Defects in two-dimensional transition metal dichalcogenides: From vacancies to substitutional random alloys

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Transition metal dichalcogenides (TMDs) are a class of layered materials, similar to graphite and BN, with promising future in nanoelectronic and photonic applications. Due to recent advances in succesful production of two-dimensional monolayers they have started to attract considerable attention. In order to take full advantage of the promise of these materials, a good control over the defect production is required. In particular, defects could be produced intentionally during chemical vapor deposition growth or by ion irradiation, whereas unintentional production may be expected during transmission electron microscope (TEM) imaging.

In this work, we first investigate vacancy formation under electron irradiation in TMD materials. Displacement thresholds are evaluated from molecular dynamics calculations and compared to the experiments in the case of S vacancy formation in MoS_2 [1]. Isolated vacancies are stable, but with increasing exposure and vacancy concentration, they are found to agglomerate to form lines. With the help of first-principles calculations, we determine their atomic structure and also discuss possible formation mechanisms.

Filling of the vacancies is observed in TEM images. Thus, we examine chalcogenide substitution processes within these materials. Substitution by other atomic species is found to be energetically favorable, thereby suggesting a way for doping of these materials [1]. Finally, as extended substitution by isoelectronic ions leads to alloying, we study the stability and electronic structure of alloys consisting of MoS_2, $MoSe_2$, and $MoTe_2$ [2].

[1] H.-P. Komsa et al., *Phys. Rev. Lett.* **109**, 035503 (2012).
[2] H.-P. Komsa and A. V. Krasheninnikov, *J. Phys. Chem. Lett.* **3**, 3652 (2012).