Project Proposal - Computational Materials Design

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January 2022

1 Scope and Aim

It is becoming clear that one of the most important technologies to deal with increasing environmental pressures and a drive to net-zero emissions, at least in the short term, is battery technology. This is reflected in the increasing research interest in the academic sphere and more importantly by increasing enthusiasm and activity in the industry. Materials research, and computational materials design is one of the pillars that will drive improvements in battery technology

Cathodes are a crucial component in the battery. The performance of these cathodes is related how readily electrons, are absorbed by the materials. Clearly, an important aspect in the design of cathodes is the topology and properties of the material. Due to constraints in current *abinitio* methods it is difficult to capture the exact behavior of these cathodic materials at a quantum level, since we can only simulate at very small spatiotemporal scales . Kinetic Monte Carlo simulations are better adapted at simulation, and allow us to deal with significantly larger spatiotemporal scales. The problem is that we lose some very important quantum information when we go up in the spatiotemporal levels. If we wish to go as far as simulating an entire topological domain of a material, we must resort to molecular dynamics (MD) simulations which are even more coarse grained than kMC models. In these cases we lose more information about the system. What if we could approximate DFT models with some alternative method, to bridge the gap between these fine resolution DFT models and lower order models such as kMC or MD models? This is where machine learning comes into play. By learning the link between atomic configurations and important microscopic properties, the idea is that the accuracy of the coarse grained model is improved without incurring excessive computational costs.

2 Methods

The idea with the project is to harvest crystal structures and precomputed DFT properties from the open quantum materials database (htts://oqmd.org). The

developers of the materials database have functioning python scripts, and extensive documentation that allows for easy data handling (https://github.com/wolverton-research-group/qmpy). With this data, the intention is to train a neural network that looks at the position, distribution, and identity of atoms and predicts important microscopic chemical and electronic properties that could improve the performance and accuracy of kMC or MD models at little computational expense. As has been showcased in several other works the incorporation of uncertainty quantification could give some estimate as to how certain the given predictions are. If time permits the goal would be to exchange the deterministic neural network for some other network using a Bayesian approach (thus incorporating this uncertainty), and for the sake of interest some random forest or optimization algorithm that suggests structures that could be of interest.