Materials Discovery using machine learning

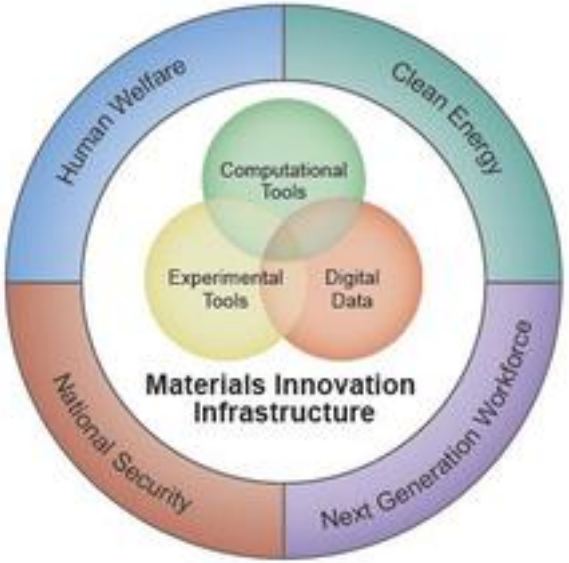
Nathan Wilson

About Me

- Originally from Minnesota and Graduated from the University of Minnesota in 2017 with a degree in material science
- 2nd year PhD student who works predominately with density functional theory calculations on materials for energy applications
- Part of the D3EM (data-enabled design and discovery of energy materials) program which is where my interest and knowledge about machine learning comes from

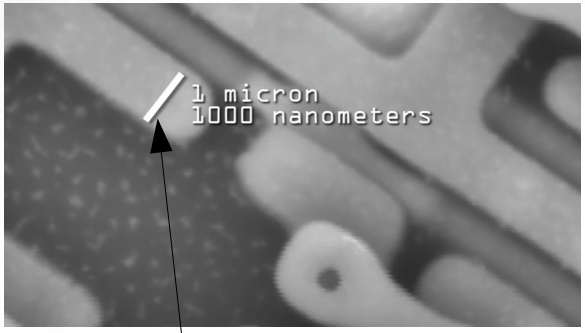
About the project

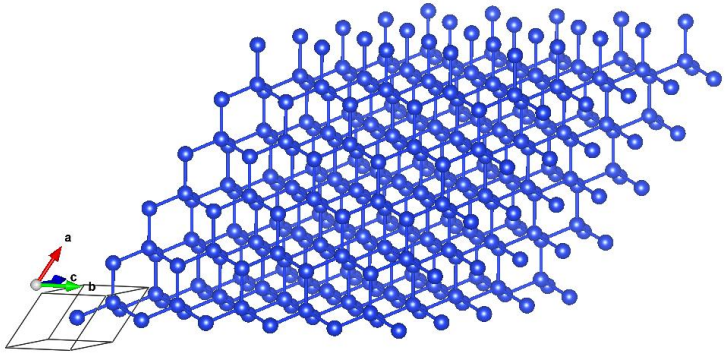
- Goal of the project is to have a machine learning algorithm that can predict if a given material will be stable based upon it’s crystal structure (more on that later)
- This project was motivated by the materials genome initative (MGI) which wants to reduce the time to get a new material into industry
- This has partly focused on increasing the data available allowing for more easier machine learning.

