

Abstract Submitted
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Electrolyte Structure near Electrode Interfaces in Lithium-Ion Batteries¹ VINCENZO LORDI, MITCHELL ONG, Lawrence Livermore National Lab, OSVALDS VERNERS, Lawrence Livermore National Lab and Penn State University, ADRI VAN DUIN, Penn State University, ERIK DRAEGER, JOHN PASK, Lawrence Livermore National Lab — The performance of lithium-ion secondary batteries (LIBs) is strongly tied to electrochemistry and ionic transport near the electrode-electrolyte interface. Changes in ion solvation near the interface affect ion conductivity and also are associated with the formation and evolution of solid-electrolyte interphase (SEI) layers, which impede transport but also passivate the interface. Thus, understanding these effects is critical to optimizing battery performance. Here we present molecular dynamics (MD) simulations of typical organic liquid LIB electrolytes in contact with graphite electrodes to understand differences in molecular structure and solvation near the interface compared to the bulk electrolyte. Results for different graphite terminations are presented. We compare the results of density-functional based MD to the empirical reactive forcefield ReaxFF and the non-reactive, non-polarizable COMPASS forcefield. Notable differences in the predictive power of each of these techniques are discussed.

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