

Nickel Phosphide (Ni₂P): An Effective Host Material for High-Performance Lithium–Sulfur Battery

*R. Amaral, N.Y. Dzade

Abstract:

High energy-density rechargeable batteries are considered critical elements for unlocking the full potential of intermittent green energy sources, such as solar and wind power. Nowadays, conventional lithium-ion batteries (LIBs) dominate the battery industry, with a market share of 63% worldwide, but with very slow improvements in their energy storage capacities since their first introduction in 1991. On the other hand, Lithium-Sulfur batteries (LSBs) appear as promising alternative that relies on the reversible redox reactions between the lightweight elements lithium and sulfur, and that can achieve an impressive theoretical energy density of 2500 Whkg⁻¹ – i.e., over six times existing LIBs. Furthermore, LSB technology replaces the expensive and short supply cathode materials of Li-ion cells, i.e. Ni, Mn, and Co (NMC), by the cost-effective and non-toxic Sulphur. The application of LSBs, however, still presents important challenges related to instabilities on the sulfur cathode, among which the low sulfur species conductivity, the diffusion of lithium polysulfides (commonly referred to as the shuttle effect), and its large volumetric expansion. These constrains compete with the priority of maximizing the energy density of the cell, demanding the rational design of multifunctional and lightweight host materials specially adapted to overcome LSB's intricate requirements. In this work, we employ accurate first-principles calculations based on Density Functional Theory (DFT) to unravel the adsorption chemistry of lithium polysulfides (LiPSs) on nickel phosphide (Ni₂P), a promising host cathode material to mitigate the shuttle effect. The binding geometries, adsorption energetics, and electronic structures (Bader charge analysis, charge density difference, and projected density of states) were systematically characterized. The results reveal a strong interaction between the LiPSs and Ni₂P material, indicating that Ni₂P is a promising potential host cathode material for Li-S battery applications.