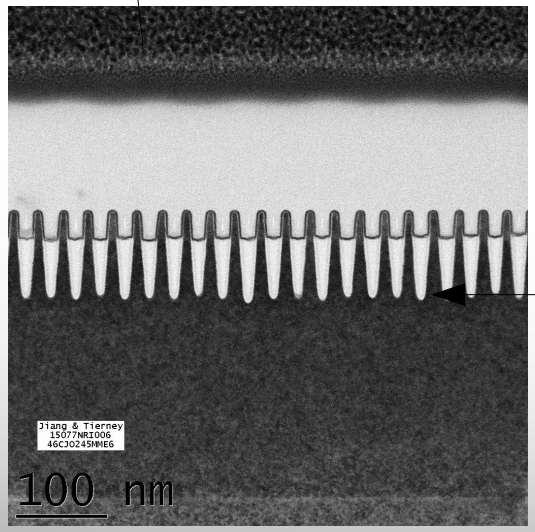


Material Science

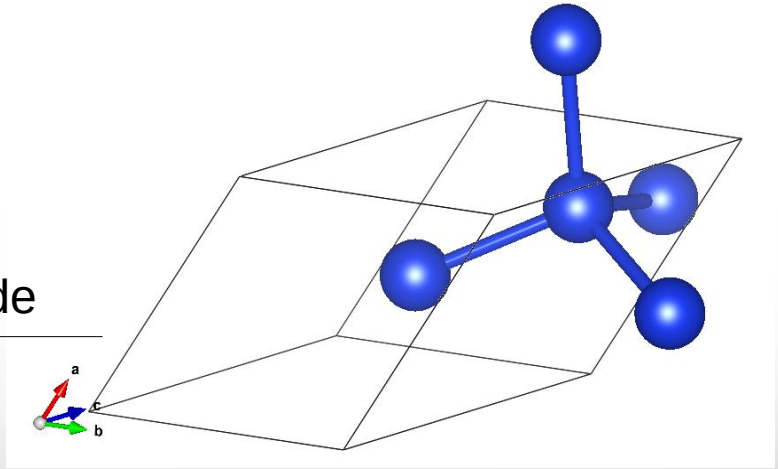
- https://www.youtube.com/watch?v=Fxv3JoS1uY8





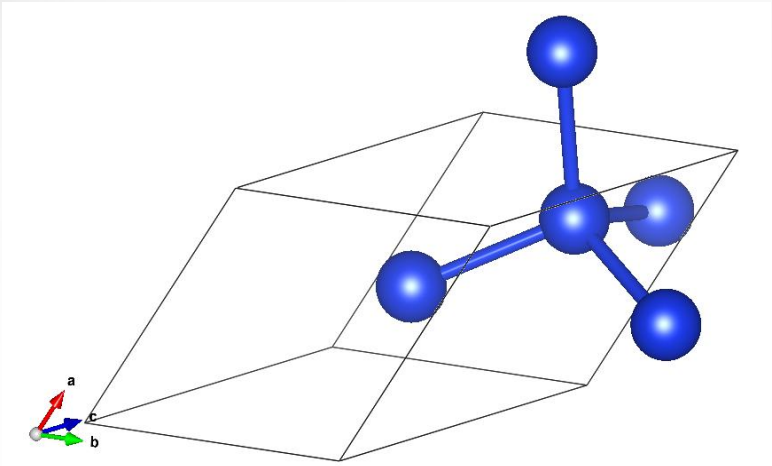


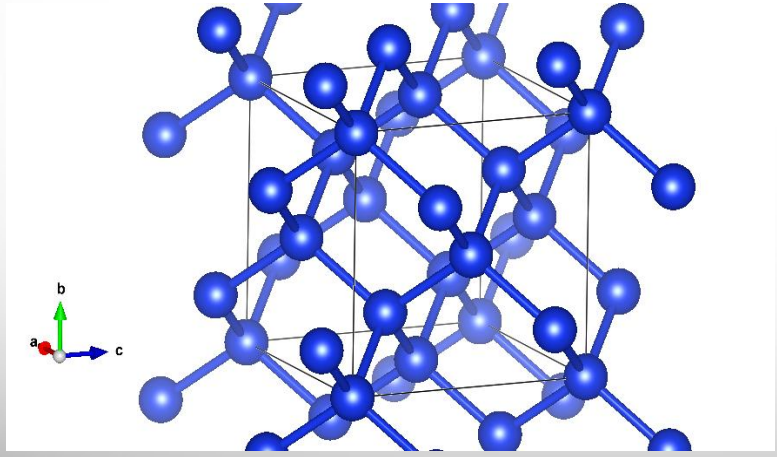
45 wide



Si

Same Structure





Lattice: 3.867 0.000 0.000
1.933 3.348 0.000
1.933 1.116 3.157

Atom Positions (fractional):
Si 0.125 0.125 0.125
Si 0.875 0.875 0.875

Lattice: 5.468 0.000 0.000
0.000 5.468 0.000
0.000 0.000 5.468

Atom Positions (fractional):
Si 0.000 0.000 0.000
Si 0.000 0.500 0.500
Si 0.500 0.000 0.500
Si 0.500 0.000 0.500
Si 0.750 0.250 0.750
Si 0.250 0.250 0.250
Si 0.250 0.750 0.750
Si 0.750 0.750 0.750

Project Objective

To create a machine learning algorithm that given a materials crystal structure, the lattice and the position and type of each atom, can predict if the structure will be stable, i.e. the forces on each atom will be below a certain threshold.

Questions?