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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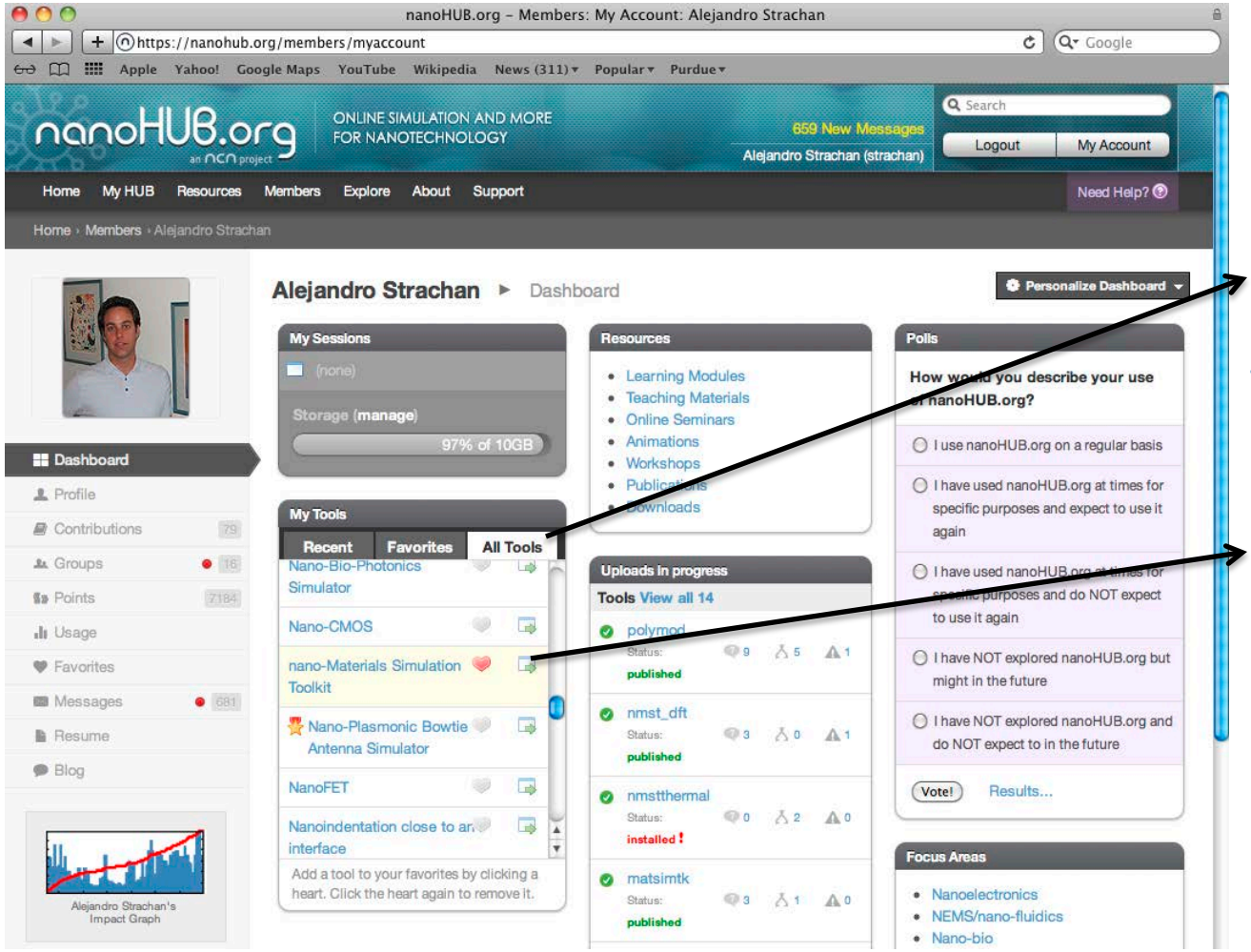
STEP 1: launch the nanoMATERIALS tool

