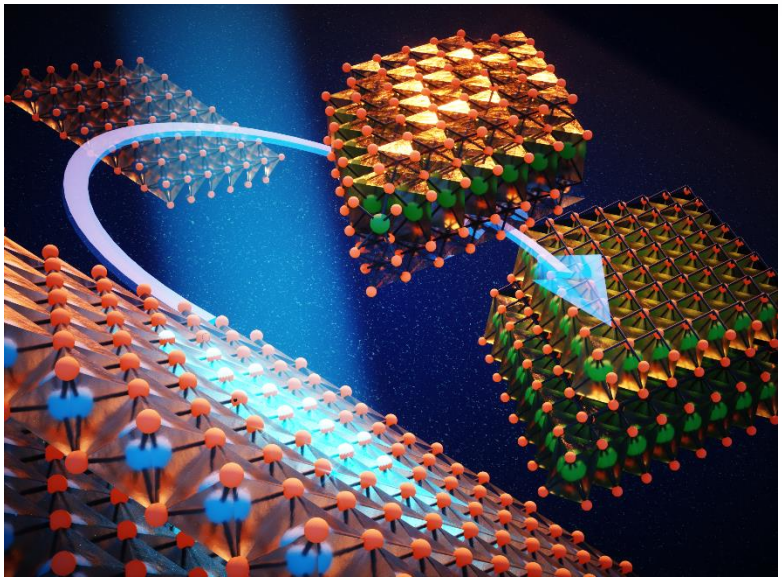
# Revealing a Reaction Mechanism in an Electrode Material



*This work was selected to be highlighted on the front cover of the Journal of Materials Chemistry A. The cover image illustrates an artistic interpretation of the transitions between three phases during battery cycling.*

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*Work was performed in part at Brookhaven National Laboratory*

## Scientific Achievement

**Scientists revealed the reaction mechanism occurring in Na–$TiS_2$ batteries with a deeper understanding of the structural evolution.**

## Significance and Impact

**This mechanism may explain why Na-$TiS_2$ has a better restoration of active materials, i.e. by restructuring after every cycle, and potentially better lifetime efficiency than lithium.**

## Research Details

- X-ray absorption spectroscopy at the TES and ISS beamlines at NSLS-II showed a redox reaction with phase transitions in both titanium (Ti) and sulfur (S), revealing the reason for the incomplete recovery of Ti after cycling.
- X-ray powder diffraction at the XPD beamline at NSLS-II showed three structurally distinct phases during cycling.
- CFN provided theoretical and experimental data analysis to resolve phase components in the reactions, which used CSI computational resources.