Excited states of charged defects in 2D semiconductors

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Charged defects in semiconductors give rise to in-gap states with a hydrogenic character. Because of the slow decay of the screened defect potential, the spatial extent of these states can be very large making first-principles calculations highly challenging. We have developed an atomistic approach to study defect states in supercells containing thousands of atoms: in particular, we first use linear-response theory to calculate the screened defect potential and then employ a large-scale tight-binding model to calculate the electronic structure. We have used this approach to study charged defects in MoS_2 and discovered an intriguing interplay of the different valence and conduction band valleys that gives rise to hybridized states, some of which have a resonant character (see Fig. 1). Our predictions were verified by STM experiments. We also developed technique to study the effect of charged defect on optical properties: for this, we solve the Bethe-Salpeter equation and find new low-energy peaks in the absorption spectrum. The energies of these peaks are in good agreement with experimental findings.

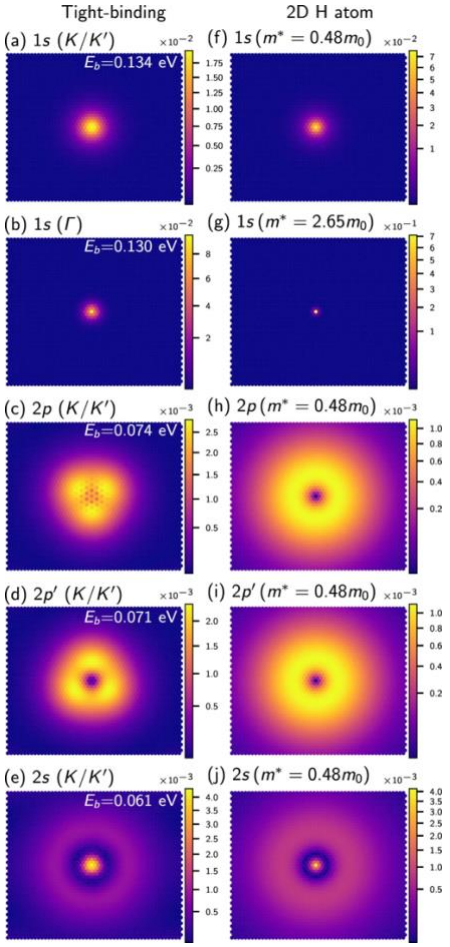

Figure 1: Hydrogenic defect states in monolayer MoS_2.

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