Quantum ESPRESSO with the MIT Atomic Scale Toolkit

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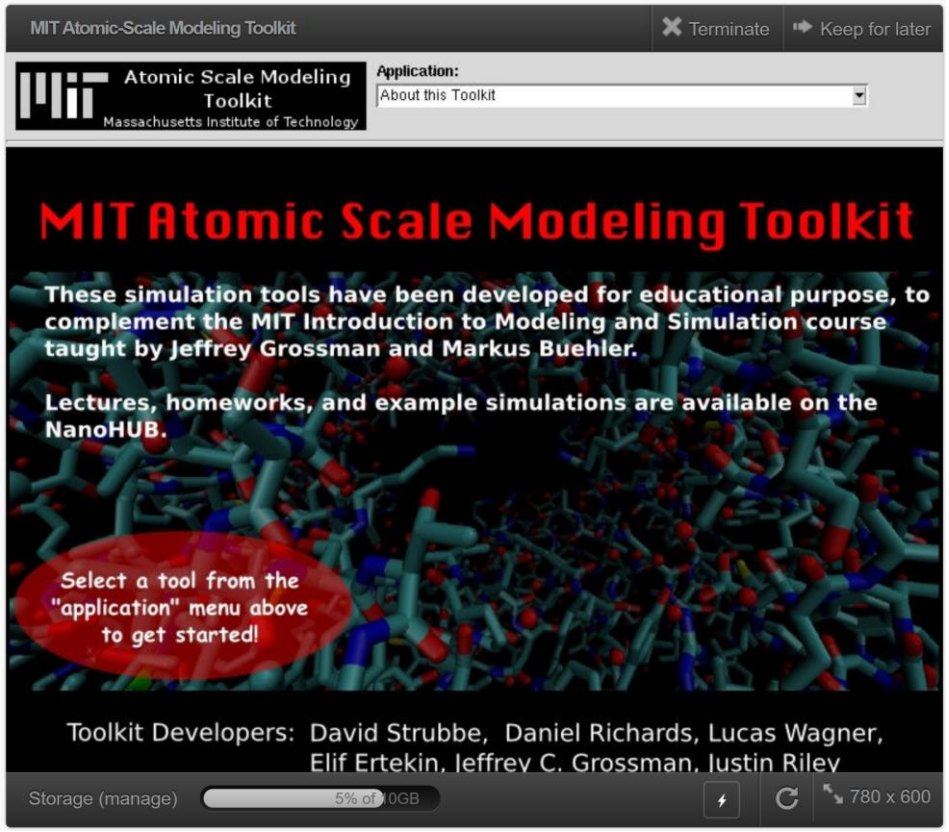
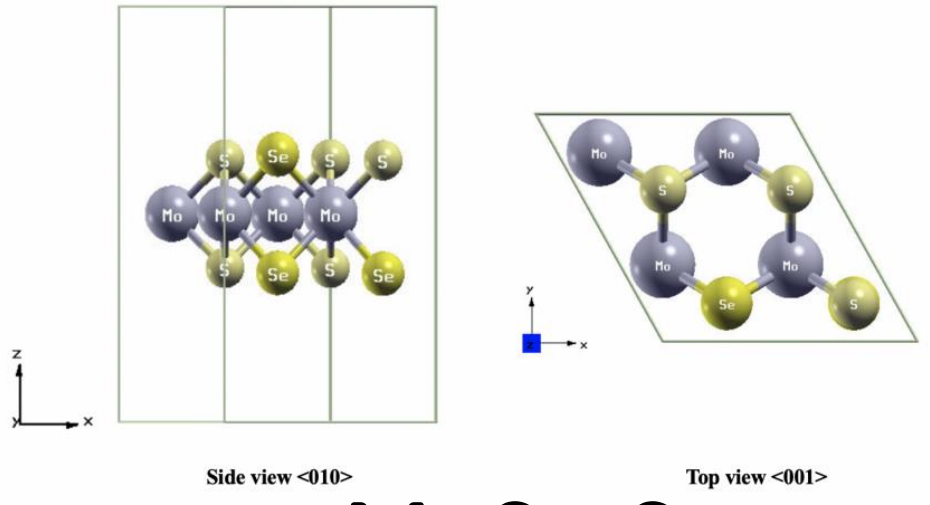
26 OCT 2022