From your *My HUB* page launch nanoMATERIALS



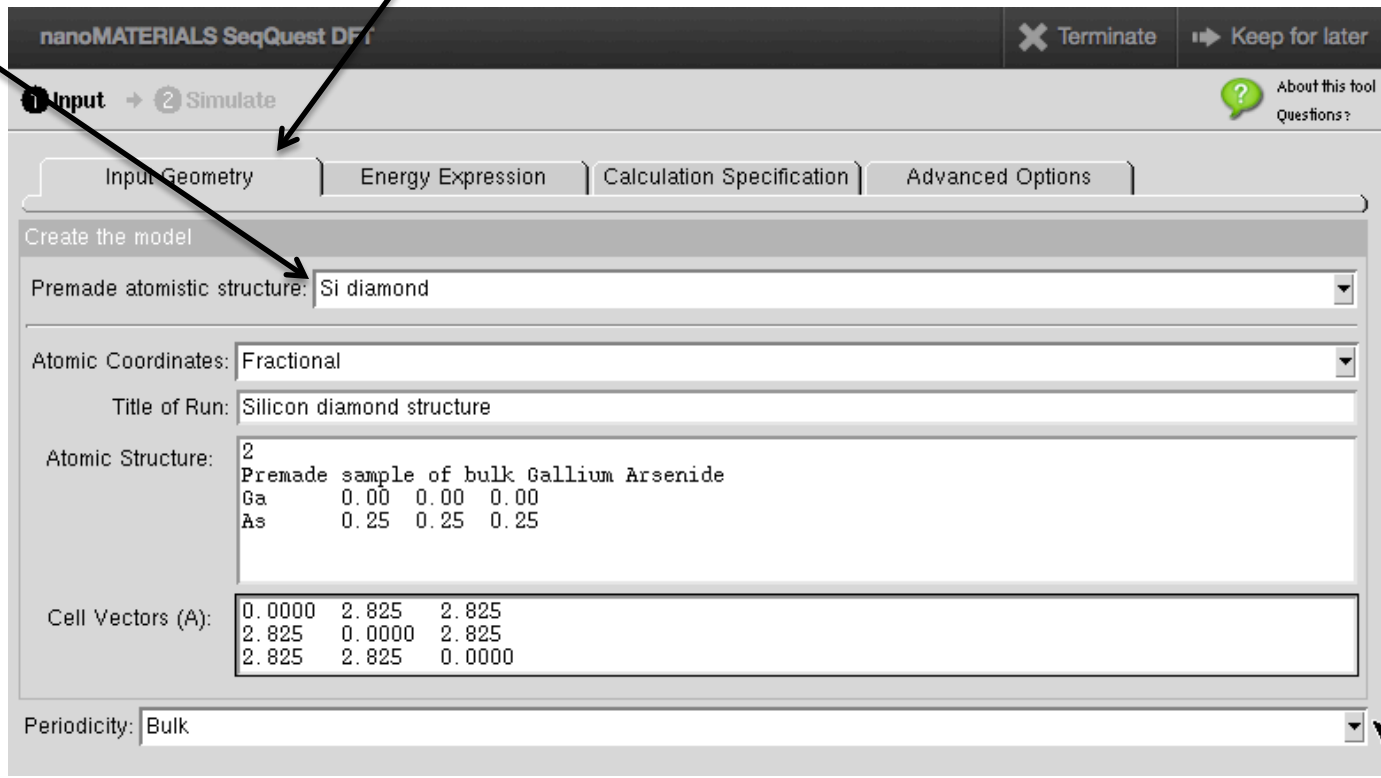
- From *All Tools* find: nano-Materials Simulation Toolkit
- Launch tool by clicking on:

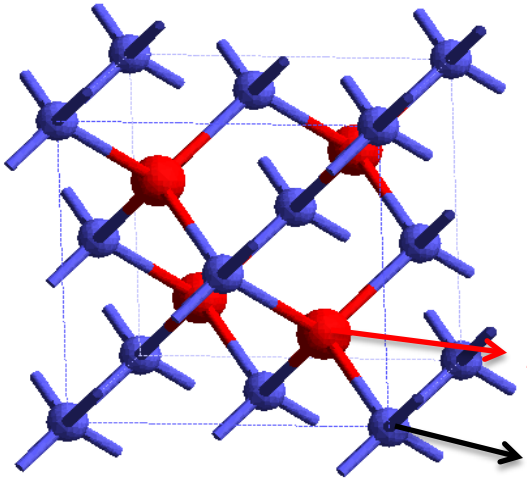
STEP 2: setup the atomistic simulation cell

- Start with an Si diamond unit cell
  - 2-atom cubic fcc cell:

From the *Input Model* tab of the tool

Fractional atomic Positions
Ga (0,0,0)
As (0.25, 0.25, 0.25)





As (0.25,0.25,0.25)

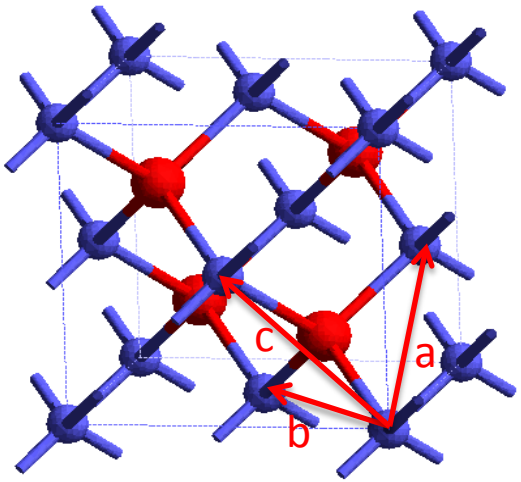
Ga (0,0,0)

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 | About this tool | Questions?

