Janus like SnWS structure and hybridized in-gap states

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Exotic quantum properties are predicted for two-dimensional (2D) derivatives of atomic tin (Sn), mainly planar or buckled hexagonal lattice called stanene. An appropriate choice of substrate is very crucial to realize 2D growth of Sn due to its large core size that prefers sp 3 hybridization over sp 2 . Transition metal dichalcogenides (TMDs) like MoS 2 or WS 2 with honeycomb lattice structure are predicted to be promising substrate candidates in this regard. We report here room temperature (RT) growth of atomic Sn under ultrahigh vacuum (UHV) conditions on the mechanically cleaved WS 2 surface and investigate the surface morphology and local electronic properties of bare WS 2 , as well as Sn/WS 2 surfaces by performing in-situ scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and first principles density functional theory (DFT) studies. Our investigations reveal an atomically flat WS 2 surface with valence band (VB) maxima at the Γ point and conduction band (CB) minima between the K-Γ line with the band edges lying at -0.2 eV and 1.19 eV respectively. Thus, an indirect band gap of 1.39 eV is demonstrated theoretically for the pristine bulk WS 2 when defects or vacancies are not consid ered. Upon considering `S' vacancies in the calculations, that are evident on the WS 2 surface during STM investigations, we find signature of in-gap electronic states directly corroborating the STS results obtained from bare WS 2 with `S' vacancies. STM studies on RT growth of Sn indicate monomer like commensurate or dimer like nearly commensurate adsorption at the `S' sites with a buckling height of 40 ± 10 pm [1], whereas emergence of modulated in-gap states are detected in the measured local density of states (LDOS) by STS [2]. These experimental observations are quantified by the DFT calculations considering substitutional doping of Sn atoms at the `S' sites revealing emergence of Janus like SnWS structural forms with a buckling height of 80 pm. Calculations also reveal Sn p and W d hybridized in-gap states that are observed in the STS measurements [2].

References

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