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

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Defects in 2D semiconductors play an important role in their electronic properties [1]. In 2D materials, defects are often present at high concentrations of 10^{13} cm^{-2} and therefore are an important area of research for understanding the properties of 2D materials. An effective way to observe defects in 2D TMDs such as MoS_2, is by using a 4 dimensional scanning transmission electron microscope (4D STEM), which allows access to atomic resolution. In this work, we combine ptychography-reconstructed 4D-STEM [2,3] datasets, of defects in 2D MoS_2, and use density functional theory (DFT) to understand the origin and dynamics of these defects. The datasets show that point defects aggregate into 1D defect lines. We employ density functional theory (DFT) with a non-local PBE0-TC-LRC functional in CP2K 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. The rhenium dopant lines have potential for high spin states (quartet) which could induce ferromagnetism in the material. We observe a relatively small energy gain from the clustering of sulphur vacancies into lines (of around 0.1 eV). Using nudged elastic band (NEB) calculations with the PBE functional, we calculate the most likely pathways for vacancy diffusion including effects of different charge states on the dynamics of the vacancies. We find that charged di-vacancies have a very low barrier for diffusion which can allow for rapid diffusion as observed with 4D STEM. This work gives insights into the dynamics of defects in 2D MoS_2 and their potential for use in doping.

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