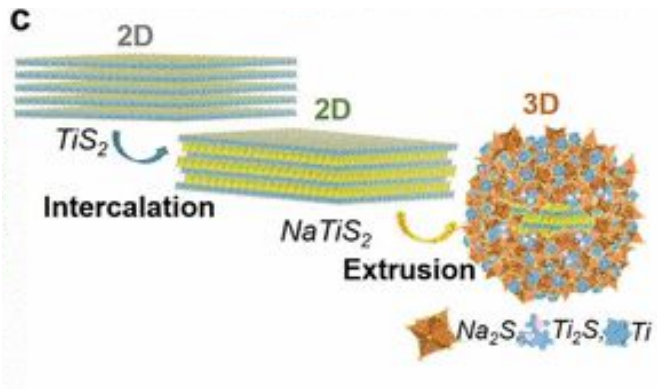
In Situ Electron Microscopy Investigation of Sodiation of Titanium Disulfide Nanoflakes



Morphological evolution during the whole reaction process has been thoroughly studied by *in situ* STEM images: These intercalation reactions are in-plane and will not destroy the Ti−S layered structure, whereas the morphological structure expands from two dimensions to three dimensions during the extrusion reaction. With Na ions' insertion, the inner volume of the particle continues to expand, then induces a morphology deformation

X. Wang, Z. Yao, S. Hwang, Y. Pan, H. Dong, M. Fu, N. Li, K. Sun, H. Gan, Y. Yao, **A. Aspuru-Guzik**, Q. Xu, D. Su, "In Situ Electron Microscopy Investigation of Sodiation of Titanium Disulfide Nanoflakes," *ACS Nano* **13**, 9421-9430 (2019).

Scientific Achievement

The fundamental mechanistic understanding of the sodiation of a two-dimensional metal-sulfide nanomaterial was elucidated. The sodiation process occurs via an intercalation phase, found to have three distinct steps, followed by an extrusion phase which alters the structure from a 2D to 3D morphology.

Significance and Impact

Much emphasis is being placed on the development of sodium-ion batteries (NIBs) as a sustainable energy source, as opposed to lithium-ion batteries; this work presents a fundamental understanding of the *in situ* reaction with an NIB electrode candidate.

Research Details

The sodiation mechanism of TiS_2 nanoflakes was investigated using *in situ* SAED and STEM imaging techniques, complemented with DFT calculations.

- Intercalation remains within the 2D morphology; extrusion, while at a slower reaction speed, alters the shape into 3D.
- First-principles DFT calculations were performed with VASP.

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Work was performed at University of Toronto.

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