Department of Chemistry: Part III Project 2017/18

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Machine learning and high-throughput screening of new functional materials

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Description of projects

Project 1: Machine learning from experimental battery data

In this project we will develop descriptors to facilitate machine learning of experimental battery cycling data, inspired by similar work utilising previous experimental data to predict crystallisation reactions [2]. There are numerous different factors that contribute to the performance of laboratory-prepared solid-state batteries, including anode and cathode chemical composition, type of cell, formulation and perparation of the cell itself, and the parameters of cycling (such as the rates of charge and discharge). Untangling the various influences from these factors on battery performance is extremely difficult, but is desirable in order to better understand how to optimise battery design. There is a large amount of data that has already been generated by the Grey group's study of novel batteries over the past decade which should prove amenable to data mining using neural network approaches, and the first step for this study is to develop a way of representing the metadata of each experiment's cell, preparation and condition. This is turn can be analysed to develop appropriate descriptors to construct the neural networks. The end goal will be producing a method that can predict the performance of batteries *in silico* based on their synthesis and preparation.

Project 2: Predicting complex order in materials

In this project we will use computer code developed within the Morris group (COMB) to predict the complex ordering within solid-state oxide materials. Current structure prediction (and theoretical calculations generally) is limited to materials with full stoichiometry, i.e. all atomic sites are fully occupied. However, there are many materials whose novel and interesting physical properties rely on non-stoichiometry, and by introducing vacancies into a material complex structural orderings can arise. COMB is able to start with a small stoichiometric cell, and then iteratively screen different defect positions, slowly moving to larger and larger cells that more accurately reflect the true structure of materials. A particularly well suited system for this approach is the transition of the perovskite $SrFeO_3$ to the brownmillerite $Sr_2Fe_2O_5$, which proceeds through the introduction of increasingly more vacancies within the perovskite structure. This reaction shows promise for use in chemical looping processes that use reversible redox reactions to deliver pure oxygen for combustion or other reaction [1], and in this project we will seek to computationally predict the structural evolution of this material at different stages of the reaction.

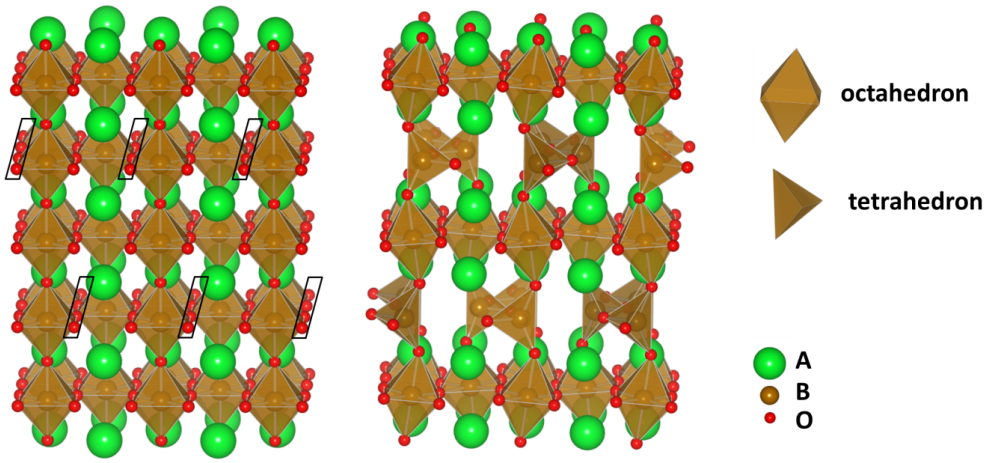

Figure 1: Removal of the highlighted oxygen atoms in the perovskite material $SrFeO_3$ on the left produces the brownmillerite material $Sr_2Fe_2O_5$ on the right. Figure reproduced from crystallography365.wordpress.com.

Project 3: Large scale screening of materials for oxide ionic conductivity

In this project we will use Voronoi mapping techniques to efficiently screen large databases of materials to predict their oxide ionic conductivity. Ionic conductivity is an important property upon which many existing materials are based, such as solid-oxide fuels and batteries. While recently new approaches have been developed to screen large databases for Li or Na ion conductivity, these are often quite expensive or limited to specific cases. Another technique that has been used successfully in other cases has been Voronoi mapping, which allows the void network within a porous material (such as within a metal-organic framework) to be characterised and the ease of movement of atoms or molecules through this material can then be calculated very quickly. In this project we will apply this approach to close packed oxide materials to determine the network available for oxide ionic conduction, and to efficiently screen large databases to rank their materials by their ionic conductivity.

References

[1] H. Falcón, J. A. Barbero, J. A. Alonso, M. J. Martínez-Lope, , and J. L. G. Fierro. $SrFeO_{3-\delta}$ perovskite oxides: chemical features and performance for methane combustion. *Chemistry of Materials*, 14(5):2325–2333, 2002.

[2] Paul Raccuglia, Katherine C. Elbert, Philip D. F. Adler, Casey Falk, Malia B. Wenny, Aurelio Mollo, Matthias Zeller, Sorelle A. Friedler, Joshua Schrier, and Alexander J. Norquist. Machine-learning-assisted materials discovery using failed experiments. *Nature*, 533(7601):73–76, 05 2016.