Design of sparse-solvated electrolyte for lithium metal anode under ultra-low temperature operation

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Operation of batteries under realistic condition, especially in ultra-low temperature, becomes an important issues for extending the capability of existing electric devices. Present LIB shows its limit due to the low ion conductivity and increased charge transfer resistance as the temperature decreases.

Lithium metal electrode, which has one-electron redox reaction, shows much faster kinetics compared to the six-electron intercalation reaction at the graphite, expecting to solve the low power density and rate capabilities issues at low temperature. However, due to the low Li ion conductivity and high charge transfer resistance hinders low-temperature operation of lithium metal batteries, exacerbating the dendrite growth of lithium and accelerating the unstable operation.

In this study, Li ion solvation free energy with diverse sparsely-coordinated was calculated using DFT calculations and MD simulations. We discuss about the importance of forming stable SEI layer at the low temperature operation in terms of reducing the interfacial resistance. The newly designed electrolyte with sparse-coordinating Li ion showed smooth Li deposition morphology and stable cell performance at -60℃.