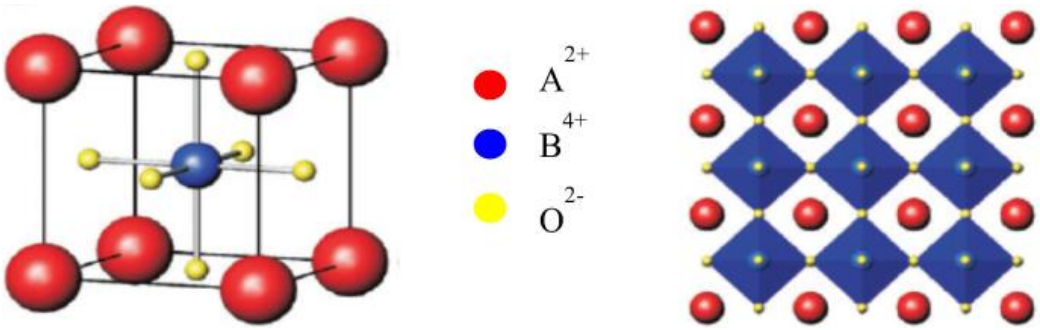

Figure 1: The ideal face-centered cubic perovskite structure. [1]

1 Perovskites

1.1 Structure

The ideal 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.

1.2 Applications

Perovskites have shown potential as efficient heterogeneous catalysts that are cheap and easy 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 potentially using wavefuntion-based methods like HF/MP2. I will compare my results to experimental data from the literature.

3 Method

3.1 Find experimental data for comparison

Look through Materials Project?

3.1.1 Choice of perovskite

I want to compute surface energies for the La series of perovskites; starting with LaMnO3, LaFeO3, and LaCoO3. I think this would be interesting because the transition metal cation is changing across the series, and I would like to see how this affects the surface energies.

3.2 Perform DFT calculations

3.2.1 Choice of DFT functional

PBE-D3

3.2.2 Basis choice

some kind of plane wave bases, tbd

3.2.3 Choice of k-point mesh

Can charles suggest something?

3.3 Perform HF/MP2 or hybrid-DFT 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 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.