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Chemical Synthesis, Computational Modeling, and Surface Reactions of Silicon Nanotube Anodes and Silicate Cathodes for Lithium Ion Batteries

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Nanostructured materials show significant promise in enhancing the performance and safety of Li-ion batteries at greatly reduced cost. We highlight certain classes of materials for next generation anodes, cathodes, and solid electrolytes in addition to interface reactions and show how advanced chemical spectroscopy and first principles modeling can be utilized to improve battery performance and stability. In this work, we utilize advanced materials characterization techniques (in-situ XPS and FTIR, Raman, AFM, XRD) to elucidate the chemical bonding, nanostructure, and electrochemical properties that lead to improved storage capabilities in these materials. We describe the recent progress in chemical synthesis methods of fabricating hydrogenated amorphous-Si nanotube anodes and tetrahedral transition metal silicate cathodes (Li_2MSiO_4), which may be well-suited for future technologies. Additionally, insight into the redox potentials and ionic and electronic conductivities has been investigated using first-principles modeling. Our findings suggest that high-voltage, multi-component Li_2MSiO_4 cathodes (M = Fe, Mn, Ni) with high Mn content are strong candidates for future Li-ion batteries. Inorganic solid electrolytes are also discussed highlighting their potential for improved safety, increased ionic conductivities, and stability against adverse reactions with the electrodes. Finally, we illustrate the complexity of interfacial chemistry in these new materials and the need for advanced spectroscopic characterization to make progress on all aspects of electrode and electrolyte development.