Accurate Static and Dynamic Properties of Liquid Electrolytes for Li-ion Batteries from ab initio Molecular Dynamics

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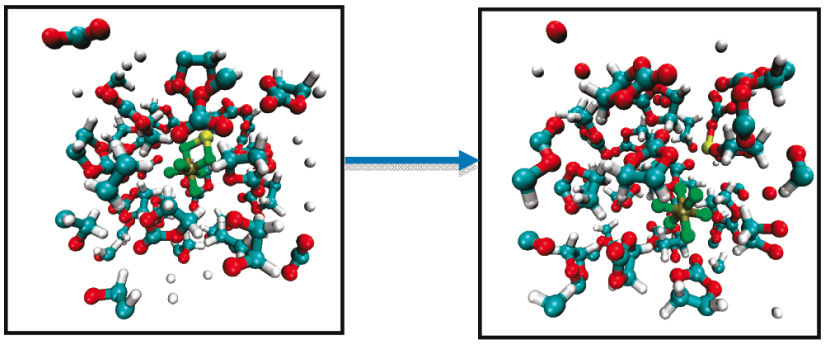
Achievement

A judicious choice of the liquid electrolytes used in Li-ion batteries is essential to achieve a good balance among high-energy storage, long cycle life and stability, and fast charging. To-date, almost all molecular-dynamics simulations of these fluids rely on classical force fields, while a complete description of the functionality of Li-ion batteries will eventually require quantum mechanics. We performed accurate quantum molecular-dynamics simulations of ethylene- and propylene-carbonate with $LiPF_6$ salt at experimental concentrations to build solvation models. These explain available neutron scattering and nuclear magnetic resonance results, and are more accurate than previous classical modeling.



Spontaneous solvation of $LiPF_6$ salt in ethylene carbonate revealed by first principles molecular dynamics simulations

Significance

Accurate models and simulation methods of known electrolytes for lithium-ion battery applications, validated against experiment, are an essential step for studies of the solid-electrolyte interphase formation at battery electrodes.

Credit

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