Atomistic Insight into Glide-Driven Phase Transformations in Layered Oxides for Sodium-Ion Batteries: A Case Study on Na$_x$VO$_2$

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Abstract

Among high-capacity, low-cost cathode contenders for Na-ion batteries, layered transition-metal oxides are particularly promising materials. Yet there is a strong need to improve their long-term stability and capacity retention due to unwanted phase transitions occurring during sodium insertion and extraction cycles. Here, using density functional theory calculations and thoroughly examining P ↔ O transitions in Na$_x$VO$_2$ as a case study, we provide atomic-level understanding into the glide-driven processes in these compounds. In particular, we rationalize the commonly observed effect of high Na contents on preventing gliding processes at low states of charge. And we identify the beneficial impact of Na ions at face-shared prismatic sites in P-type phases to specifically hinder P → O transitions. We put forward that the gained new insights can help to focus and guide the current research efforts to design layered transition-metal oxides with enhanced long-term stability for practical applications.