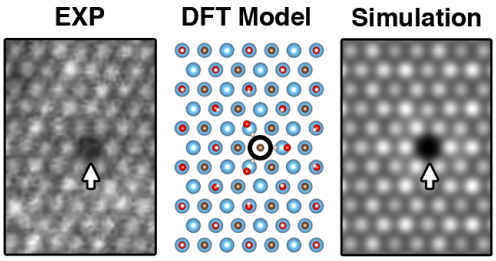
Tuning Defects in Monolayer Titanium Carbide ($Ti_3C_2T_x$) "Mxene" at the Atomic Level

Achievement: Aberration-corrected STEM showed that Ti vacancy density could be controlled by the etchant concentration during preparation of single-layer $Ti_3C_2T_x$ MXene.



Comparison between experimental (EXP) HAADF-STEM image, defect crystal structure from DFT, and simulated HAADF-STEM image of a single Ti vacancy.

Significance and Impact: The presence of defects strongly influences materials properties; thus, a detailed understanding of the MXene single layer structure and point defects is foundational for unlocking physiochemical properties.

Research Details:

- Atomic structure of single-layer MXene $Ti_3C_2T_x$ was investigated using STEM, EELS, and DFT.
- Ti vacancies and vacancy clusters are the primary point defects.
- DFT confirmed defect formation mechanism and revealed surface modification from defects.

Sponsor/Facility: This work was conducted at the Center for Nanophase Materials Sciences, a U.S. Department of Energy (DOE) Office of Science user facility.

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Overview:

The 2D transition metal carbides or nitrides, Mxene phases, are emerging as a group of materials showing great promise in lithium ion batteries and supercapacitors. Until now, characterization and properties of single layer MXenes have been scarcely reported. Here, using scanning transmission electron microscopy (STEM), we determined the atomic structure of freestanding monolayer $Ti_3C_2T_x$ flakes prepared via the minimally intensive layer delamination (MILD) method and characterized the different point defects that are prevalent in the monolayer flakes. We determine that the Ti vacancy concentration can be controlled by the etchant concentration during preparation. Density function theory-based calculations confirm the defect structures and predict that the defects can influence the surface morphology and termination groups, but do not strongly influence the metallic conductivity. Using devices fabricated from single and few-layer $Ti_3C_2T_x$ MXene flakes, the effect of the number of layers in the flake on conductivity has been demonstrated.