

# Online simulations via nanoHUB: Density functional theory calculation on Gallium Arsenide with SeqQuest

In this tutorial:

- Setup a DFT calculation on GaAs
- Extract the total energy and stress tensor

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# STEP 1: launch the nanoMATERIALS tool

From your *My HUB* page launch nanoMATERIALS

The screenshot shows the nanoHUB.org website interface. The top navigation bar includes links for Home, My HUB, Resources, Members, Explore, About, and Support. The user's account name, Alejandro Strachan, is displayed. The dashboard is divided into several sections: My Sessions, Resources, Polls, My Tools, Uploads in progress, and Focus Areas. The 'My Tools' section is highlighted, showing a list of tools including Nano-Bio-Photonics Simulator, Nano-CMOS, nano-Materials Simulation Toolkit, Nano-Plasmonic Bowtie Antenna Simulator, NanoFET, and Nanoindentation close to an interface. The 'nano-Materials Simulation Toolkit' is highlighted with a red heart icon. An arrow points from the text 'From All Tools find: nano-Materials Simulation Toolkit' to the 'All Tools' tab in the 'My Tools' section. Another arrow points from the text 'Launch tool by clicking on:' to the 'nano-Materials Simulation Toolkit' entry.

• From *All Tools* find:  
nano-Materials Simulation  
Toolkit

• Launch tool by clicking  
on: 

# STEP 2: setup the atomistic simulation cell

- Start with an Si diamond unit cell

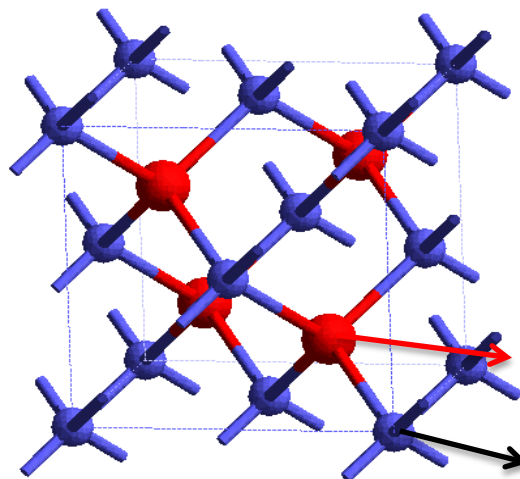
From the *Input Model* tab of the tool

- 2-atom cubic fcc cell:

Fractional atomic  
Positions

Ga (0,0,0)

As (0.25, 0.25, 0.25)



nanoMATERIALS SeqQuest DFT

Terminate Keep for later

1 Input → 2 Simulate

Input Geometry Energy Expression Calculation Specification Advanced Options

Create the model

Premade atomistic structure: Si diamond

Atomic Coordinates: Fractional

Title of Run: Silicon diamond structure

Atomic Structure: 2  
Premade sample of bulk Gallium Arsenide  
Ga 0.00 0.00 0.00  
As 0.25 0.25 0.25

Cell Vectors (Å):  
0.0000 2.825 2.825  
2.825 0.0000 2.825  
2.825 2.825 0.0000

Periodicity: Bulk

As (0.25,0.25,0.25)

Ga (0,0,0)

# STEP 2: setup the atomistic simulation cell

- Start with an Si diamond unit cell
    - 2-atom cubic fcc cell:
- From the *Input Model* tab of the tool

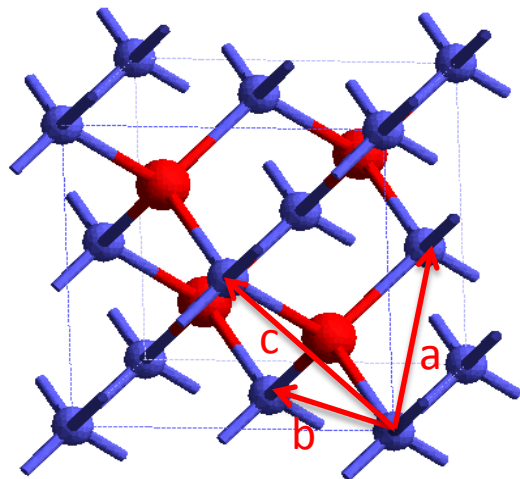
Cell vectors:

$$a = a_0(0, 0.5, 0.5)$$

$$b = a_0(0.5, 0, 0.5)$$

$$c = a_0(0.5, 0.5, 0)$$

With  $a_0 = 0.565$  nm



nanoMATERIALS SeqQuest DFT

Terminate Keep for later

1 Input → 2 Simulate

Input Geometry Energy Expression Calculation Specification Advanced Options

Create the model

Premade atomistic structure: Si diamond

Atomic Coordinates: Fractional

Title of Run: Silicon diamond structure

Atomic Structure: 2

Premade sample of bulk Gallium Arsenide

Ga	0.00	0.00	0.00
As	0.25	0.25	0.25

Cell Vectors (Å):

0.0000	2.825	2.825
2.825	0.0000	2.825
2.825	2.825	0.0000

Periodicity: Bulk

Simulation cell will be infinitively periodic with no free surfaces

# STEP 3: setup the run parameters

From the *Energy Expression* tab of the tool

- Choice of the exchange and correlation functional:

- LDA
- GGA
- SP...

