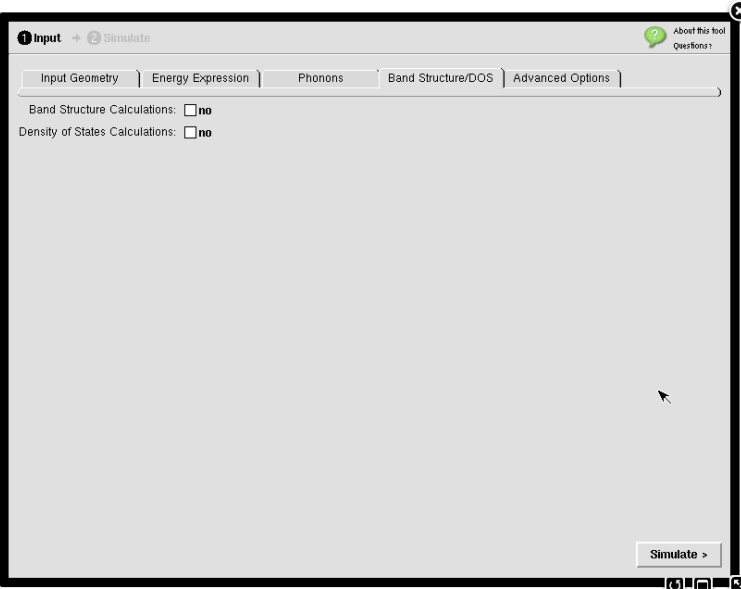
The screenshot shows the 'Band Structure/DOS' tab selected. Under 'Band Structure Calculations', the checkbox is checked (yes). Below it, a 'Path' table is visible with values: 0.5 0.5 0.5, 0.0 0.0 0.0, and 1.0 0.0 0.0. The 'Number of Points' is set to 11. Under 'Density of States Calculations', the checkbox is also checked (yes). Below it, 'minimum Energy (eV)' is -6, 'maximum Energy (eV)' is 10, and 'energy grid step (eV)' is 0.1. Blue arrows point to the 'yes' checkboxes. A 'Simulate >' button is at the bottom right.

