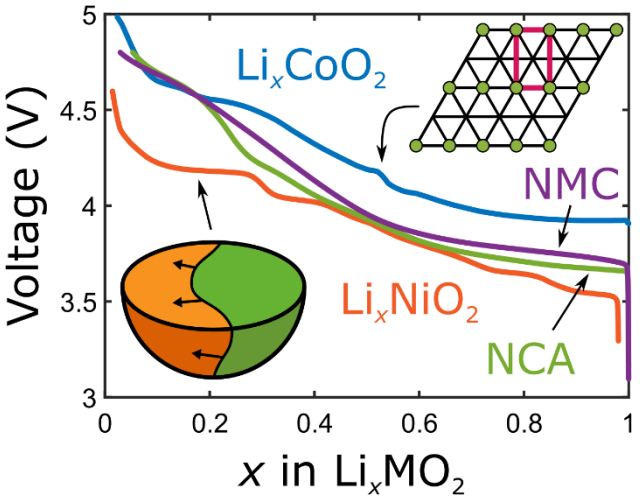
Narrowing the Gap Between Theoretical and Practical Capacities in Li-ion Layered Oxide Cathode Materials



Superimposing the voltage curves for different layered-oxide cathode materials illustrates the fundamental physical effects of alloying transition metals. The Ni-Co-Al (NCA) and Ni-Mn-Co (NMC) alloys are dominated by Ni redox at low voltages and Co redox at high voltages. Alloying also disrupts lithium/vacancy ordering, resulting in smoother voltage curves for NCA and NMC compared to pure Li_xCoO_2 and Li_xNiO_2.

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Work was performed at UCSB, UCSD, & Binghamton

Scientific Achievement

Performed a comprehensive review and critical analysis of literature related to layered-oxide cathode materials, focusing on the synthesis of new insights by comparing different materials.

Significance and Impact

Identified key pathways to closing the gap between theoretical and practical energy densities, and defined critical research questions and best practices to set the stage for forthcoming NECCES work.

Research Details

- Pathways to closing the gap between theoretical and practical energy densities. Tailoring electrode/electrolyte interactions to be self-limiting; mitigating mechanical damage; optimizing materials for Li diffusion.
- Key research questions. Role of aluminum in NCA; the physical origin of first-cycle capacity loss; the influence of particle mesostructure on electrochemical performance.
- Recommended best practices. Careful selection of experimental parameters when comparing electrochemical cells; monitoring beam damage at high states of charge; judicious use of corrections for dispersion & self-interaction in simulations.

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