Harnessing Two-Dimensional Materials for High-Performance Metal-Sulfur Batteries

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Room-temperature metal-sulfur batteries (Li-S and Na-S) are promising next-generation energy storage technologies beyond conventional Li-ion batteries (LIBs) due to their exceptionally high theoretical energy density and the natural abundance of sodium and sulfur. However, their commercialization is hindered by polysulfide shuttling and sluggish electrochemical kinetics. This talk explores the potential of generic two-dimensional (2D) materials as cathode hosts to address these challenges. Using density functional theory (DFT), we systematically investigate interfacial interactions between lithium/sodium polysulfides (Li_2S_n and Na_2S_n, $1 \leq n \leq 8$) and 2D materials, along with their role in sulfur reduction reaction (SRR) mechanisms. Our findings reveal that nanoporous graphene[1], MoSTe[3], and MoS_2/electride heterostructures[3] effectively suppress polysulfide shuttling by strongly binding polysulfides, preventing their dissolution in electrolytes. Additionally, these materials catalyze electrochemical reactions, lowering SRR intermediate conversion barriers and reducing Na^+- and Li^+-ion diffusion barriers, thereby enhancing charge transfer kinetics. This work highlights the novel functionality of 2D materials as cathode hosts in metal-sulfur batteries, providing a pathway to high-performance, scalable energy storage solutions.

References

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