Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Webinar

Electronic Structure of Y-doped H-MoS_2 in Isolation and in Conjunction with Au(111) Surface

Arpita Sen

TIFR, Hyderabad

MoS_2 is a promising material in electronic devices due to several tunable properties. Experimentally, doping H-MoS_2 with Yttrium (Y), where Y replaces Mo atoms, at various concentrations in a heterojunction with Au(111) changes the Schottky barrier. After confirming with CI-NEB calculations that Y-doped mono-layer H-MoS_2 is sufficiently stable, we built a heterostructure with Au(111) surface and calculated the Schottky barrier. We also computed the change in electronic structure of Y doped H-MoS_2 as a function of the doping percentage.

Wednesday, May 13th 2026

09:30 Hrs