Understanding the electronic properties and mechanisms of formation of 1D defects observed in 2D MoS_2

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Defects in 2D semiconductors exist either in the dilute limit, or can form lines or clusters. Their nature can critically determine the electronic structure of their host material. The most effective way to image defects at atomic resolution is using a scanning transmission electron microscope (STEM) with aberration correction and 4D STEM acquisition with ptychographic processing. This latter technique can determine the location of the atoms with great precision, down to a few pico-meters. However, STEM imaging can induce defects over time due to the impact of the high energy beam on the sample. We have identified several defects in 4D STEM images of pristine and rhenium doped monolayer MoS_2 samples. We use density functional theory (DFT) with a non-local PBE0-TC-LRC functional in order to calculate the electronic properties of 1D defects including sulphur vacancy lines, kinks and rhenium (which substitutes molybdenum) lines. We find that vacancy aggregation results in areas of increased electron density localized at the line defect sites and observe an increase in the number of defect states present when the 'kink' limit is reached. Whilst the rhenium dopant lines have potential for high spin states (quartet) which could induce ferromagnetism in the material. We predict some of the defects we observe are nucleation sites for the 1T phase, with metastable, mobile, sulphur interstitial-like atoms. There is a small (approx. 0.1 eV) energy gain from the clustering of sulphur vacancies. Using nudged elastic band calculations with the PBE functional we calculate different pathways for vacancy migration which can lower the barrier and make defect clustering more favourable, considering effects of dopants and different charge states. This work gives insight into creation of 1D defects in MoS_2 and their potential for uses in doping.

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