جامعة عبد المالك السعدي
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Université Abdelmalek Essaadi

Pole for Doctoral Studies
Center for Doctoral Studies Sciences, Technologies, and Medical Sciences

ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE

Centre des Etudes Doctorales Sciences et Techniques et Sciences Médicales

Ms. ZIANI Hanan

Will present their research work with the aim of earning a Doctorate

Doctoral program: Mathematical and Physical Sciences and New Technologies (SMPNT)
Discipline: Physics
Specialty: Physics of materials and Renewable energy

On 02/05/2026 at 10H30 at the Marrakech Hall, Faculty of Sciences of Tetouan, UAE
Under the Theme

Investigation of the Optoelectronic Properties of 2D/2D van der Waals Heterostructure as Semiconductor Materials for Photovoltaic Applications: The case of Black-Phosphorene and Janus monolayers

Front of the jury composed of :

First Name & Last Name	Establishment	Designation
Pr. ACHAHBAR Abdelfettah	FS of Tetouan , UAE	President
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Pr. SAMOUDI Bouselham	FS of Tetouan, UAE	Reviewer
Pr. BOUTAHIR Mourad	ENS of Meknes, UMI	Reviewer
Pr. ESSAOUINI Hilal	FS of Tetouan , UAE	Examiner
Pr. BRESSON Serge	UniLaSalle Polytechnic Institute, France	Examiner
Pr. BEN ABDELOUAHAB Farid	Independent Researcher	Expert
Pr. MARJAOUI Adil	FST of Tangier, UAE	Co-Supervisor
Pr. EL HADRI Mustapha	FS of Tetouan, UAE	Supervisor

Host Research Structure: Condensed Matter Physics Team/UAE/SU05FS

Abstract

Two-dimensional (2D) van der Waals heterostructures have emerged as promising materials for next-generation photovoltaic applications due to their tunable electronic properties, strong light absorption, and reduced thickness. In this thesis, the photovoltaic potential of 2D heterostructures based on Janus monolayers and black phosphorene is systematically investigated, with the aim of understanding how heterostructuring affects their structural stability, electronic structure, and optical properties, and how these features can be exploited to design efficient heterojunction photovoltaic solar cells (HJSCs). The study begins with the establishment of the theoretical and methodological framework, including electronic structure theory based on density functional theory (DFT) and fundamental photovoltaic models. These approaches provide the basis for analyzing material properties at the atomic scale and for evaluating photovoltaic performance at the device level.

Three families of 2D heterostructures are then examined. First, Janus GaXY (X/Y = S, Se, Te)/GeAs heterostructures are investigated to assess the effects of chemical asymmetry and stacking configuration on their electronic and optical behavior. The results show that the intrinsic polarity of Janus monolayers enables effective tuning of band alignment, band-gap values, and carrier effective masses. Most of the studied systems exhibit direct band gaps and high optical absorption coefficients in the visible and ultraviolet regions, confirming their strong potential as 2D photo absorbing materials. The second part focuses on the Black-P/Si_2SeS heterostructure, which exhibits a direct band gap of 1.26 eV, lying within the optimal range for photovoltaic energy conversion. A type-II band alignment is obtained, promoting efficient separation of photogenerated electron–hole pairs, while the pronounced anisotropy of carrier mobilities provides favorable conditions for efficient charge transport. The theoretical power conversion efficiency estimated using the Shockley–Queisser model reaches 18.05%, positioning this heterostructure among the most promising 2D photovoltaic candidates. Finally, black phosphorene/GaSeS heterostructures are studied by combining the high carrier mobility of phosphorene with the intrinsic out-of-plane asymmetry of Janus materials. Both SeGaS and SGaSe configurations demonstrate good structural stability and distinct electronic characteristics. In particular, the black phosphorene/SGaSe heterostructure exhibits strong interfacial charge transfer, enhanced optical absorption in the visible region compared to the individual monolayers, and a simulated power conversion efficiency of 20.40% obtained using the SCAPS-1D device simulator.

Overall, this thesis demonstrates that Janus/black phosphorene–based 2D heterostructures constitute a versatile and efficient platform for ultrathin photovoltaic technologies. Their tunable band alignment, chemically induced internal electric fields, enhanced visible-light absorption, and compatibility with heterojunction solar cell architectures make them highly promising candidates for future high-efficiency photovoltaic applications.

Keywords: Two-dimensional (2D) - Janus - Black-P - Power Conversion Efficiency (PCE) - Density Functional Theory (DFT - photovoltaic applications