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
```

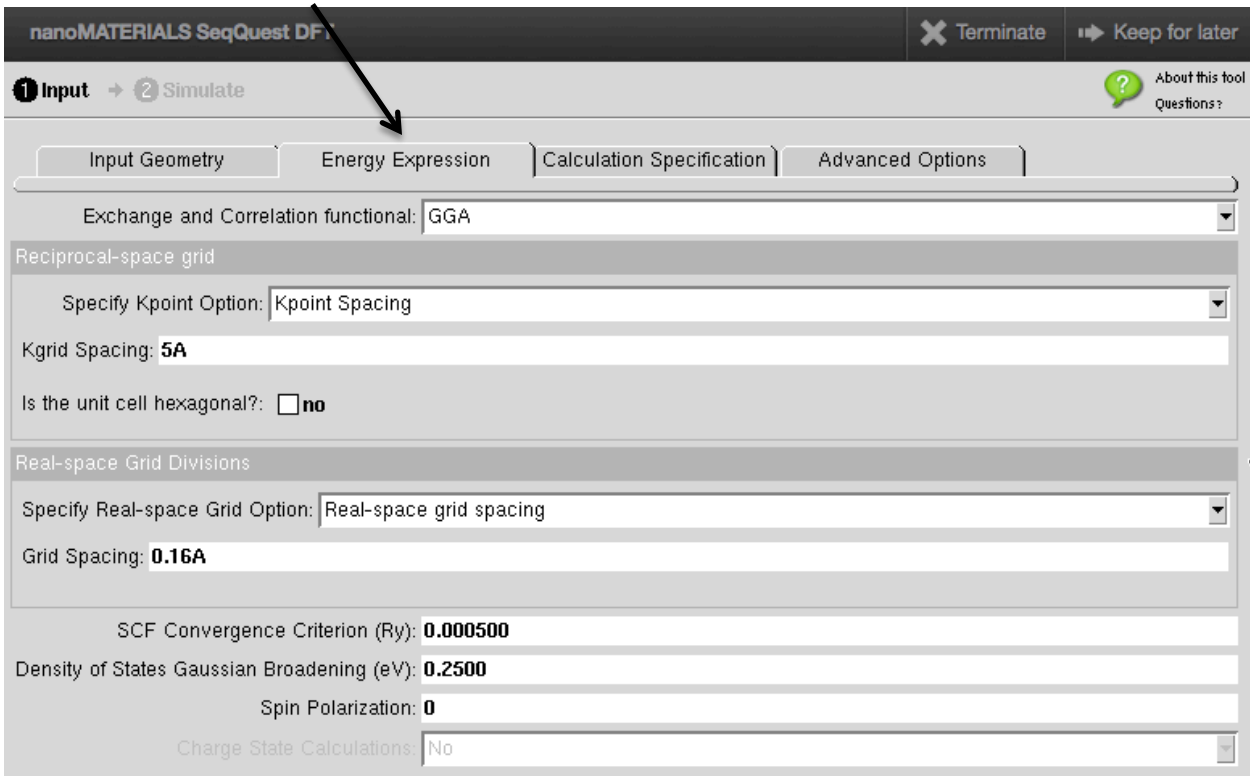
Cell Vectors (A):
```
0.0000   2.825   2.825
2.825    0.0000  2.825
2.825    2.825   0.0000
```

Periodicity: Bulk

Simulation cell will be infinitively periodic with no free surfaces

STEP 3: setup the run parameters

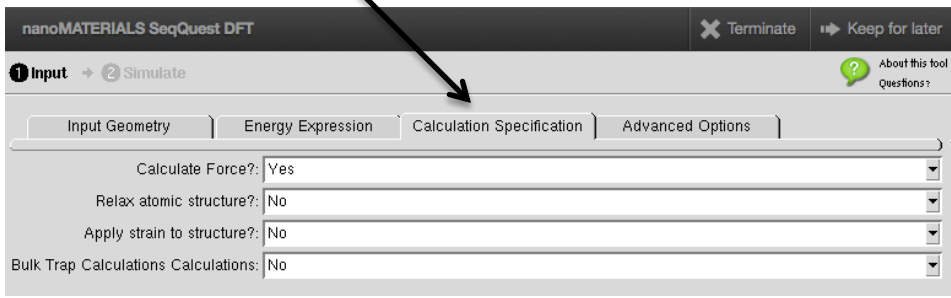
From the *Energy Expression* tab of the tool



- Choice of the exchange and correlation functional:
