

NanoMATERIALS SeqQuest DFT tool at nanoHUB.org

User guide

This guide describes the nanoHUB.org graphical user interface to the simulation code SeqQuest, developed at Sandia National Laboratories by Peter A. Schultz and collaborators. For more information about SeqQuest please visit: dft.sandia.gov/Quest/

Input geometry

This panel sets up the initial atomic structure for the simulation.

- Select a pre-built model (you can also create your own with the fields below)
- Select whether atomic coordinates are given in Cartesian or fractional coordinates
- Provide a title for the run
- Atomic structure
 - Number of atoms in the simulation cell
 - Second line is a comment (xyz format)
 - The element and position (Cartesian or fractional) of each atom in the simulation cell
- Simulation cell parameters (needed for all simulations)
- The dimensionality of your material. 0 for molecules (no periodic boundary conditions); 1 for wires (periodic along x), 2 for slabs or films

Energy expression

This panels lets users select the exchange and correlation functional used during the simulation, numerical parameters and the total spin of the system.

- Select the exchange and correlation function. LDA for local density approximation, GGA for the PBE gradient corrected functional. *-SP are for spin polarized calculations
- Reciprocal space grid. Number of k-points for calculations in reciprocal space can be specified as numbers along each periodic direction or as a density
- Real space grid for calculations in real space can also be given as a density of numbers along each direction of the simulation cell
- SCF convergence criterion (read the SeqQuest webpage for an explanation of this parameter)
- Spin polarization determines the difference in electrons between majority and minority populations

Driver specification

- Specific whether to calculate force (and stress) or not
- Relax the atomic structure (energy minimization)
- Force convergence criterion (Ryd/Bohr)
- Deform cell by applying a strain

Advanced options

- Simulation venue specifies where to run your simulation
- Users familiar with SeqQuest input files can paste it there