جامعة عبد المالك السعدي
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Université Abdelmalek Essaadi

Pole for Doctoral Studies
Center for Doctoral Studies Sciences and Techniques and Medical Sciences

ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE

M. ASSIOUAN Kamal

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: Materials Physics and Renewable Energy

On 26/09/2026 at 11H00 at the Meetings Hall of the Chemistry Department, Faculty of Sciences of Tetouan, UAE
Under the Theme

Investigation of Novel Halide Double Perovskite Compositions for Single-Junction and Tandem Solar Cells: First-Principles and Device-Scale Modelling

Front of the jury composed of :

First Name & Last Name	Establishment	Designation
Pr. LAAZIZ Yassin	ENSA of Tanger, UAE	President
Pr. El HADRI Mustapha	FS of Tetouan, UAE	Reviewer
Pr. ESSAOUINI Hilal	FS of Tetouan, UAE	Reviewer
Pr. FAHMI Atika	FS of Kenitra, UIT	Reviewer
Pr. SAMOUDI Bousselham	FS of Tetouan, UAE	Examiner
Pr. ZANOUNI Mohamed	FST of Tangier, UAE	Examiner
Pr. EL KHAMKHAMI Jamal	FS of Tetouan, UAE	Co-Supervisor
Pr. ACHAHBAR Abdelfattah	FS of Tetouan, UAE	Supervisor

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

Abstract

Solar energy is one of the most prominent renewable energy sources and is widely investigated as a solution for reducing carbon emissions. However, conventional silicon-based solar cells face limitations associated with intrinsic material properties and high manufacturing costs, which drive the search for alternative absorber materials. In this context, inorganic halide double perovskites have emerged as promising candidates due to their enhanced structural stability and strong resistance to moisture and thermal degradation.

Solar energy is one of the most popular renewable energy sources, and it is also being actively investigated as an approach to reducing carbon emissions. However, traditional silicon-based solar cells have limits due to inherent material qualities and high production costs, leading to a desire for alternate absorber materials. Inorganic halide double perovskites have exhibited promise in this regard, considering that they can be more resistant to moisture and heat degradation and also have much more remarkable structural stability. This thesis work presents computational methodologies to examine new rubidium-based halide double perovskite properties for single-junction and tandem solar cells' absorber layer.

The proposed materials are carefully investigated utilising the density functional theory (DFT) as applied to Quantum ESPRESSO. The structural, mechanical, optoelectronic, and photovoltaic properties are assessed. Rb2AuBiCl6, Rb2CuAsCl6, and Rb2InRhCl6 has intriguing potential for solar applications due to its outstanding thermodynamic and mechanical stability, as well as its optical properties in the visible band. The replacement of Rb2AuBiCl6 by Rb2CuAsCl6 boosts carrier mobility and, as a result, device performance. Rb2InRhCl6 exhibits a wide band gap, making it appropriate for use in tandem solar cells.

The SCAPS-1D simulator is also used to assess the devices' performance in terms of the most important photovoltaic parameters, shortcircuit current density (Jsc), open-circuit voltage (Voc), fill factor (FF), and power conversion efficiency (PCE), as well as the effect of different layer thicknesses, series and shunt resistances, and temperature on the solar cell efficiency. Rb2AuBiCl6, Rb2CuAsCl6, and Rb2InRhCl6 have estimated power conversion efficiencies of 17.38%, 21.57%, and 26.66%, respectively. These findings suggest that rubidium-based double perovskites can be used as a stable, high-performance, lead-free absorber material in next-generation solar technology.

Keywords: Halide double perovskites; Rubidium-based perovskites; Density Functional Theory (DFT); Photovoltaic performance; Tandem solar cells.