Path
0.5 0.5 0.5
0.0 0.0 0.0
1.0 0.0 0.0

Number of Points: 11

minimum Energy (eV): -6  
maximum Energy (eV): 10  
energy grid step (eV): 0.1

Before

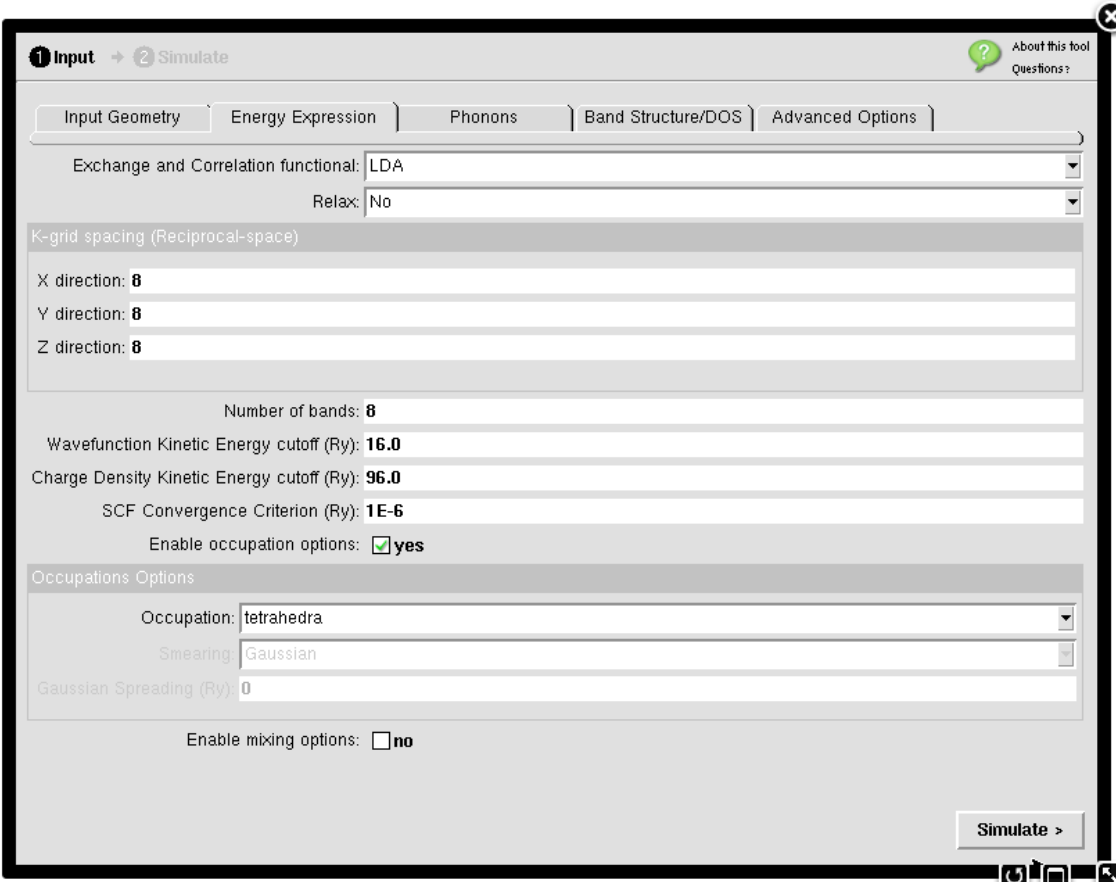


The screenshot shows the same 'Band Structure/DOS' tab, but the checkboxes for 'Band Structure Calculations' and 'Density of States Calculations' are now unchecked (no). The 'Simulate >' button remains at the bottom right.

After

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4. Click on the Energy Expression tab. The window should look like this.



The screenshot shows the 'Energy Expression' tab in a software interface. At the top, there are tabs for 'Input Geometry', 'Energy Expression' (which is selected), 'Phonons', 'Band Structure/DOS', and 'Advanced Options'. Below these tabs, the 'Exchange and Correlation functional' is set to 'LDA' and 'Relax' is set to 'No'. A section titled 'K-grid spacing (Reciprocal-space)' contains three input fields: 'X direction: 8', 'Y direction: 8', and 'Z direction: 8'. Below this, 'Number of bands' is set to '8'. Further down, 'Wavefunction Kinetic Energy cutoff (Ry)' is '16.0', 'Charge Density Kinetic Energy cutoff (Ry)' is '96.0', and 'SCF Convergence Criterion (Ry)' is '1E-6'. The 'Enable occupation options' checkbox is checked, with 'yes' selected. An 'Occupations Options' section follows, with 'Occupation' set to 'tetrahedra', 'Smearing' set to 'Gaussian', and 'Gaussian Spreading (Ry)' set to '0'. At the bottom, 'Enable mixing options' is unchecked, with 'no' selected. A 'Simulate >' button is located in the bottom right corner. The interface also features a top bar with '1 Input' and '2 Simulate' indicators, a help icon with 'About this tool' and 'Questions?' links, and standard window controls at the bottom right.

1 Input → 2 Simulate

Input Geometry | **Energy Expression** | Phonons | Band Structure/DOS | Advanced Options

Exchange and Correlation functional: LDA

Relax: No

K-grid spacing (Reciprocal-space)

X direction: 8

Y direction: 8

Z direction: 8

Number of bands: 8

Wavefunction Kinetic Energy cutoff (Ry): 16.0

Charge Density Kinetic Energy cutoff (Ry): 96.0

SCF Convergence Criterion (Ry): 1E-6

Enable occupation options: ☒ yes

Occupations Options

Occupation: tetrahedra

Smearing: Gaussian

Gaussian Spreading (Ry): 0

Enable mixing options: ☐ no

Simulate >

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5. Change the K-grid spacing to 6 (or another desired value) in each direction. Change the Wavefunction Kinetic Energy cutoff (Ry) to 24 (or another desired value). Leave other settings to default values. The screen should now look like this. (Note that Generalized Gradient Approximation (GGA) can be selected here if desired, but we will only use Local Density Approximation (LDA) in this module.)

