The University of Texas at San Antonio

UTSA Physics and Astronomy

Solar cells using 2H-MoS_2 and beyond!

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Dr. Manuel Ramos

Molybdenum disulfide (MoS_2) has been intensively studied over the past 20 years. Chemist Linus Pauling first reported its chemical structure by proposing a series of two-dimensional sheets stacked by weak van der Waals interactions. The mineral was first used as a lubricant to prevent wear on mechanical parts and as a "workhorse" in the catalytic process known as crude oil hydrodesulfurization and, more recently, in the field of nanoelectronics. This talk will provide a comprehensive overview of the exceptional properties of this low-dimensional material, with particular emphasis on the electronic structure upon interaction with indium tin oxide (ITO), using theoretical and experimental data from ITO RF sputter deposits 2H-MoS_2 thin films (100–300 nm). In addition, the talk presents data from I-V curves, atom probe tomography (APT), scanning and transmission electron microscopy, and density functional theory (DFT) calculations. Microscopy shows that the ⟨110⟩ orientation is aligned perpendicular to the ITO film with the main reflections at (002), (100), (101), (201). APT detects MoS^{+2} and MoS^{+3} as the primary evaporated molecular ions, indicating no significant diffusion/segregation of Mo or S species within the ITO layer. DFT calculations suggest that ITO and MoS_2 form a Schottky barrier. Thanks to d-orbital interactions that create an ohmic contact with the n-type Schottky barrier height (Φ_n) of −1.6eV for 2H and −1.2eV for 3R MoS_2 and contact resistance of ~1cm^2 when in contact with transparent ITO, MoS_2 can achieve 2.48% conversion efficiency measured in the proposed hybrid organic semiconductor solar cell prototype.

Bio: Prof. Dr. Manuel Ramos is a Mexican-American native of Ciudad Juárez and a full-time professor in the Department of Physics and Mathematics at the Autonomous University of Ciudad Juárez. He was a research assistant at the National High Magnetic Field Laboratory in Tallahassee, FL, a Research Professor at the Materials Institute of UTEP, and is currently a visiting researcher at the Center for Integration of Nanotechnologies of Sandia National Labs at Albuquerque, NM, and Karlsruhe Nano and Micro Facility in Germany. His area of research combines theory and experiment to study the structure/functionality of energy and catalytic materials. He is the author of 35 peer-reviewed manuscripts and conference proceedings. He has been a member of the National System of Researchers of CONACyT-Mexico since 2010. From 2013 to the present, he has served as co-organizer and director of the Advanced Catalytic Materials Symposium held within the framework of IMRC, a joint scientific meeting between the Mexican Society of Materials and Materials Research Society (USA). In addition, he has served as special editor for the Journal of Materials Research, Catalysis Today, MRS Advances, and Springer Book Series. He is a peer reviewer for more than 20 JCR journals.

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