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New Theory Tools for Modeling Growth of TMD Materials

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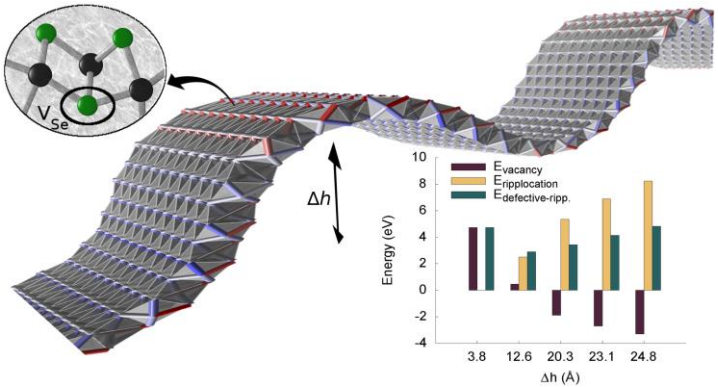
Project Summary: The first ReaxFF force field developed for 2D-WSe_2 provides the community with a highly efficient means that describe material growth, phase transitions, defect formation and migration and thus can provide valuable atomistic insights into experimental efforts on growth, phase, and defect engineering as a function of the local chemical environment. This potential can elucidate further the morphological evolution of monolayers in different environments in terms of loading conditions and defect concentrations/distributions. Interactions between vacancies and ripples in a 2D layers ("ripplocations") suggest that vacancies could stabilize buckled structures by modulating the strain energy and possibly open a venue for sweeping out undesirable defects such as vacancies from 2D WSe_2.



$MoSe_2$ and WS_2 force fields were also trained and will be made available to the 2D community. A new ReaxFF potential for TMD heterostructures ($W_xMo_{1-x}S_ySe_{2-y}$ where x=0–1, y=0,1,2) is under active development to enable simulations for the growth of in-plane and vertically stacked TMD heterostructures to understand how defects and grain boundaries impact nucleation, domain orientation, lateral growth and chalcogen/metal exchange.

2DCC Role: The 2DCC Theory/Simulation/Data facility has developed three different ReaxFF potentials for WSe_2, $MoSe_2$, and WS_2 by training against extensive first-principles data on periodic and non-periodic systems. The 2DCC Experiment/Characterization facility has also provided data to validate the performance of the new potentials.

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