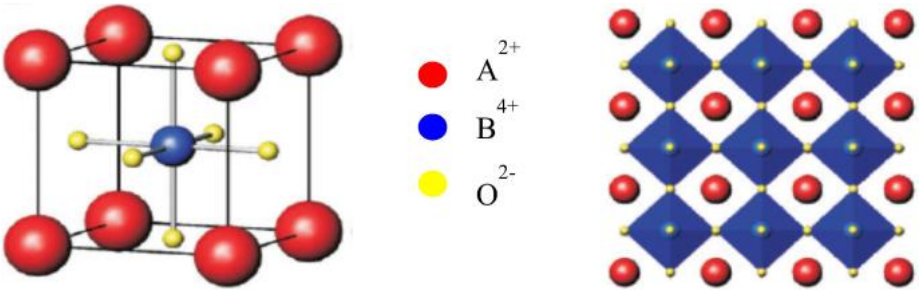

Figure 1: The ideal face-centered cubic perovskite structure. [1]

1 Perovskites

1.1 Structure

The ideal perovskite stucture is ABO_3, 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]. They show promise in Catalytic NO Decomposition, catalytic NO Reduction, Catalytic N2O Decomposition, Catalytic Complete Oxidation of CO and CH4, Catalytic Oxidative Reforming of Hydrocarbon, Soot Oxidation, and Catalytic Combustion of Volatile Organic Compounds (VOCs) to name a few. [3]

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 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. I will compare my results to experimental/computational data from the literature (material project).

3 Method

3.1 Perform DFT calculations

3.1.1 Choice of DFT functional

PBE-D3

3.2 Perform HF/MP2 or hybrid-DFT calculations

This might be a good continuation into Ch121b. 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.

[3] Junjiang Zhu, Hailong Li, Linyun Zhong, Ping Xiao, Xuelian Xu, Xiangguang Yang, Zhen Zhao, and Jinlin Li. Perovskite oxides: preparation, characterizations, and applications in heterogeneous catalysis. *Acs Catalysis*, 4(9):2917–2940, 2014.