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Activation Energies of Rotational Defects in 2D Transition Metal Dichalcogenides[1] ANTHONY YOSHIMURA, MICHAEL LAMPARSKI, NEERAV KHARCHE, VINCENT MEUNIER, Rensselaer Polytechnic Institute —
Owing to their outstanding electrical and optical properties, two-dimensional (2D) transition metal dichalcogenides (TMDs) are promising for a wide array of applications in electronics, photonics, and energy harvesting. As with any material, 2D TMDs are subject to structural defects, which can modify their physical properties. It is therefore important to understand the conditions in which these defects can occur. Here we examine a rotational defect in the pristine trigonal-prismatic TMD lattice, arising from a 60-degree rotation about the surface normal of the bonds of a transition metal atom. The resulting structure is a three-fold symmetric set of three 8-membered rings subtended by the central transition metal. This defect has been recently observed in WSe_2, WS_2 and $MoSe_2$. Using density functional theory (DFT), we calculate the activation energy for these defects in several TMDs: MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2, and WTe_2. We find that the activation energy of the defect depends primarily on the chalcogen species, with sulfur having the largest and tellurium the smallest. Furthermore, we find that the chalcogen species also determines the defects thermodynamic stability, with tellurium being the most stable and sulfur the least.

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