Abstract:

In the evolving field of battery technologies, the demand for safer, higher-capacity, and faster rechargeable devices drives the exploration of new materials and modeling techniques. High-performance batteries form a crucial Solid Electrolyte Interface (SEI), essential for functionality but limiting lifespan and capacity [1]. The reactive SEI environment complicates the experimental investigation, emphasizing the role of modeling [2]. This study develops an accurate atomistic model using advanced force fields to improve the understanding of lithium transport. We compare the semi-empirical Reactive Force Field (ReaxFF) and the Machine Learning Force Field (ML-FF) for lithium diffusivity in lithium fluoride (LiF), a key SEI component [3]. Trained with ab initio data from Density Functional Theory (DFT), our results show ReaxFF's limitations and ML-FF's high accuracy [4]. ML-FF significantly enhances the prediction of lithium transport properties and offers deeper insights into ion diffusion mechanisms. In conclusion, innovative force fields are crucial for accurately modeling SEIs, improving battery safety and efficiency, and enabling in-silico material screening [5]. We acknowledge partial support from MUR through the "Progetto Ministeriale Continuativo" entitled "Better Measurements for Energy Storage."

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