

Abstract Submitted
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Understanding Complex Ion Dynamics in Lithium-Ion Battery Electrolytes from First Principles¹ MITCHELL ONG, VINCENZO LORDI, Lawrence Livermore National Laboratory, TIMO BREMER, ATTILA GYULASSY, Lawrence Livermore National Laboratory, University of Utah, ERIK DRAEGER, Lawrence Livermore National Laboratory, HARSH BHATIA, Lawrence Livermore National Laboratory, University of Utah, JOHN PASK, Lawrence Livermore National Laboratory — Lithium-ion secondary batteries are commonly used to power many consumer devices such as handheld phones, laptops, portable music players, and even electric vehicles. One of the key properties that influence the performance of lithium-ion batteries is the ionic conductivity of the electrolyte. This is dependent on the mobility of the Li ion in solution and also related to their solvation structure. In this work, we have performed first principle molecular dynamics of an LiPF_6 salt solvated in different organic solvents such as ethylene carbonate (EC), ethyl methyl carbonate (EMC) and a mixture of the two. We observed that the diffusivity of Li^+ is correlated to the degree of Li^+ solvation. Corresponding analysis for PF_6^- shows greater diffusivity than Li^+ associated with a weakly-bound, poorly defined first solvation shell. Using a recent analysis method to study the distribution of directional change from relative angles at successive time intervals, we also characterize the complex motion of these ions and find distinct patterns for each ion in different organic solvents. These results provide valuable insight that can be used to improve the cycling rate of Li-ion batteries and potentially lead to the design of new electrolytes for better overall battery performance.

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