

Materials Day

Understanding rare earth point defects in MoS₂

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Abstract: Rare earth point defect in 2D materials such as MoS₂ have recently attracted interest for use as single photon emitters. However, the defect chemistry of rare earth dopants is not well studied. In this poster, we investigate the formation energies and electronic properties of various types of point defects in these systems. We show that apart from the expected f-electron states in the gap, there are other states that originate from hybridization between host and rare earth states. We discuss the generality of the findings, particular the potential impact on the optical properties and the consequences for downfolding methods.