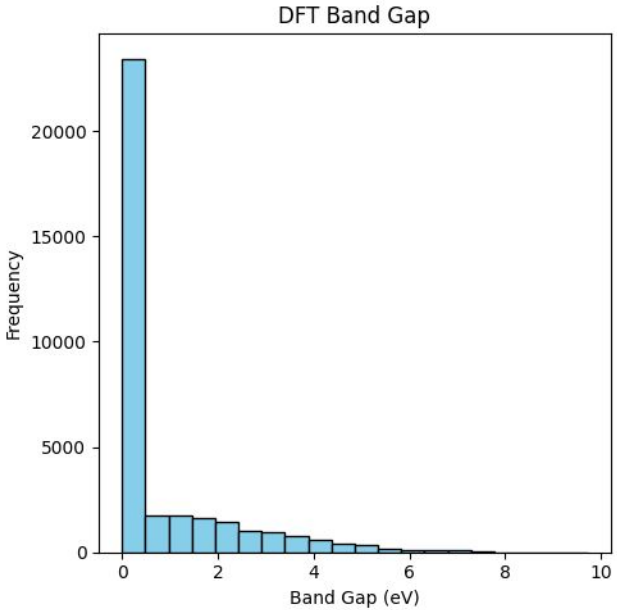
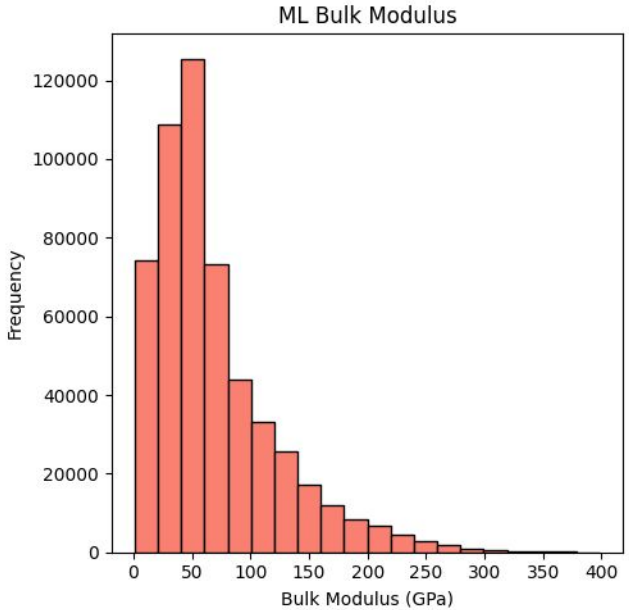
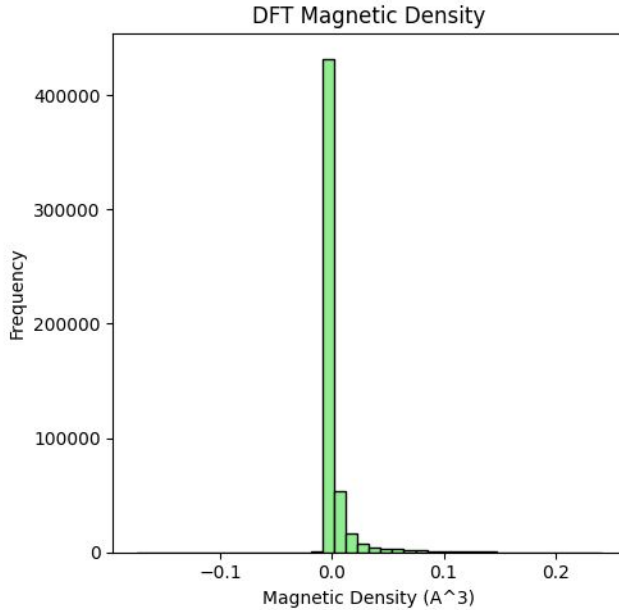
Materials Discovery Meeting

Alex-MP-20

- Significantly smaller dataset for band gap
  - (probably why MatterGen isn't great in generating materials for a specific band gap)
- Magnetic density seems to be very condensed around 0







Mattergen evaluation bug

- Issue with the MatterSim library
  - There is an issue opened without comments on the library already
  - Broken due to changes to ASE requiring a gradient to check if training has converged
- Fix:
  - mattersim/src/mattersim/batch_relax.py
  - add to line 126: gradient = opt.optimizable.get_gradient()
  - edit next line: if opt.converged(gradient) and …

Generated materials

Completed some experiments with extreme values (16 materials generated per)

- Band gap: 8 eV
  - Avg energy above hull: 0.05279652665039114
- Bulk modulus: 400GPa
  - Avg energy above hull: -0.03082677114843868
- Magnetic density: 0.2 A^-3
  - Avg energy above hull: 0.008682207041015744

Need to see if we can get properties with DFT/Mattersim

Plan to run:

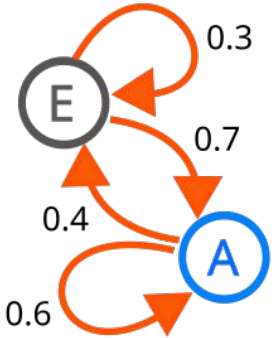
- Conditioned on bulk modulus with certain elements (aluminum) included

Diffusion Methods

Crystal structures are defined by:

- Atoms
- Lattice structure
- Coordinates

Atom Type Diffusion



Atomic species are discrete

- We have an input sample a_0
  - a_t denotes our atom type after t diffusion steps
  - Model the transition as a Markov process - this allows us to do efficient calculations about the next steps

Coordinate Diffusion

Lattice Diffusion

Questions

- What is the best way to get properties from a structure?
  - DFT
  - Mattersim should be able to do some initial predictions
- What is the HHI score?
  - How risky is the supply?
  - Check how abundant a material is, basically how much potential there is to commercialize it at large scales.
- What experiments would be interesting?
  - Property condition + including/excluding some element
  - We can see if we can add a search-based method to improve searching for materials with out-of-distribution properties

TODOs

- Generate materials conditioned on both property and material
- Select best materials from tail distribution experiments from this week
  - Try mattersim to get initial property predictions
  - Do DFT from this
- Roadmap:
  - Find a space where there are lots of global minima
  - Should lead to a better material
- We want to find significant deviations to mattergen's generations
  - Materials don't properly meet what we try to condition on
  - Materials aren't stable
- What is a good candidate material?
- Can we use a search to get global minima?