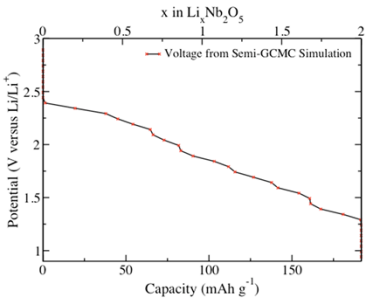
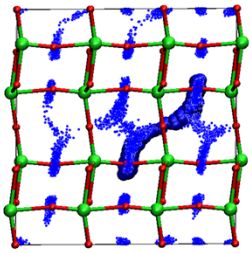
Understanding the origin of high-rate intercalation pseudocapacitance in Nb_2O_5 crystals





Top: Computed CV profile shows a pseudocapacitative slope over the entire range of Li-ion intercalation in Nb_2O_5.

Left: Overlapped lithium (blue) trajectories from *ab initio* molecular dynamics show diffusion pathways through the Nb_2O_5 crystal.

Work was performed at the Center for Nanophase Materials Sciences, ORNL.

Scientific Achievement

Using first principles calculations, we unravel a detailed mechanism explaining the high-rate pseudocapacitance in niobium pentoxide (Nb_2O_5).

Significance and Impact

Our modern energy ecosystem demands that we overcome fundamental bottlenecks in materials and design that limit simultaneous high energy density and power-density with long cycle life. The detailed mechanism for high-rate pseudocapacitance in niobium pentoxide materials provides a blueprint for efficient design/discovery of greatly improved energy storage materials.

Research Details

- First principles simulation of pseudocapacitance.
- Improved computational workflow to reliably predict the stability and dynamics of ions in solids at finite temperatures.
- Insights and approach enable opportunities for designing new materials exhibiting improved energy storage capacities.

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Highlight Narrative

Electrochemical energy storage is an essential means of storing/retrieving energy with ubiquitous use in applications from powering portable electronics to vehicular transportation. Our current energy ecosystem demands that we overcome fundamental bottlenecks in materials and design that limit simultaneous high energy density and power-density with long cycle life. The present work highlights a detailed mechanism explaining the origins of high-capacity pseudocapacitance in niobium pentoxide, where local oxidation/reduction reactions occur along with electrostatic charge storage coupled to efficient mass mobility. This new mechanism provides a means for future design/discovery of new energy storage materials with greatly improved energy capacity and very long cycle life.

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