STS and DFT studies on atomic adsorption of Sn on the WS_2 surface

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With enormous research interest presently being focussed on to fabricate various two-dimensional (2D) derivatives of atomic tin (Sn), mainly planar or buckled hexagonal lattice called stanene, it is of fundamental importance to study their structure, local electronic properties and hybridization with the substrates. 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 points 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 considered. Upon considering `S' vacancies in the calculations, that are evident on the $WS_2$ surface in the 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 commensurate or nearly commensurate adsorption at the `S' sites with a buckling height of 40 ±10 pm, whereas, emergence of modulated in-gap states are detected in the measured local density of states (LDOS) by STS. These experimental observations are quantified by the DFT calculations considering substitutional doping of Sn atoms at the `S' sites that exhibit a buckling height of 80 pm. The calculations also reveal Sn *p* and W *d* hybridized in-gap LDOS as are observed in the STS measurements.

References

[1] Manu Mohan, Vipin Kumar Singh, Reshmi S., Sudipta Roy Barman, Kuntala Bhattacharjee, Atomic adsorption of Sn on mechanically cleaved WS_2 surface at room temperature, Surf. Sci. **701** 121685 (2020).
[2] Manu Mohan, Vipin Kumar Singh, Reshmi S., Mihir Ranjan Sahoo, Sudipta Roy Barman, Kuntala Bhattacharjee, Local hybridized states of adsorbed atomic Sn on WS_2 substrate, Appl. Surf. Sci (under consideration).

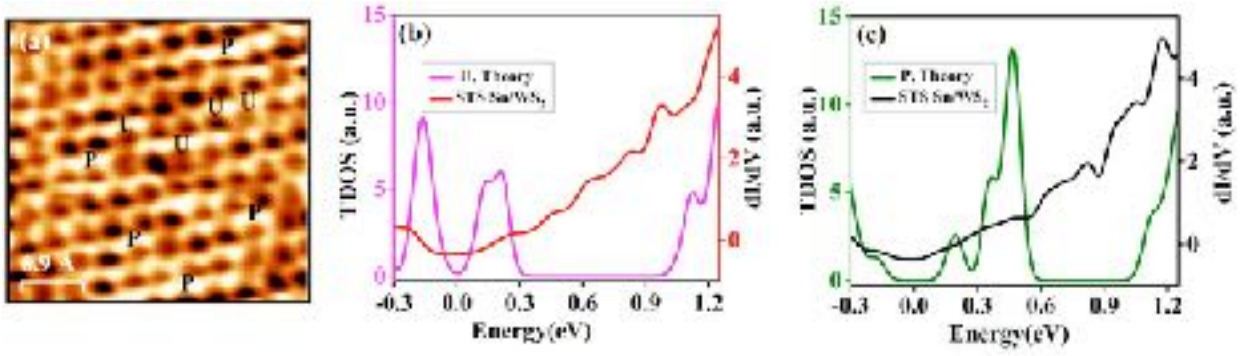

Fig.1. *(a) STM image of Sn adsorbed WS_2 surface. 'P' and 'U' represent dimer and monomer adsorption of Sn respectively. STS data taken on (b) 'U' and (c) 'P' configurations along with the corresponding calculated TDOS are shown.*