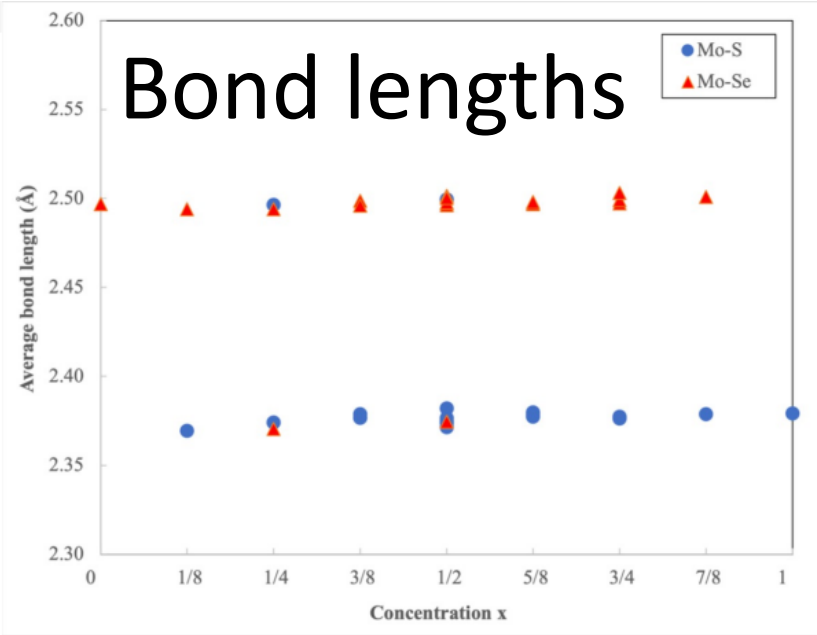
Overview

* Practice using the Quantum ESPRESSO density functional theory application within the MIT Atomic Scale Modeling Toolkit, especially if integrating this application for classroom use.

Previously… C.U.R.E. (Course Undergraduate Research Experience)



$MoS_{2-x}Se_x$



* Student work computing properties of new material configurations
* Toolkit removes some teaching overhead (e.g. no need to teach Linux or Bash)

Resources for introduction to density functional theory

* nanoHUB DFT Users' Group: https://nanohub.org/groups/dft_users

* **PBS Space Time (Beginner friendly): https://www.youtube.com/watch?v=55c9wkNmfn0**
  - "How To Simulate The Universe With DFT" – PBS Space Time

* Lecture series by nanoHUB: https://www.youtube.com/watch?v=DEJwRLHtyqQ
  - "nanoHUB-U Atoms to Materials L5.1: Ab Initio Electronic Structure Calculations" – nanohubtechtalks

* D. S. Sholl and J. A. Steckel, Density Functional Theory: A Practical Introduction. Wiley (2009)

* M. C. Payne et al. "Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients" Rev. Mod. Phys. **64**, 1046-1077 (1992)

DFT with Quantum ESPRESSO

Schrödinger Equation

* If solved in a material, we know all about the material properties. Difficult to solve because electrons interact with each other.

Hohenberg-Kohn

* You need only the correct electron density, not wavefunctions, to have accurate system energies (and properties that result)

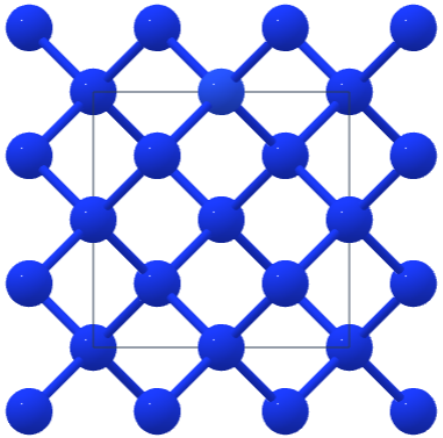
Kohn-Sham

* An auxiliary non-interacting system with a fictitious mean-field can give the same electron density (solvable)

Plane Wave basis set

* Plane waves are a natural basis set for Kohn-Sham wavefunctions in extended/periodic systems

Example density functional theory computations of diamond silicon



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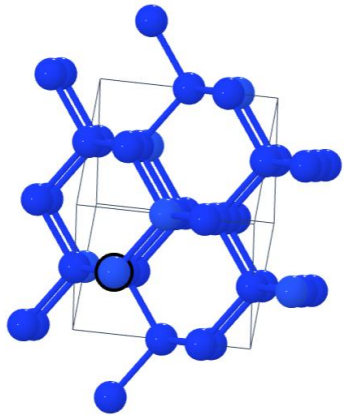
Diamond Si



