2D Crystal Consortium
NSF Materials Innovation Platform

PennState
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MIP: 2D Crystal Consortium
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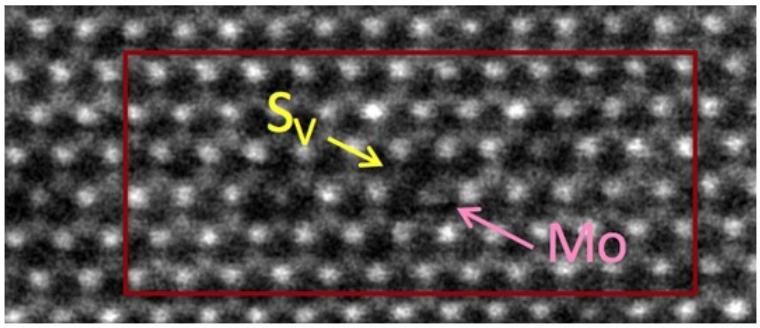
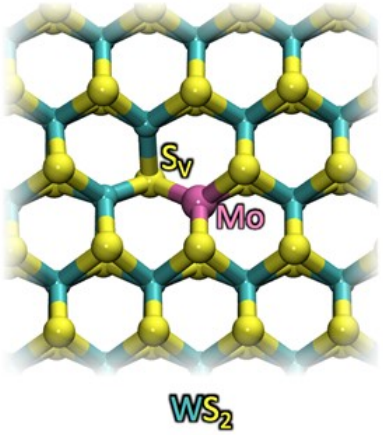
Coupling distinct defect species in 2D crystals





Doping modulates the electronic, chemical, and mechanical properties of materials. For a two-dimensional tungsten disulfide, although an isolated molybdenum substitution only perturbs the host lattice negligibly, it couples strongly to common lattice defects such as sulfur vacancies, as verified by state-of-the-art electron microscopy and atomistic modeling techniques. This coupling can be potentially exploited to controllably segregate undesirable defects away from the active areas of 2D crystalline devices.

NSF DMR DIVISION OF MATERIALS RESEARCH
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Azizi, Wang, Stone, Elías, Lin, Terrones, Crespi, Alem, Penn State

Left Figure Title: Electron Microscope Image.
Left Figure Caption: A sulfur vacancy can be seen to pair with a molybdenum dopant in a electron microscope image.

Right Figure Title: Defect-Pair Structure.
Right Figure Caption: Defect-pair structure is confirmed by quantum chemical calculations as shown in the right panel.

What Has Been Achieved: A new type of strong coupling between isoelectronic substitutional dopants (Mo dopants) and common lattice defects (sulfur vacancies) has been identified in WS2 by their ~80% probability of co-localization using aberration-corrected scanning transmission electron microscopy. The coupling mechanism and the Mo dopant's ability to facilitate the charging of sulfur vacancies is identified using first-principles density functional theory calculations.

Importance of Achievement: Innocuous isoelectronic dopants can act as "vacancy collectors" that attract undesirable vacancies to inactive areas of a 2D chalcogenide device, thanks to their strong coupling with vacancies.

Unique Features of the MIP That Enabled Project: Close collaboration between synthesis, characterization, and theory efforts.

Publication: A. Azizi, Y. Wang, G. Stone, A. L. Elias, Z. Lin, M. Terrones, V. H. Crespi, and N. Alem, "Defect Coupling and Sub-Angstrom Structural Distortions in W1–xMoxS2Monolayers", Nano Lett. 17, 2802 (2017).

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