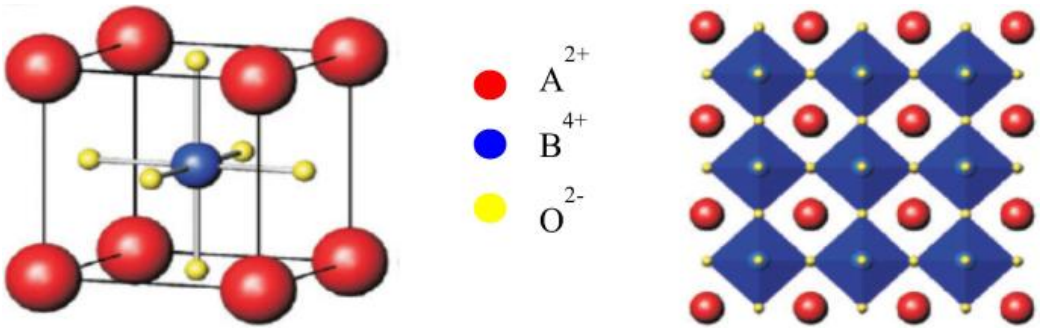

Figure 1: The ideal face-centered cubic perovskite structure. [1]

1 Perovskites

1.0.1 Structure

The perovskite stucture is ABO3, where A is a large cation, B is a smaller cation, and O is an oxygen anion. The B cation is typically a transition metal, and the A cation is typically an alkali metal or alkaline earth metal. The structure is face-centered cubic, with the B cation at the center of the cube, the A cation at the corners of the cube, and the O anion at the center of each face of the cube. The structure is shown in Figure 1.

1.0.2 Applications

Perovskites have shown potential as efficient heterogeneous catalysts, and could be used to replace platinum-group metal (PGM) catalysts as they are cheaper and easier to synthesize. Additionally, the structure of perovskites allows for a wide range of substituting and doping, allowing to tailor their properties to better target applications [2].

2 Objectives

I will be using VASP to compute surface energies of perovskites, first using DFT and then using the wavefuntion-based methods HF and MP2. I will compare my results to experimental data from the literature.

3 Method

3.1 Find experimental data for comparison

Materials Project looks promising.

3.1.1 Choice of perovskite/quantity

Leaning toward computation of surface energies, as opposed to adsorption energies. Thinking that it will be good to focus on the material itself, and leave the adsorbates out. the materials I have in mind are LaMnO3, LaFeO3, and SrTiO3. Thinking to choose one of these three, and then choose a quantity to compute for that material. How many systems do I want to choose for study given my somewhat limited time frame (this isn't a SURF project that I can spend 45 hrs/week for 10 weeks on)?

3.2 Perform DFT calculations

3.2.1 Choice of DFT functional

any advice here? I could try and educate myself on this point, but thinking that you gus might have easy answer that might be most appropriate.

3.3 Basis choice

To be compatible with both DFT and later the wavefunction-based methods HF and MP2. Any advice here?

3.3.1 Choice of k-point mesh

Any advice here? Or do I simply need to look through the computational literature to find out what has been done in the past? The later is probably good idea for me to look into, but I am not completely aware of the timeline for Ch121 project as a whole, as you probably are.

3.4 Perform HF and MP2 calculations

I was speaking with Charles and we agreed that this might be a good continuation into Ch121b, where I will start on DFT now in Ch121a, and then move on to HF and MP2 in Ch121b.

References

[1] Eman Abdul Rahman Assirey. Perovskite synthesis, properties and their related biochemical and industrial application. *Saudi Pharmaceutical Journal*, 27(6):817–829, 2019.

[2] Sebastien Royer, Daniel Duprez, Fabien Can, Xavier Courtois, Catherine Batiot-Dupeyrat, Said Laassiri, and Houshang Alamdari. Perovskites as substitutes of noble metals for heterogeneous catalysis: dream or reality. *Chemical reviews*, 114(20):10292–10368, 2014.