Optimizing Silicon Anodes: Investigating Ultra-High Carboxyl Density Binders

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Electric vehicles solve for fossil fuel-induced environmental damage, but 70% of consumers cite limited battery capacity as a major drawback. Replacing traditional graphite anodes with silicon (Si) can solve this gap by expanding capacity 11-fold. However, Si expansion during charging can compromise battery integrity, prompting the aim of this study–improving Si-anode stabilization with polymeric binders. Data-driven models suggest that binders with ultra-high carboxyl (COOH) density (.33 COOH/monomer) could optimize Si-stabilization despite opposing mechanisms–adhesion and electrolyte consumption. This study resolves these mechanisms, examining their relationship at ultra-high COOH densities, to predict and optimize Si-anode functionality. Utilizing Density Functional Theory (DFT), interaction energy (IE) quantified binder adhesion while pKa quantified electrolyte consumption. COOH density was strongly correlated with IE ($r = .90$), as opposed to pKa ($r = -.15$), indicating enhanced binder adhesion without high electrolyte consumption at ultra-high COOH densities. Qualitative molecular analysis, using DFT simulations, revealed coordinate covalent bonding as a novel adhesion mechanism, with unpaired t-tests indicating a significant increase in IE ($p < .01$). Silicon anodes with standard ($n=2$) and ultra-high COOH ($n=1$) density binders were then physically synthesized and measured for true performance, confirming that ultra-high COOH density improves battery performance by 90% ($p < .01$). Demonstrating that ultra-high COOH density binders achieve unprecedented adhesion without simultaneously increasing electrolyte consumption, this study establishes proof of concept for ultra-high COOH density binders in next-generation Si-anodes to meet global, sustainable energy demands.

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