Structural insights into Li-based energy storage by metastable niobates

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As batteries are employed in larger numbers and for increasingly diverse applications, there is interest in electrode materials with improved safety, availability, and cost relative to commercial electrodes. Early transition metal oxides are one alternative material family showing promise, especially for high rate applications. However, we do not yet have a strong understanding of the role of composition, structure, and structural evolution with cycling for these materials, which tend to have large unit cells and complex structures.

We report here the synthesis, energy storage behavior, and atomic structure evolution during cycling for several metastable niobates featuring crystallographic shear planes. Ex situ and operando X-ray diffraction, along with complementary methods and first principles calculations, allow us to identify atomic structure changes and relate them to cycling performance and properties, especially ionic conductivity. The fundamental understanding established through study of these are related materials can help to establish new fundamental understanding of the atomic structure and chemical motifs that support fast ion transport, thus supporting the selection and design of electrode materials for the quickly-evolving energy landscape.