Atomic structure of defects in 2D materials

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The presence of defects and dopants in 2D materials influences their properties and therefore understanding their atomic structure is important for accurate predictions of their behaviour. In this talk I will discuss recent work on resolving the atomic structure of defects in the monolayer transition metal dichalcogenides (TMDs) MoS₂ and WS₂ using aberration corrected transmission electron microscopy. The aggregation of individual sulphur vacancies results in line defects that have compression and strain the local lattice. These can stack up to form larger regions of sulphur deficient 2D material. I will discuss the analysis of bilayer TMDs and reveal the detailed structure of 2H and 3R stacking phases and the impact this has on the defect migration and reconstruction. The edges of monolayered 2D WS₂ and MoS₂ are also imaged and we resolve the reconstruction that occurs from the dangling bonds. Dopants are identified in the lattice by variations in contrast in the metal sites and also in the S sites.