1 Input → 2 Simulate

Input Geometry | Energy Expression | Phonons | Band Structure/DOS | Advanced Options

Exchange and Correlation functional: LDA

Relax: No

K-grid spacing (Reciprocal-space)

X direction: 6

Y direction: 6

Z direction: 6

Number of bands: 8

Wavefunction Kinetic Energy cutoff (Ry): 24

Charge Density Kinetic Energy cutoff (Ry): 96.0

SCF Convergence Criterion (Ry): 1E-6

Enable occupation options: ☒ yes

Occupations Options

Occupation: tetrahedra

Smearing: Gaussian

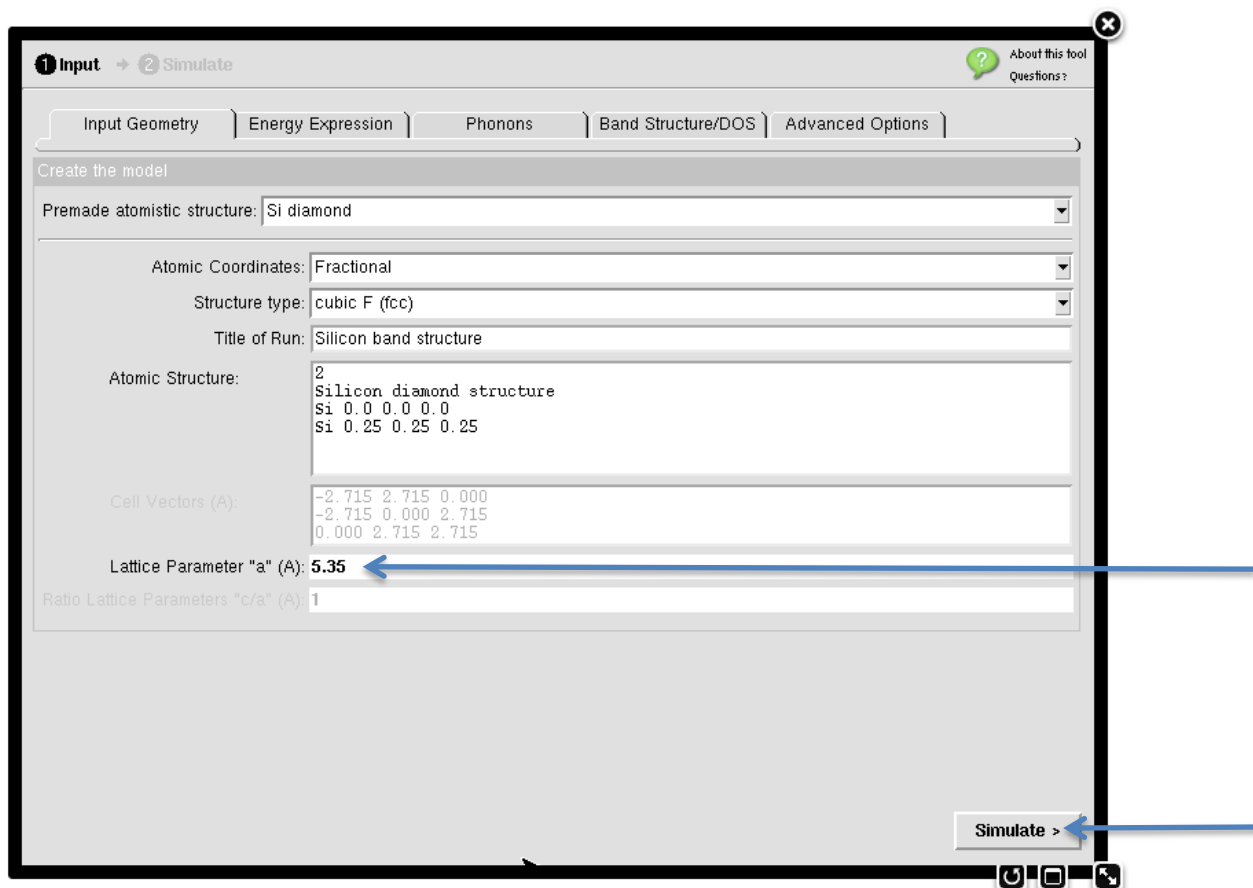
Gaussian Spreading (Ry): 0

Enable mixing options: ☐ no

