

Abstract Submitted
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Adsorption of Fluorine on single layer MoS₂: a first principles study¹ CONRAD TROHA, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — One of the effective methods for tuning properties of single layer MoS₂ is to impose interactions with adsorbates. Using density functional theory, with the optB88-vdW exchange correlation functional, we have studied the adsorption of fluorine atoms on a single layer MoS₂. We find that fluorine atoms prefer to adsorb on top of sulfur atoms in (2×2) , (3×3) , and (4×4) overlayer structures and that at $1/9$ ML or smaller coverage, the interactions between fluorine atoms are small and can be ignored. The band structures of the considered overlayer structures suggest that the adsorption of fluorine atoms introduces defect state inside the band-gap of MoS₂. This state disperses near the Fermi level in the (2×2) overlayer structure and is dispersionless in the (3×3) or larger overlayer structures.

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