Estimation of the Charge Carrier Density of Transition Metal Dichalcogenides (TMDs) by X-ray/Ultraviolet Photoelectron Spectroscopy

Abstract: 2D materials beyond graphene such as Transition metal dichalcogenides (TMDs) have gained tremendous attention due to their excellent properties much work has been done for the development of next generation TMDs based electronic and optoelectronic devices. Many of the key electronic parameters such as work function, concentration of charge carries, density of states are calculated through density functional theory (DFT) based simulations and are utilized for experimental findings. The reports demonstrate for the first time, the experimental determination of electronic properties and the pristine band structure for the family of TMDs materials (MoS_2, $MoSe_2$, $SnSe_2$, $MoSe_2$, SnS, $NiSe_2$) using sophisticated Ultraviolet Photoelectron Spectroscopy (UPS) technique. Further, utilizing the hall effect measurements, effective masses have been experimentally approximated and utilized for estimating the carrier concentration for all pristine TMDs. Successful demonstration of the experimental extraction of the electronic properties of all TMDs would provide a detailed understanding of the band structures and further band alignment and to develop more optimized 2D TMDs based electronic and optoelectronic devices.

Introduction

Transition Metal Dichalcogenides (TMDs) are post graphene 2D materials which have gained significant interest in the electronics and material science research community due to their excellent optoelectronic properties especially the modulation of the bandgap with the number of layers. Even though these materials have been extensively synthesized and utilized at device level for various exciting applications, basic electronic properties are not well reported and most of values in literature are through density functional theory based first principle simulations. Most of the work reported on the 2D materials based photodetector display the band structure and the values such as work function, electron affinity etc. are either estimated or simulated values. This certainly create a bit of ambiguity as these values depend a lot of factors such as synthesis procedure, temperature, oxygen content and substrate etc. and hence cannot be taken as simulated values. Understanding and experimentally extracting the basic electronic properties and further the carrier concentration is essential to better understand the transport and physics of the fabricated device.

X-ray and Ultraviolet Photoelectron Spectroscopy is a strong analytical tool to (please elaborate about the XPS and UPS technique here, at least ¾ page). Write the basic of how UPS estimates it (not the procedure) but the actual physics (like knocking the electron from the outer shell etc etc.)

(Last paragraph is what we did)

Experimental

(Add the details of the synthesis procedure)

Results and Discussions