Mechanistic Insights into Electrolyte Stability towards Li/Na Anode

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Lithium (Li) and sodium (Na) metal batteries are considered as promising next-generation energy storage devices due to their ultrahigh energy densities. However, the high reactivity of alkali metal toward organic solvents and salts renders inevitable side reactions, which further leads to undesirable electrolyte depletion, cell failure, and evolution of flammable gas. A novel multiscale calculation, in combination with in situ optical microscopic observations, was applied to investigate the intrinsic instability of normal organic electrolytes (PC, DOL, DME, and TEGDME) towards Li and Na metal anodes. Once complexed with Li/Na ions, solvent molecules exhibit a significantly reduced the lowest unoccupied molecular orbital level, facilitating the electrolyte decomposition and gas evolution. Based on this mechanistic insight, novel strategies are proposed to build a stable Li/Na anode-electrolyte interphase and thus long-life safe Li/Na metal batteries.

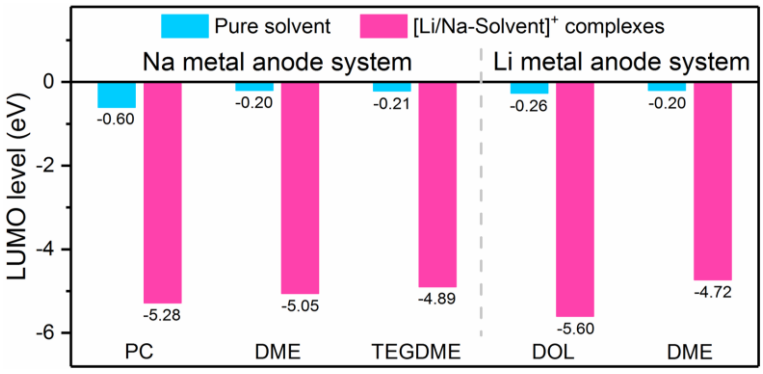

Fig. 1. Comparisons among the LUMO levels of pure solvent and ion-solvent complexes.

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