# The electronic structure of Indium-Tin-Oxide/$MoS_2$ interface


Oscar A. López-Galán*[1], Manuel Ramos*[1], John Nogan[2], Torben Boll[3,4], Martin Heilmaier[3]

[1]Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, 450, Av. del Charro, Cd. Juárez, CHH, México.
[2]Center for Integrated Nanotechnologies, 1101 Eubank Bldg. SE, Albuquerque, NM 87110, USA
[3]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Engelbert-Arnold-Str. 4, D-76131 Karlsruhe, Germany
[4]Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany.

## Introduction

Molybdenum Disulfide-Indium Tin Oxide ($MoS_2$/ITO) heterojunctions were studied under the DFT scheme based on experimental evidence on the formation of an abrupt heterojunction between $MoS_2$ and ITO[1].

The development of high-performance electronic devices based on 2D semiconductors require the formation of reliable ohmic contacts. Schottky barrier (SB) formation is a key parameter that determines the transport phenomena at the interface. Reliable ohmic contacts require low values of SB.

Numerous works report the lack of reliable ohmic behavior in metal-$MoS_2$ interfaces due molybdenum electronic disruption and the formation of SB[2,3]. Recently, Li et al.[4] and by Gao & Gupta[5] report the fabrication of trustworthy ohmic contacts by using titanium carbide and titanium disulfides as contact material with transition metal dichalcogenides like $MoS_2$ and $WS_2$.

We predict the formation of consistent ohmic contacts with SB of around -5.0 eV at the $MoS_2$/ITO van der Waals interface [6,7]. Electronic structure indicates little electron orbital hybridization without the disruption of molybdenum electronic structure by the ITO which commonly found in metal-$MoS_2$ leading to poor ohmic contacts.

Our calculation were based on experimental evidence of $MoS_2$/ITO interface prepared by RF sputtering and characterized by APT. XRD shows the presence of (002) preferential growth in both 2H and 3R $MoS_2$ phase[1].

## Methods

- DFT + CASTEP code within the Materials Studio Suite 2018.
- GGA + RPBE
- ITO ($In_2Sn_2O_7$) in the (222) and (400) planes.
- $MoS_2$ (2H and 3R phases) in the (002) plane.
- Interfaces were modelled by placing a 2H/3R $MoS_2$ surface atop of (222)/(400) ITO

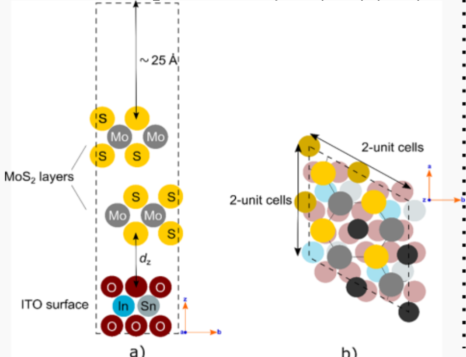


Figure 1. Schematic of the interfaces modelled.

## Results

- All the interface models behave as a van der Waals heterojunction lacking any chemical bonding between ITO and $MoS_2$ with an equilibrium distance ($d_{eq}$) of ~3.0 Å (see Table 1).
- The $n$-type SBH is defined as $\Phi_n = E_g - \Phi_p$ where $E_g$ is the band gap of $MoS_2$, measured with respect to the vacuum level. $\Phi_p = E_V - W_{ITO} + \Delta_{ps}$. $E_V$ is the valance band position, $W_{ITO}$ the work function of the ITO surface and $\Delta_{ps}$ the potential dipole at the interface.
- SB estimation at the $MoS_2$/ITO interface is resumed in Table 1.

