# $MoSe_2/MoS_2$ type I heterojunction deposited by RF-sputtering for photovoltaics applications

Oscar A. López-Galán[1], Manuel Ramos[1], John Nogan[2], Torben Boll[3,4], Martin Heilmaier[3], Roberto C. Ambrosio[5]

[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.
[5]Facultad de Electrónica, Benemérita Universidad Autónoma de Puebla, Puebla, México.

## Introduction

We obtained molybdenum disulfide - molybdenum diselenide ($MoS_2/MoSe_2$) heterojunctions whereby RF magnetron sputtering using ITO as transparent top and contact material and using $Si/SiO_2$ substrate.

Numerical modelling of current vs voltage shows that these heterojunctions performed close to the ballistic regime of electron transport.

These materials has potential application in electronic devices as active layer due to the low dimensions and the conservation of their electronic properties [1].

## Methods

- **RF-sputtering** at 275 W using 99.9% purity targets of $MoS_2$ and $MoSe_2$.
- **Deposits** of $MoS_2$ and $MoSe_2$ at 150 nm, 250 nm, and 350 nm.
- **CASTEP** code was used for all **DFT-D2** calculations.
- **GGA + RPBE** exchange-correlation functional.
- **Landauer approach** describe the electron transport throughout the heterojunction.

## Results

- $MoS_2/MoSe_2$ heterojunctions deposited at 250 nm presents a higher crystallinity compared to the deposits made at 150 nm and 350 nm (Figure 1.)
- Comparing the simulated and experimental XRD spectroscopy, shows that in our obtained heterojunction exist both lateral and Van der Waals unions between $MoS_2$ and $MoSe_2$.

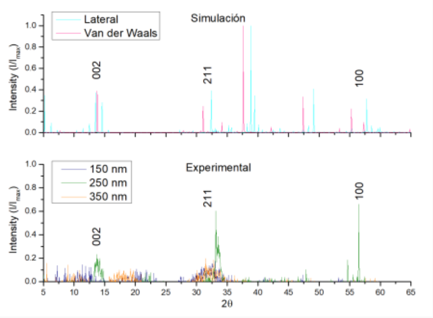


Figure 1. XRD spectroscopy of the samples deposited at 150 nm, 250 nm, and 350 nm.

- SEM micrographs confirm the obtention of stacked layers of ITO, $MoS_2$, and $MoSe_2$.

EDS mapping shows a clear and uniform distribution of the constituent parts of the heterojunction, achieving a vertical stacking which is highly desirable in photovoltaic applications

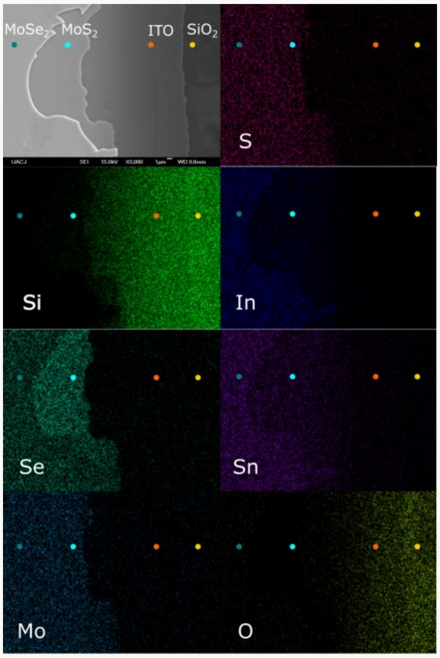


Figure 2. SEM micrographs and EDS element mapping of the obtained heterojunction.

We estimated the band alignment between $MoS_2$ and $MoSe_2$ finding a type I alignment. This arrangement confines charge carriers in the low-band gap material. Figure 3 shows the drain to source current ($I_{DS}$) as a function of a gate voltage ($V_G$) modeled using the Landauer approach. We consider that the device uses three different threshold voltages ($V_T$), -10 V, -5 V, and -1 V. using parameters of previous devices [4,5].

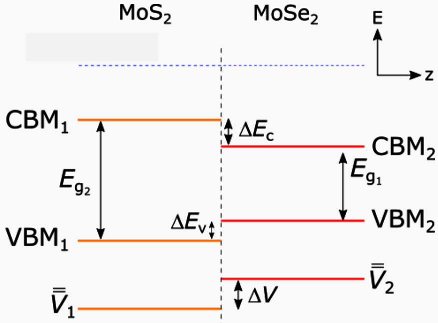


Figure 2. Schematic of land alignment of the obtained heterojunction.

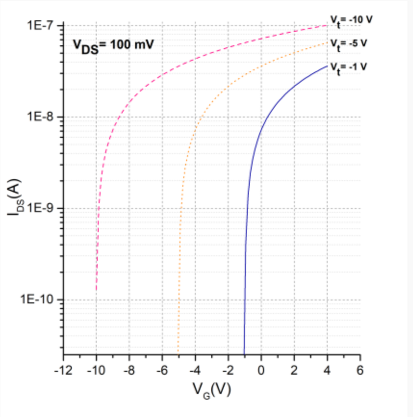


Figure 3. Drain to source current as a function of a gate voltage at different threshold voltages.

## Conclusions

- $MoS_2/MoSe_2$ heterojunctions deposited at 250 nm have a higher crystallinity.
- **SEM and EDS** show a uniform deposition of ITO, $MoS_2$, and $MoSe_2$ in a vertical architecture
- **Landauer approach** and **ballistic transport regime** describes the charge phenomenon in the $MoS_2/MoSe_2$ heterojunction.
- **Band alignment** analysis indicates the potential application of such material in photovoltaic applications.

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