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Properties of Liquid Electrolytes for Li-ion Battery Applications from First Principles Molecular Dynamics Simulation PAUL KENT, PANCHAPAKESAN GANESH, DEEN JIANG, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — A judicious choice of the liquid electrolytes used in battery systems is required to achieve a good balance between high energy storage, fast charging and long lifetime. Ethylene-carbonate (EC) and propylene-carbonate (PC) are popular electrolytes used for this purpose. To date, molecular-dynamics simulations typically rely on classical force-fields, which do not capture the true quantum-mechanical nature of the electrons, most important for the charging/discharging dynamics. We perform accurate first principles molecular-dynamics simulations of EC and PC with LiPF_6 at experimental concentrations to build solvation models which explain available Neutron and NMR results as well as to compute Li-ion solvation energies and diffusion constants. Our results throw light on why EC is a more popular choice for battery applications over PC. Insights into the formation of solid-electrolyte interphases in the presence of carbon electrodes in conventional Li-ion batteries will also be discussed, and perspectives into the likely future scope of these simulation methods presented. Supported by the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Basic Energy Sciences under Award Number ERKCC61.

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