MRS Spring 2022

View Abstract

CONTROL ID: 3672556

PRESENTER: Nidhish Sagar

AUTHOR PREFERRED PRESENTATION TYPE: Oral Presentation Preferred

Symposium: DS01: Integrating Machine Learning and Simulations for Materials Modeling, Design and Manufacturing

Abstract

TITLE: Constructing Machine Learned Interatomic Potentials for Multi-component Oxides

AUTHORS (FIRST NAME, LAST NAME): Nidhish Sagar[1], Sai Gautam Gopalakrishnan[1]

INSTITUTIONS (ALL): 1. Indian Institute of Science, Bangalore, KA, India.

ABSTRACT BODY:

Abstract Body: Lithium-ion batteries (LIBs) have disrupted the energy storage technology space by promoting the use of portable electronics, electric vehicles, and grid-scale storage. The state-of-the-art positive electrodes (or cathodes) used in commercial LIBs are layered (and ordered) transition-metal-oxides (TMOs), where the lithium and the redox-active transition-metal cations occupy distinct sites. However, layered TMOs are often susceptible to irreversible phase transformations and oxygen release (leading to fires), especially under towards top-of-charge. Recent research has shown that cation-disordered oxides, which can exhibit a large diversity in their compositions and configurations, allow for facile, reversible lithium intercalation yielding high capacities, eventually resulting in high energy density batteries. However, disordered materials are hard to accurately model using conventional density functional theory (DFT) calculations, because of their configurational complexity, which is especially relevant to understand and predict their dynamic behaviour over large-length and long-time scales. Hence, we have constructed machine learned interatomic potentials (ML-IAPs) on a large dataset (>10,000 unique configurations) of multi-component oxides, to yield robust predictions of electrochemical and thermodynamic properties on this diverse chemical space. Specifically, we have benchmarked the computational accuracy and cost of different ML-IAP frameworks (against our DFT-calculated dataset) to identify the most optimal training regimen and subsequently used the optimal ML-IAP to scan through a wider compositional and configurational space to identify new candidates. Our predictions will not only guide experimentalists to prepare new electrodes in the lab (eventually resulting in better LIBs), but also aid in accelerating the computational screening and modelling of configurationally-complex systems.

Attendance Preference: I would prefer to present in person in Honolulu