# LOCAL ELECTRONIC STATES OF ATOMIC TIN (Sn) GROWN ON TUNGSTEN DISULFIDE ($WS_2$) SURFACE

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*By*

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# ABSTRACT

The exfoliation of graphene from graphite led to the new area of research in physics and material science known as two-dimensional materials (2DM). Today, the class of 2DM is constituted by different materials like transition metal dichalcogenides (TMDs), monoelemental Xenes, hexagonal boron nitride (hBN) etc. These materials show superior structural and electronic characteristics which makes them important in the field of electronics and optoelectronics. Different exotic properties like Quantum spin Hall effect (QSH), Quantum anomalous Hall effect (QAH), topological properties, presence of mass less Dirac fermions, spin orbit coupling (SOC) induced electronic properties etc. demonstrated by these materials forced current research to look for new low dimensional candidates with distinctive structures and intriguing properties.

Atomic layers of Sn have drawn immense interest recently owing to their structurally driven quantum nature and novel properties. The practical realization of extended flawless two-dimensional (2D) sheets of Sn remains a challenge even with today's sophisticated fabrication techniques and depends largely on the substrate. The synthesis of 2D Sn like stanene and other allotropes of Sn have obtained special deliberation lately due to exceptional physical properties predicted and many of these anticipated properties have recently been demonstrated successfully. However, practical realization of 2D Sn in buckled or planar form largely relies on the choice of the substrate due to preferred $sp^3$ hybridization over $sp^2$ owing to the large core size which can influence the physical properties. Therefore, the choice of substrate for 2D Sn growth is very critical.

Transition metal dichalcogenides (TMDs) such as $WS_2$ with honeycomb lattice and thickness dependent tunable electronic properties is proposed to be a suitable substrate candidate for the growth of Sn and its 2D derivatives. Recent studies on TMDs reveal tuning of physical properties by engineering materials configuration via doping of foreign atoms. Doping of foreign atoms into the TMD layers can lead to the formation of Janus forms of 2D TMDs, which can have fascinating properties. The successful experimental

realization of Janus TMDs via substitutional doping have been reported recently. Motivated by these different strategies for tuning the different properties of materials, we have carried out our work of the growth of Sn on $WS_2$ substrate.

In this thesis, we study the growth of Sn and the local electronic properties of Sn grown $WS_2$ surfaces by in-situ scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and first principles density functional theory (DFT) calculations. Our investigations suggest substitutional doping of Sn at the S sites, with Sn atoms occupying a slightly elevated position of 80 pm on the $WS_2$ surface. These results agree well with our STM observations on room temperature growth of atomic Sn, indicating commensurate or nearly commensurate adsorption at the S sites with a buckling height of 40 ± 10 pm. This is a case of substitutional doping of Sn mostly indicating emergence of Janus like SnWS structural form. Pristine $WS_2$ without any S vacancies on the surface exhibits a bandgap of 1.39 eV, while ingap local density of states comprised of W *d* and S *p* orbitals are detected when S vacancies are considered. Upon adsorption of Sn atoms, we find the signature of modulated hybridized ingap electronic states of Sn *p* and W *d* orbitals with a spin orbit coupling interaction up to 38 meV at the K point of the Brillouin zone. These results throw important light on the future fabrication of Janus like SnWS vertical heterojunctions with atomic level doping accuracy, which will have enormous device applications.