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Author: Mr. Karun Kumar Rao
University of Houston, United States, karun.kumar.rao@gmail.com

USING ARTIFICIAL NEURAL NETWORKS TO MODEL DIFFUSION IN SOLID STATE ELECTROLYTES

Abstract

For many aeronautical and space applications energy storage is a key component for a successful mission where reliability, energy density, and safety are paramount. There is great interest in developing solid state electrolytes (SSE) to replace the flammable liquid electrolyte in traditional Li-ion batteries to improve safety and use metallic lithium as the anode to greatly increase the specific capacity and energy density of the battery. Previous efforts trying to understand the structure-function relationships resulting in high ionic conductivity materials have relied on ab-initio molecular dynamics (AIMD). Such simulations, however, are computationally demanding and cannot be reasonably applied to large systems containing more than a hundred or so atoms. Herein, we propose using machine learning artificial neural networks (ANN) to supply the forces and energies used during the molecular dynamics (MD) simulations, to eliminate the need for costly ab-initio force and energy evaluation methods, such as density functional theory (DFT). After carefully training a robust ANN for four and five element systems, we obtain nearly identical lithium ion diffusivities for Li10GeP2S12 (LGPS) when benchmarking the ANN-MD results with DFT-MD. To demonstrate the power of the outlined ANN-MD approach we apply it to a doped LGPS system to calculate the effect of concentrations of chlorine on the lithium diffusivity at a resolution that would be unrealistic to model with DFT-MD. Our trained neural network predicts the optimal concentration of Li doping to be 1% and a similar conductivity at 24.22 mS/cm2, which is comparable to experimental results[1]. We additionally test the overall robustness of these ANNs and find their accuracy is highly dependent upon the training data with some force fields being unable to reproduce 0 K structure optimization while others accurately reproduce both 0 K and finite temperature effects. Overall, we find that ANN-MD simulations can provide the framework to study systems that require a large number of atoms more efficiently and with high accuracy within the trained regime. Ref: [1] Y. Kato, et al Nat. Energy 2016, 1, 16030.