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Accelerating Molecular Dynamics Simulations of Electrolytes with Neural Network: Bridging the Gap between Ab Initio Molecular Dynamics and Classical Molecular Dynamics

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Abstract : Classical molecular dynamics (CMD) simulations are highly efficient for material simulations but have limited accuracy. In contrast, ab initio molecular dynamics (AIMD) provides high precision by solving the Kohn–Sham equations yet requires significant computational resources, restricting the size of systems and time scales that can be simulated. To address these challenges, we employed NequIP, a machine learning model based on an E(3)-equivariant graph neural network, to accelerate molecular dynamics simulations of a 1M LiPF6 in EC/EMC (v/v 3:7) for Li battery applications. AIMD calculations were initially conducted using the Vienna Ab initio Simulation Package (VASP) to generate highly accurate atomic positions, forces, and energies. This data was then used to train the NequIP model, which efficiently learns from the provided data. NequIP achieved AIMD-level accuracy with significantly less training data. After training, NequIP was integrated into the LAMMPS software to enable molecular dynamics simulations of larger systems over longer time scales. This method overcomes the computational limitations of AIMD while improving the accuracy limitations of CMD, providing an efficient and precise computational framework. This study showcases NequIP's applicability to electrolyte systems, particularly for simulating the dynamics of LiPF6 ionic mixtures. The results demonstrate substantial improvements in both computational efficiency and simulation accuracy, highlighting the potential of machine learning models to enhance molecular dynamics simulations.

Keywords : lithium-ion batteries, electrolyte simulation, molecular dynamics, neural network
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