COMPUTATIONAL SCREENING OF SOLVENTS FOR Li-ION BATTERIES

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The reduction potential of the electrolyte solution plays a crucial role in the performance of Li-ion batteries, influencing reactions at the electrode surface and the formation of the solid electrolyte interface (SEI).

A computational screening of reduction potentials for 300 candidate solvents was conducted using a density functional theory (DFT)-based approach. This methodology integrates constrained DFT with a cluster-continuum model to evaluate the reduction behavior of potential solvents.

The study reveals that molecules can be categorized into two groups: those with reduction potentials above the lithium electrode potential and those below it. These categories correspond to electrochemically stable and unstable molecules, respectively. For small molecules, a strong correlation is observed between the reduction potential and molecular deformation during reduction reactions, whereas this correlation is weaker for larger molecules.

Additionally, DFT simulations were complemented by classical molecular dynamics calculations to assess the dielectric permittivity of the solvents. The findings indicate that most electrochemically stable solvents exhibit low dielectric permittivity.

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