All the numerical parameters can be left to their default values

The screenshot shows the 'Energy Expression' tab of the nanoMATERIALS SeqQuest DFT tool. The interface includes a top bar with 'nanoMATERIALS SeqQuest DFT', 'Terminate', and 'Keep for later' buttons. Below the top bar are tabs for 'Input', 'Simulate', 'Input Geometry', 'Energy Expression' (selected), 'Calculation Specification', and 'Advanced Options'. The 'Energy Expression' section contains the following parameters:

- Exchange and Correlation functional: GGA
- Reciprocal-space grid
  - Specify Kpoint Option: Kpoint Spacing
  - Kgrid Spacing: 5A
  - Is the unit cell hexagonal?: ☐ no
- Real-space Grid Divisions
  - Specify Real-space Grid Option: Real-space grid spacing
  - Grid Spacing: 0.16A
- SCF Convergence Criterion (Ry): 0.000500
- Density of States Gaussian Broadening (eV): 0.2500
- Spin Polarization: 0
- Charge State Calculations: No

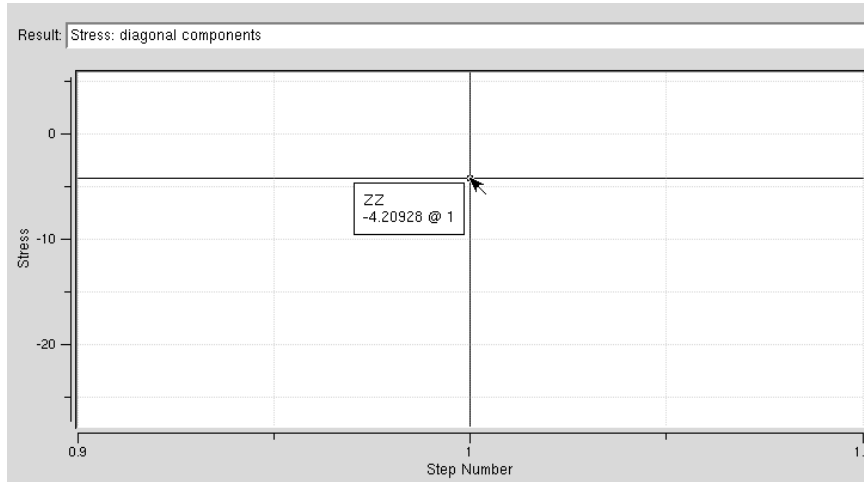
From the *Calculation specification* tab of the tool

- No need to relax the structure

The screenshot shows the 'Calculation Specification' tab of the nanoMATERIALS SeqQuest DFT tool. The interface includes a top bar with 'nanoMATERIALS SeqQuest DFT', 'Terminate', and 'Keep for later' buttons. Below the top bar are tabs for 'Input', 'Simulate', 'Input Geometry', 'Energy Expression', 'Calculation Specification' (selected), and 'Advanced Options'. The 'Calculation Specification' section contains the following parameters:

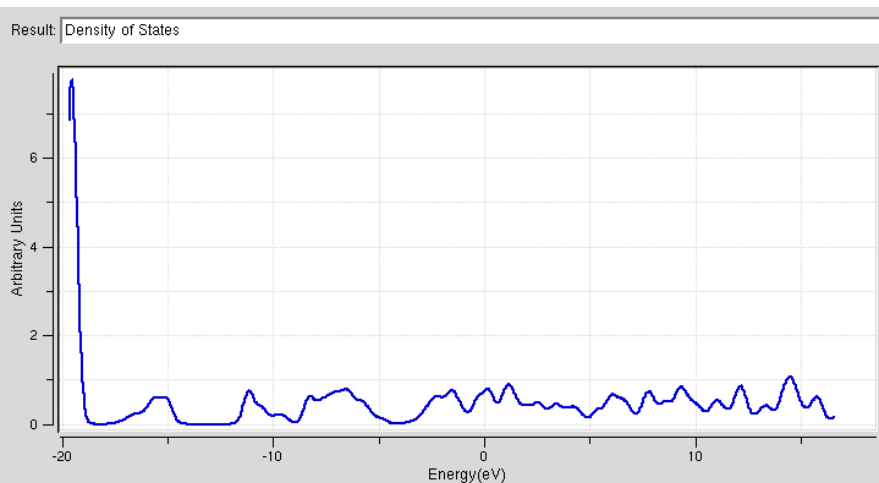
- Calculate Force?: Yes
- Relax atomic structure?: No
- Apply strain to structure?: No
- Bulk Trap Calculations Calculations: No

# STEP 4: explore the results interactively



Stress: diagonal component

## Density of states



## Data

