Lithiated Organic Coverages on SiO_x Anodes: Promoting Li_2O Formation and Suppressing Lithium Silicate Growth for Stable Lithium-Ion Batteries

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Silicon oxide (SiO_x) is a high-capacity anode material for lithium-ion batteries. SiO_x offers lower irreversible capacity loss, improved cycling stability, and reduced volume expansion, which facilitate practical electrode design and manufacturing. Nevertheless, SiO_x faces challenges such as the formation of inactive lithium silicates, the need for conductive carbon composites, and a relatively high lithiation potential plateau. Prelithiation has proven particularly effective, as it mitigates irreversible reactions associated with solid electrolyte interphase (SEI) formation and lithium intercalation. In this study, two lithiated organic coatings (LiOCs) were developed and applied onto the SiO_x surface for long-term stability. The LiOCs introduce additional Li^+ species and functional groups containing O and N atoms, which strongly interact with the surface Si-O-Si bonds of SiO_x. This interaction redistributes the local electron density, resulting in partial electron withdrawal from oxygen atoms and alters the structural distortion of the local asymmetry of the Si-O-Si as well as promotes the formation of extended Si clusters prior to electrochemical cycling. The LiOCs effectively suppress the formation of lithium silicates (Li_xSiO_y) while promoting Li_2O generation. Consequently, the LiOCs@SiO_x anode exhibits significantly improved cycle retention, attributed to the minimized formation of small Si clusters and enhanced interfacial Li^+ transport. Li_2O offers superior Li^+ diffusivity compared to Li_xSiO_y. Combining with direct contact prelithiation from Li metal during conventional prelithiation, the LiOC-modified SiO_x anode demonstrates twin synergistic effects with Ni-rich cathodes.

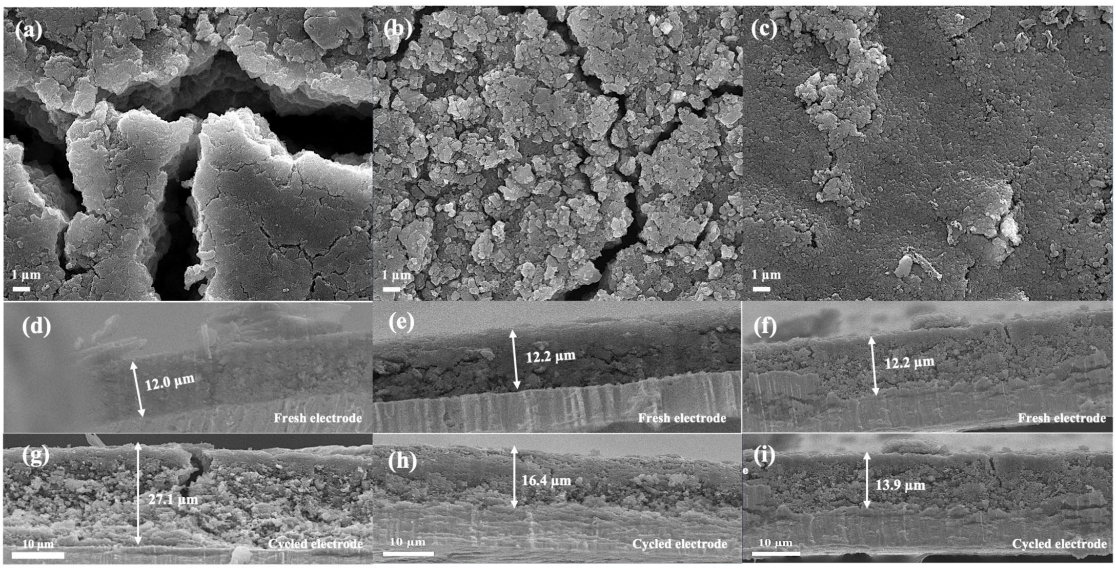

Figure 1 Top view SEM image of (a) pristine SiO_x, (b) SALi@SiO_x, and (c) DTPALi@SiO_x after 200 cycles in Figure 7(a). Cross section SEM image of (d) pristine SiO_x, (e) SALi@SiO_x, and (f) DTPALi@SiO_x before cycling. Cross section SEM image of (g) pristine SiO_x, (h) SALi@SiO_x, and (i) DTPALi@SiO_x after 200 cycles.

Reference

[1] Fu-Ming Wang et al, "Lithiated Organic Coverages on SiO_x Anodes: Promoting Li_2O Formation and Suppressing Lithium Silicate Growth for Stable Lithium-Ion Batteries", *Small Structure* (2026) https://doi.org/10.1002/sstr.70501