Simulate >

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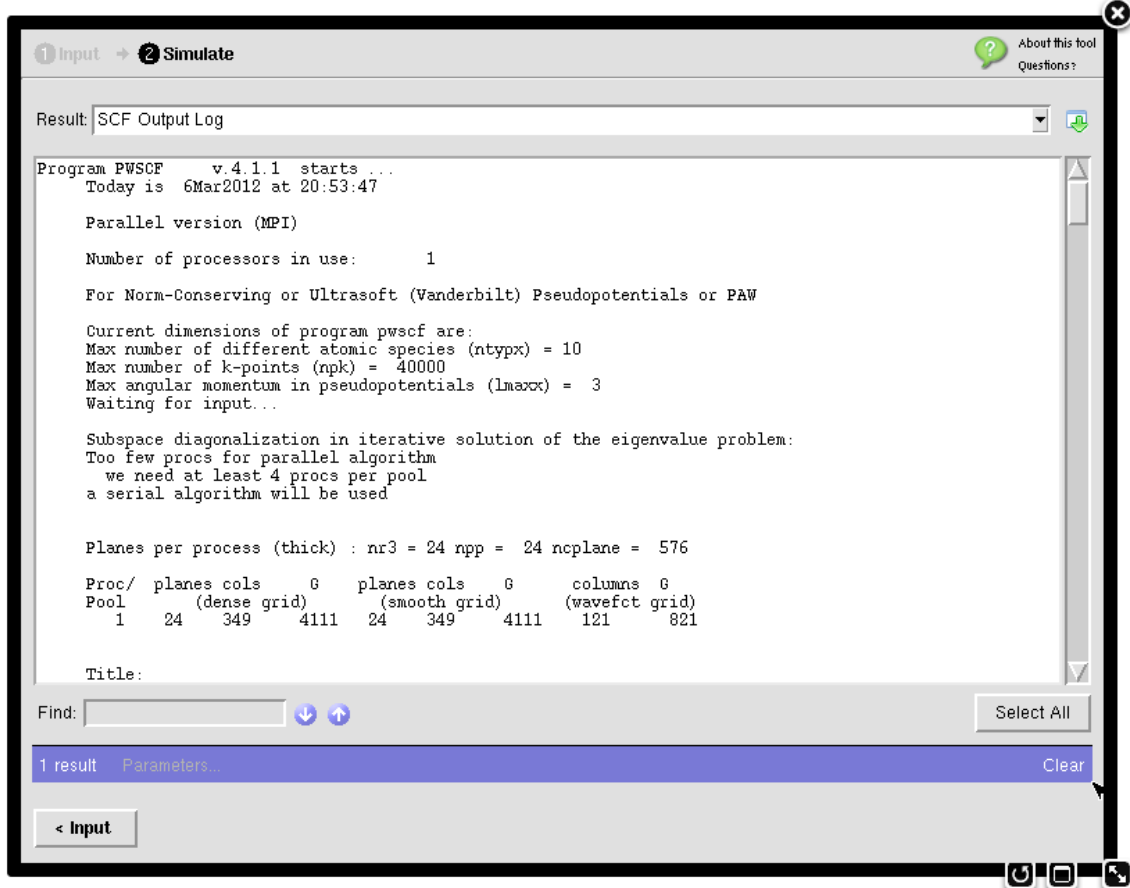
6. Go back to the Input Geometry tab. Set the lattice parameter to the desired value (e.g., 5.35Å).



7. Click on the Simulate button (see above) to perform the calculation.

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8. The simulation will run on the nanoHUB server, and the results will be printed on the output window. The output includes many pieces of information, including the intermediate results during the calculation's iterative steps. The window will look like this.