  - LDA
  - GGA
  - SP…

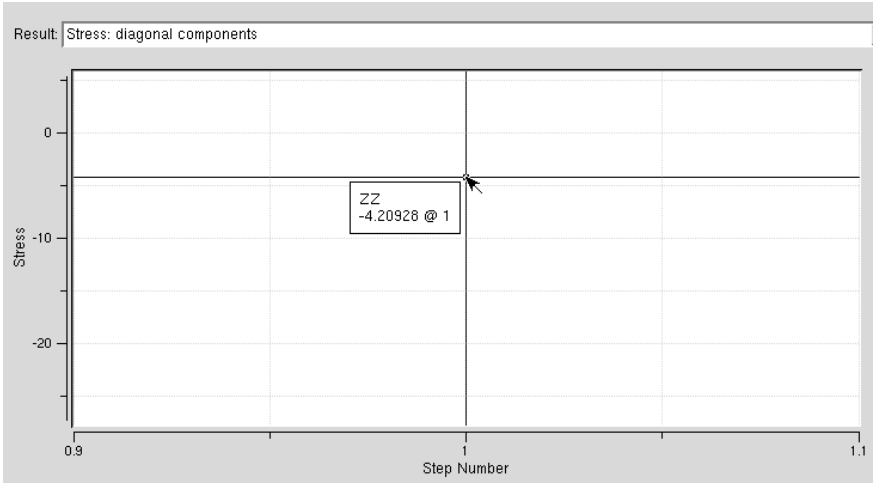
All the numerical parameters can be left to their default values

From the *Calculation specification* tab of the tool



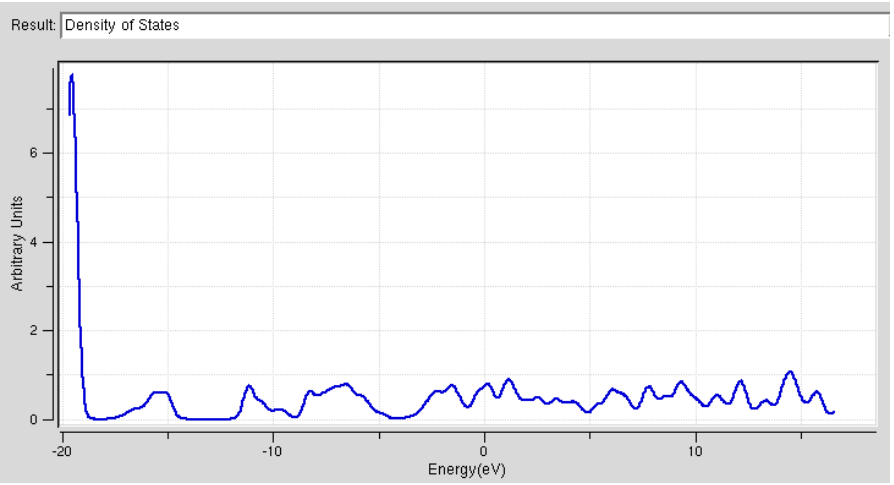
- No need to relax the structure

STEP 4: explore the results interactively

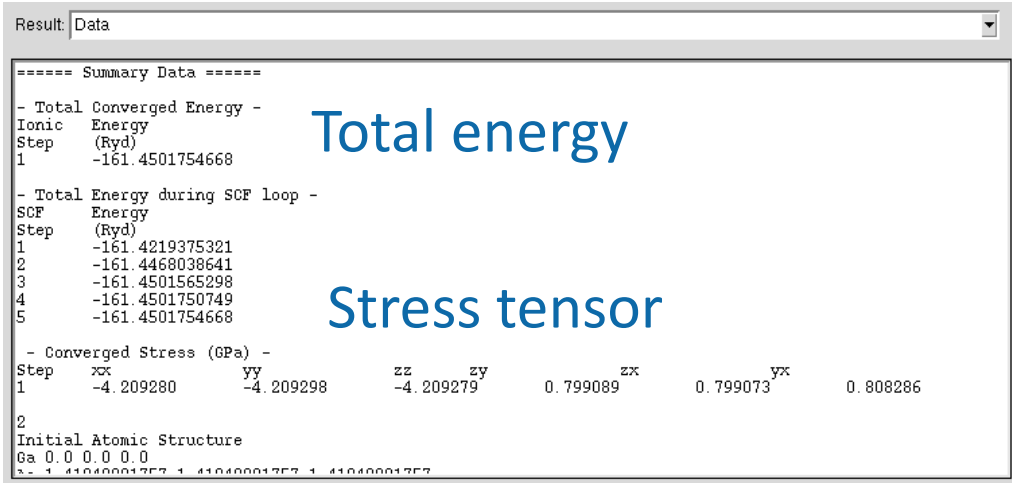


Stress: diagonal component

Density of states



Data



Total energy

Stress tensor