

Battery Materials Innovation: Toward High-Energy Li-S Systems

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Abstract (Arial 10)

Lithium-sulfur (Li-S) batteries, known for their high energy density and low cost, are promising candidates for next-generation energy storage. However, their practical application is hindered by the high solubility of lithium polysulfide (LiPS) intermediates, which leads to rapid capacity decay and severe self-discharge. While previous efforts have focused on electrolytes with low LiPS solubility to suppress the shuttle effect, we report that electrolytes with moderate LiPS solubility (F4DMB) are more effective in balancing shuttle suppression and Li-S reaction kinetics. To this end, we further propose a solvation-catalysis coupling strategy, which synergistically combines electrolyte solvation energy regulation with atomic cobalt-mediated trapping and conversion on hydrogen-substituted graphdiyne (Co-HGDY). By tuning the solvation energy of the electrolyte, a sustained adsorption-conversion equilibrium is achieved at the Co-HGDY interface. As a result, the assembled cells demonstrate high capacity and excellent long-term cycling stability under both room temperature and elevated conditions, outperforming systems with mismatched solvation and catalytic regulation. Moreover, this talk will discuss the role of artificial intelligence in guiding catalyst and electrolyte design, highlighting its transformative potential in the development of high-energy battery systems.

References

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