The screenshot shows the 'Simulate' tab of a nanoHUB interface. The 'Result' dropdown is set to 'SCF Output Log'. The output text is as follows:

```
Program PWSCF v.4.1.1 starts ...
Today is 6Mar2012 at 20:53:47

Parallel version (MPI)

Number of processors in use: 1

For Norm-Conserving or Ultrasoft (Vanderbilt) Pseudopotentials or PAW

Current dimensions of program pwscf are:
Max number of different atomic species (ntypx) = 10
Max number of k-points (npk) = 40000
Max angular momentum in pseudopotentials (lmaxx) = 3
Waiting for input...

Subspace diagonalization in iterative solution of the eigenvalue problem:
Too few procs for parallel algorithm
we need at least 4 procs per pool
a serial algorithm will be used

Planes per process (thick) : nr3 = 24 npp = 24 ncplane = 576

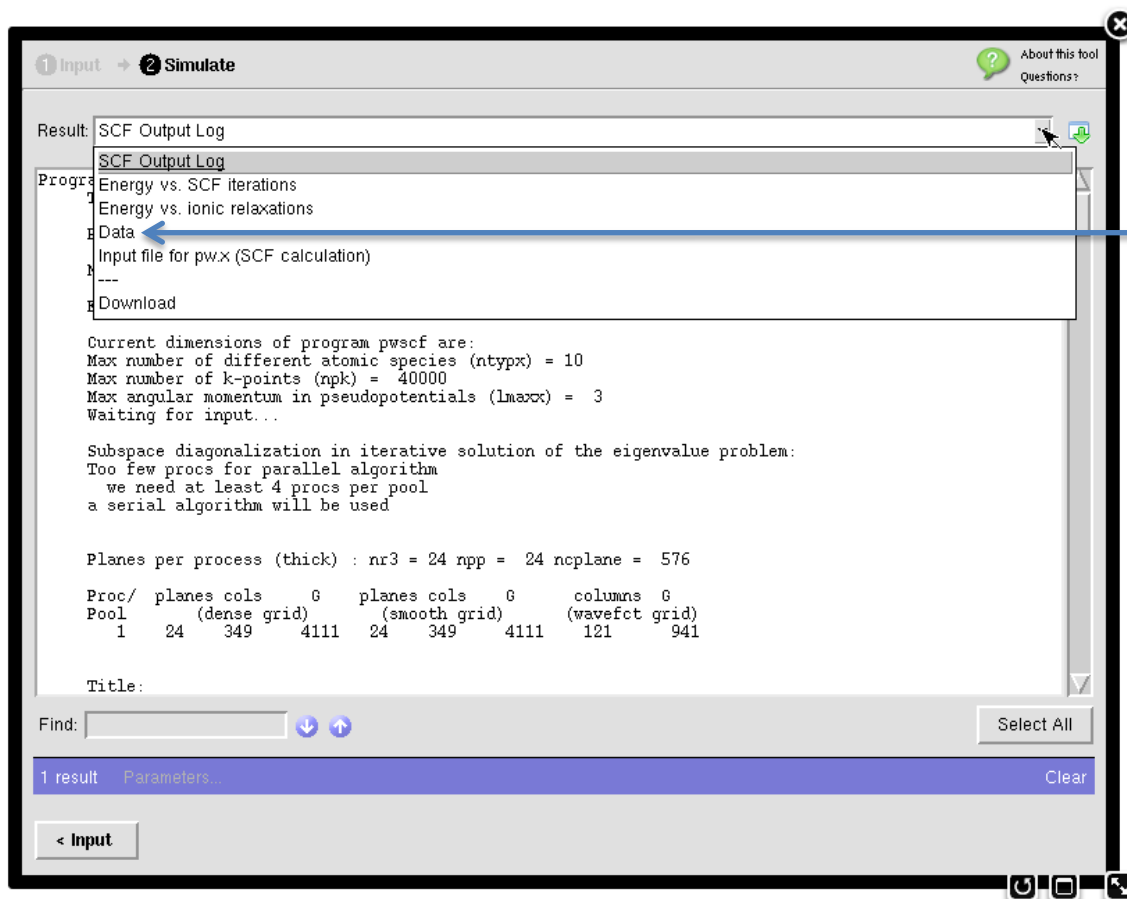
Proc/ planes cols 0 planes cols 0 columns 0
Pool (dense grid) (smooth grid) (wavefct grid)
1 24 349 4111 24 349 4111 121 821

Title:
```

Below the output text is a 'Find:' search bar with up/down arrows and a 'Select All' button. At the bottom, there is a status bar showing '1 result Parameters...' and a 'Clear' button. A '< Input' button is located at the bottom left of the window.

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9. In the drop-down menu, select Data.



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10. Find the final total energy and pressure values. Record the values in the appropriate table entries.

The screenshot shows the 'Simulate' window of a Quantum Espresso interface. The 'Result' dropdown is set to 'Data'. The main text area displays the following output:

```
==== Summary Data =====
- Total Energy during SCF loop -
SCF Step      Energy (Ryd)
1 -15.84411939
2 -15.84826858
3 -15.84837106
4 -15.84837943

- Final Forces -
Forces acting on atoms (Ry/au):
atom 1 type 1 force = 0.00000000 0.00000000 0.00000000
atom 2 type 1 force = 0.00000000 0.00000000 0.00000000
Total force = 0.000000 Total SCF correction = 0.000000

- Final Stress -
total stress (Ry/bohr**3) (kbar) P= 26.67
0.00018133 0.00000000 0.00000000 26.67 0.00 0.00
0.00000000 0.00018133 0.00000000 0.00 26.67 0.00
0.00000000 0.00000000 0.00018133 0.00 0.00 26.67

- Fermi Energy -
```

Two blue arrows point to the final energy value (-15.84837943 Ryd) and the final pressure value (P= 26.67 kbar). The interface includes a 'Find' search bar, 'Select All' and 'Clear' buttons, and a '< Input' button at the bottom left.

11. Repeat with other parameters as necessary.