Colloidal and Interfacial Properties of Silicon Nanocrystals and Their Impact on Lithium Ion Battery Performance

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Silicon nanocrystals (SiNCs) are promising candidates for next-generation energy and hybrid materials, yet their practical integration is often limited by interfacial instability, aggregation, and sensitivity to aqueous environments. In this work, we investigate SiNCs of 6, 20, 55, and 100 nm to understand how surface chemistry, particle size, and solid-state properties jointly influence their colloidal behaviour and functional performance. Using hydrogen-terminated SiNCs as a starting point [1], we show that functionalization with poly(acrylic acid) (PAA) and phytic acid (PhA) produces covalent and ionic Si–O–C and Si–O–P linkages that substantially enhance dispersion stability. Spectroscopic analysis (FTIR, XPS), dynamic light scattering, and zeta-potential measurements demonstrate that controlled surface chemistry stabilizes surface charge and suppresses aggregation across a broad pH range, highlighting the central role of interfacial speciation in colloidal control.
Extending this strategy across all investigated sizes enables a direct comparison of how curvature, accessible reactive sites, and initial oxidation state affect functionalization efficiency and colloidal stability. Incorporation of size-defined SiNCs into hydrogel-derived polypyrrole (PPy) networks further reveals the interplay between colloidal stabilization and electrochemical behaviour [2]. Smaller SiNCs show the most favourable electrochemical response, achieving capacity retention up to 85% after 100 cycles, whereas physically blended electrodes display weaker cohesion and accelerated degradation. Electrochemical analyses (GCD, CV, EIS) confirm that optimised interfacial environments enhance charge-transfer stability and mitigate irreversible degradation pathways.
Overall, this work provides a unified framework demonstrating how surface functionalization, size effects, and solid-state properties together determine the colloidal and electrochemical performance of Si nanomaterials. These insights support the development of stable, high-performing Si-based colloids relevant to colloid and interface science, sustainable processing, and next-generation lithium-ion energy technologies.

References:

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