9/23 Materials Discovery

Purpose of dft:
- give an approximate of electron properties (electron density?)

If dft is already calculated, is it easy to calculate properties (conductivity, band gap, etc)?
- it's hard, still need quite a few calculations

Problem from past collab:
- already characterized a large amount of materials
- only found 10-20 materials that meet the criteria
- ML methods are hard to deal with due to low number of true positives

Idea:
- narrow down search size with smth similar to mattergen
- classifier guided diffusion would be interesting

new paper: https://chemrxiv.org/engage/chemrxiv/article-details/685057d9c1cb1ecda05e9aec
- highlights limitations of mattergen

Limited number of lattice systems?
- honeycomb structures
    - https://en.wikipedia.org/wiki/Honeycomb_(geometry)
- think about symmetry
- look at materials that we have
    - find distribution of those materials
    - https://contribs.materialsproject.org/

Possible direction: is it possible to do predictions based on how dft is calculated?
- make the dft calculation itself part of the neural net (maybe pinn)

- get the property that we're interested in from jerry
    - do a mix of search + generation

TODO:
- talk about the architecture for the diffusion model
    - what parameters go into the model
- look at a property from Jerry and look at the distribution within a dataset
    - look at bandgap, electron transport property, thermoelectric (maybe dead end), catalysis?

read to catch up on chemistry terms:
- https://www.sciencedirect.com/science/article/pii/S0927025622006000