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Modeling ion solvation in ethylene carbonate and propylene carbonate[1] AYSE ARSLANARGIN, THOMAS BECK, University of Cincinnati — Lithium-ion batteries (LIBs) and supercapacitors are expected to have important roles in renewable energy generation and in electric vehicles as electrochemical storage systems. Non-aqueous solvents such as ethylene carbonate (EC), and propylene carbonate (PC) are widely used as liquid electrolytes in LIBs. The electrolyte structure affects the efficiency of the ion transport, and understanding the solvent structure is essential for battery performance enhancements. This work investigates the thermodynamics of ion solvation in EC and PC. Free energy and enthalpy of solvation calculations have been conducted employing different force fields. Simulated annealing calculations have been performed to fit classical ion-solvent dimer interaction energies to quantum data. Non-bonded energy parameters are altered during the fitting process. The new parameters result in good agreement with the experimental free energy of solvation values, while the enthalpy of solvation results show deviations from the experimental data. These results suggest that classical models often do not accurately predict basic interactions in ion-solvent systems.

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