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Lithium Ion Solvation and Diffusion in Bulk Organic Battery Electrolytes from First Principles Molecular Dynamics MITCHELL ONG, VINCENZO LORDI, ERIK DRAEGER, JOHN PASK, Lawrence Livermore National Laboratory — Lithium-ion batteries are commonly used to power many consumer devices. 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 speed at which Li ions diffuse across the cell and related to the solvation structure of the Li ions. The choice of the electrolyte can greatly impact both solvation and diffusivity of Li ions. In this work, we use first principles molecular dynamics to examine the solvation and diffusion of Li ions in several bulk organic electrolytes. We find that differences in the local environment throughout the liquid can lead to solvation of Li ions by either carbonyl or ether oxygen atoms. In addition, we examine the differences in solvation of associated and dissociated $Li(PF_6)$ salts, showing that the bulky PF_6 group blocks complete solvation of Li^+ by solvent oxygen atoms. Finally, we calculate Li diffusion coefficients in each electrolyte, finding slightly larger diffusivities in a linear carbonate such as ethyl methyl carbonate (EMC) compared to a cyclic carbonate like ethylene carbonate (EC). Results from this work can be used to design new bulk electrolytes that will improve the performance of current Li-ion batteries.

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