Table 1: Resulted equilibrium distance between $MoS_2$ and ITO ($d_{eq}$) and estimated p-type and n-type Schottky barrier labelled as $\Phi_p$ and $\Phi_n$, respectively.

| Interface | $d_{eq}$/Å | $\Phi_p$/eV | $\Phi_n$/eV |
|---|---|---|---|
| ITO222/2H$MoS_2$ | 3.0 | 7.45 | -5.65 |
| ITO222/3R$MoS_2$ | 3.1 | 7.50 | -5.70 |
| ITO400/2H$MoS_2$ | 3.14 | 7.0 | -5.19 |
| ITO400/3R$MoS_2$ | 3.5 | 7.01 | -5.19 |

- Low values of $\Phi_n$ predicts the formation of ohmic contacts at the $MoS_2$/ITO interface.
- By determining the electronic structure, we attribute negative $\Phi_n$ to the low hybridization between ITO and Mo-S orbitals.

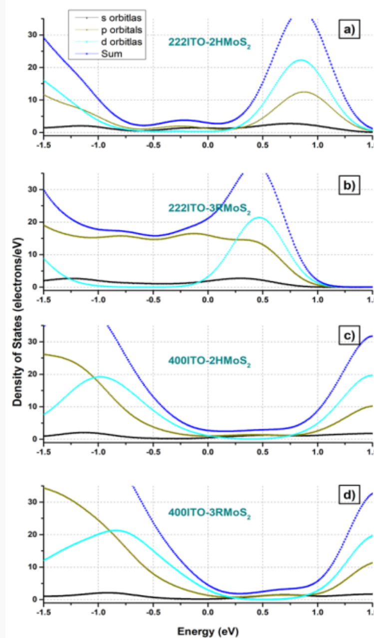


Figure 2. Calculated Density of States for the a) ITO222-2HMoS2, b) ITO222-3RMoS2, c) ITO400-2HMoS2 and d) ITO400-3RMoS2 models

- From Figure 2 we observed low insertion of states around the Fermi level indicating a minimal hybridization process between ITO orbitals and Mo-S orbitals.
- Expected low presence of metal-induced gap states (MIGS) due semiconducting character of ITO and the low density of states around the Fermi level.
- Contribution from d orbitals remains low around the Fermi level an increase rapidly at the upper and bottom part of the $MoS_2$ band gap.
- In contrast, p orbitals have a considerably higher contribution to the density of states around the Fermi level. Their contribution became less dominant at the extremes of the band gap.
- Metal contact disturbs the electronic distribution of sulfur atoms weakening the Mo-S bonding which resulted in an increase of d orbitals density around the Fermi level coming from Mo[2].

## Conclusions

- In this work we predict the formation of Ohmic contact at the $MoS_2$/ITO interface by means of DFT through CASTEP code based on experimental evidence.
- By determining the density of states of the van der Waals interfaces modelled we concluded that the low insertion of states around the Fermi level leaves almost undisrupted Mo and S orbitals allowing a high carrier injection from ITO to $MoS_2$.
- Achieving ohmic contacts at interfaces comprising 2D semiconductors like $MoS_2$ is crucial for successful integration of such materials in high-efficiency next generation electronic devices, like solar cells, high-speed devices, and self-powered devices.

## Acknowledgements


This work is supported by Universidad Autónoma de Ciudad Juárez for licensing BIOVIA Materials Studio 2018 and providing high performance computing facilities. Authors thanks CONACyT-Mexico for graduate scholarship (#735528). Special thanks to CINT for providing access to RF sputtering equipment under contract #2019BU0090. Author appreciate the support of KIT for APT characterization.


## References


[1]MRS Communications, 9(4), 1261-1266, 2019
[2]Nano Lett, 14 (4), 1714–1720, 2013
[3]Nat Mater, 14 (12), 1195-1205. 2015
[4]Carbon, 135, 125–133, 2018
[5]NPJ 2D Mate & Appl, 4 (1), 26-31, 2020
[6]Appl Phys Lett, 108 (8), 2016
[7]Nanomaterials, 10 (3), 579-585, 2020


## Contact us


*oscar.lopez@uacj.mx
*manuel.ramos@uacj.mx