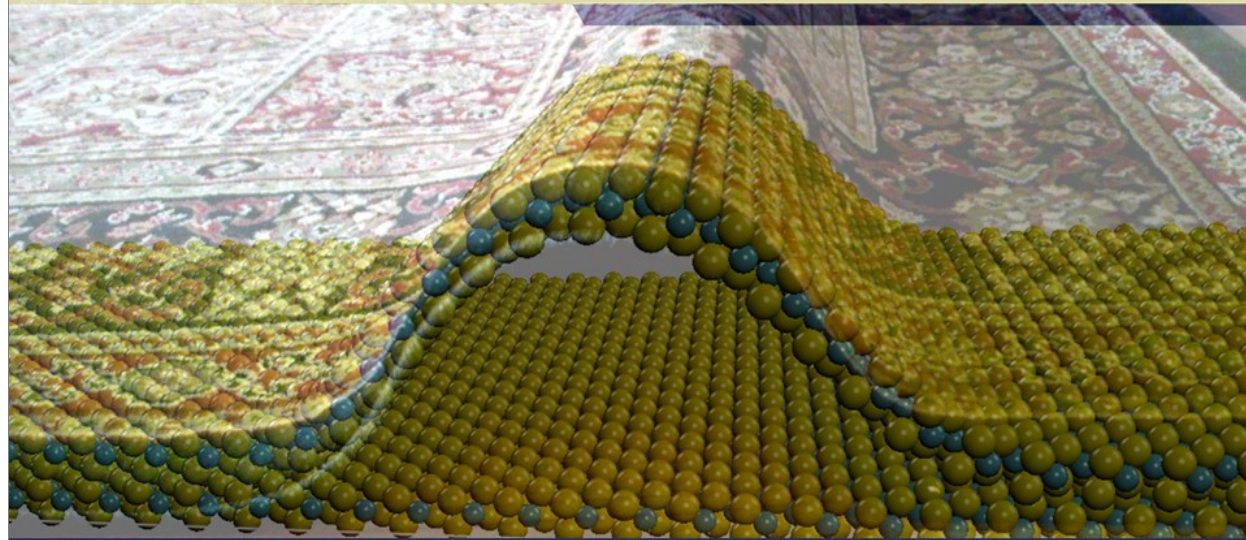



MIP: 2DCC at Penn State University
DMR-1539916, CMMI-1462980

Can ripples in monolayer sheets “sweep out” unwanted defects?

2017



Atomically thin two-dimensional layers such as molybdenum disulfide, MoS₂, are promising materials for nanoelectronics due to their exceptional electronic and optical properties. An inter-atomic potential has been developed that can accurately describe the thermodynamic and structural properties of MoS₂ sheets, including defects and transitions between different structural phases. A new type of “ripple” defect has been identified as a favorable host for sulfur vacancy defects. A train of moving ripplocation defects may be able to “sweep out” sulfur vacancy defects from key regions within 2D devices.



DMR DIVISION OF
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Ostadhossein, Rahnamoun, Wang, Zhao, Zhang, Crespi, van Duin, Penn State

Figure Title: Can ripples in monolayer sheets “sweep out” unwanted defects?

Figure Caption: Atomistic rendering of a ripplocation defect within a single MoS₂ layer that sits on a lower, flat layer also composed of MoS₂. The upper layer has three extra unit cells of material, hence the tendency to buckle upwards in a ripple-shaped defect.

What Has Been Achieved: The new ReaxFF reactive potential developed for this project accurately describes both equilibrium properties and also mechanical deformations and structural defects within MoS₂, a promising material for nanoelectronics. A new type of “ripple” defect has been identified as a favorable host for sulfur vacancy defects.

Importance of Achievement: Since sulfur vacancy defects have lower energy when they reside within the ripple, it may be possible to transport these defects by transporting the ripple across the 2D layer through controlled mechanical deformations that create a pulse train of propagating ripplocations. Sulfur vacancies degrade the properties of 2D devices, so a means to remove them from key regions of a device may prove useful in the long term. In a broader sense, this new reactive interatomic potential provides a means to model structural fatigue, defect mobility, mechanical response, and other properties of transition metal dichalcogenide systems much more efficiently than is possible with more computationally intensive first-principles methods..

Unique Features of the MIP That Enabled Project: Tight coupling of cross-disciplinary theory in both first principles and empirical methods.

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