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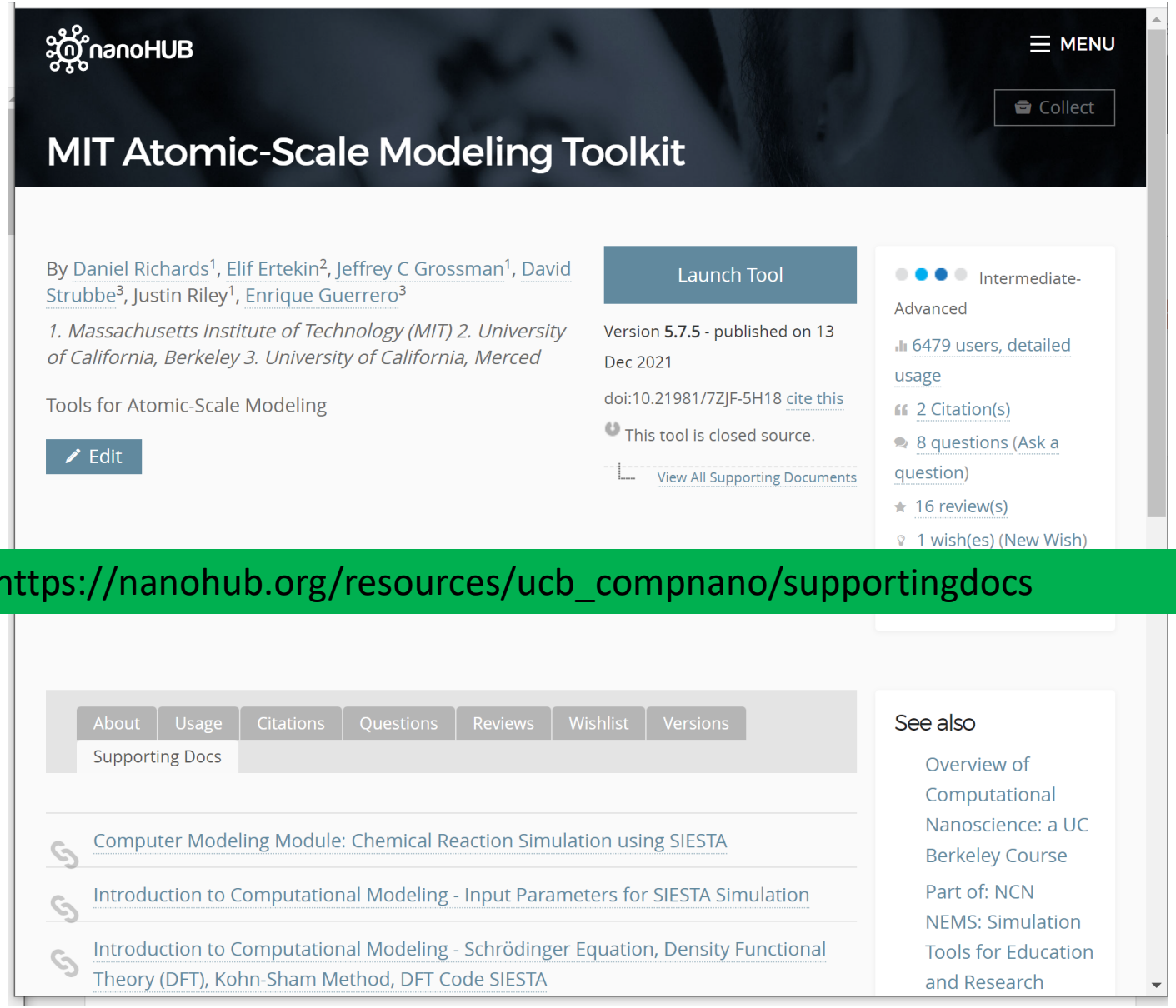
0. Getting acquainted with the MIT Atomic Scale Modeling Toolkit

1. Find ideal computation parameters (Kinetic energy cutoff)

2. Compute Density of States and Band Structure

3. Compute Phonon Frequencies and Raman Intensities



To follow along:

* Go to https://nanohub.org/resources/ucb_compnano/supportingdocs

- Alternatively
  - Go to nanohub.org and sign into an account
  - Click on “Menu” on the top-right corner
  - “Search” for “MIT Atomic Scale Toolkit”
  - Click on the “Supporting Docs” tabs
- Download Quantum_ESPRESSO_guide_26_OCT_22

On to nanoHUB…

https://nanohub.org/resources/ucb_compnano/