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Nanostructures and thin films of metal-organic complexes and hybrid perovskites for applications in optoelectronics and photovoltaics

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Amina LAOUID

TABLE OF CONTENTS

ABSTRACT

This PhD thesis makes a significant contribution to the fields of natural sciences and engineering and technical sciences in the disciplines of physical sciences and materials engineering by investigating the potential of perovskites and metal-organic complexes in optoelectronic and photovoltaic applications.

The research focused on the development and characterization of materials in the form of nanostructures and thin layers, intending to enhance efficiency and stability and accelerate the sustainable development of next-generation solar cells and light-emitting devices.

The presented work covers the study of linear and nonlinear optical properties as well as morphological features of functional materials, using experimental techniques supported by calculations and theoretical simulations.

The thin films were fabricated by physical vapor deposition (PVD) technique and analyzed using advanced characterization techniques, including Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Photoluminescence (PL), Fourier Transform Infrared Spectroscopy (FTIR), UV-Vis Spectroscopy, and X-ray Fluorescence (XRF). Perovskite materials, particularly $RbSn_{0.5}Ge_{0.5}I_3$ and $MAPbI_3$, exhibited exceptional light absorption properties and significant photovoltaic potential upon integration into solar cells.

In addition, thin films of Znq_2, a metal-organic complex doped with organic molecules (red-dye-DCM), were studied for their structural, linear and non-linear optical properties, demonstrating energy transfer by Förster resonance, which is crucial for optoelectronic applications.

Furthermore, Density Functional Theory (DFT) calculations have provided a detailed analysis of the electronic structure of these materials, contributing to a better understanding of the mechanisms involved and leading to improved stability and performance in practical applications.

Through experimental as well as computational research, this work discovered promising materials for making solar cells having sub-micrometer thickness with efficiency comparable to silicon solar cells but with environmental compatibility. Those findings in this thesis are an important achievement towards building future-generation photovoltaic as well as optoelectronic photovoltaic devices, allowing innovative as well as sustainable industrial applications.

Abstract (Polish)

Niniejsza rozprawa doktorska wnosi istotny wkład w dziedziny nauk ścisłych i przyrodniczych oraz nauk inżynieryjno-technicznych w dyscyplinach nauki fizyczne i inżynieria materiałowa, badając potencjał perowskitów i kompleksów ligandów organicznych z metalami w zastosowaniach optoelektronicznych i fotowoltaicznych. Przeprowadzone w trakcie jej realizacji badania koncentrowały się na opracowaniu i charakteryzowaniu materiałów w postaci nanostruktur i cienkich warstw i miały na celu zwiększenie wydajności i stabilności oraz przyspieszenie zrównoważonego rozwoju nowej generacji ogniw słonecznych oraz urządzeń emitujących światło.

Tematyka prezentowanej pracy obejmuje badania liniowych i nieliniowych właściwości optycznych, a także cech morfologicznych materiałów funkcjonalnych, przy zastosowaniu technik eksperymentalnych popartych obliczeniami i symulacjami teoretycznymi.

Cienkie warstwy zostały wytworzone metodą fizycznego osadzania z fazy gazowej (PVD) i poddane analizie przy użyciu różnych technik charakteryzacji, w tym mikroskopii sił atomowych (AFM), skaningowej mikroskopii elektronowej (SEM), fotoluminescencji (PL), spektroskopii UV-Vis, spektroskopii w podczerwieni z transformacją Fouriera (FTIR) oraz fluorescencji rentgenowskiej (XRF). Materiały perowskitowe, szczególnie $RbSn_{0.5}Ge_{0.5}I_3$ oraz $MAPbI_3$, wykazały wyjątkowe właściwości pochłaniania światła oraz znaczący potencjał fotowoltaiczny jako warstwy aktywne w ogniwach słonecznych.

Z kolei cienkie warstwy Znq_2, kompleksu organometalicznego domieszkowanego cząsteczkami organicznymi (czerwony barwnik DCM), zostały zbadane pod kątem ich właściwości strukturalnych i optycznych, wykazując Försterowski rezonansowy transfer energii istotny w zastosowaniach optoelektronicznych. Dodatkowo obliczenia w ramach teorii funkcjonału gęstości (DFT) pozwoliły na dokładniejszą analizę struktury elektronowej tych materiałów, przyczyniając się do lepszego zrozumienia mechanizmów w nich zachodzących i prowadzących do zwiększenia stabilności i wydajności w zastosowaniach praktycznych. Poprzez integrację prac eksperymentalnych i obliczeniowych, badania te identyfikują obiecujące materiały do rozwoju ogniw słonecznych o grubości mniejszej niż mikrometr, wydajności porównywalnej z ogniwami krzemowymi a jednocześnie przyjaznych dla środowiska. Wyniki przedstawione w niniejszej rozprawie stanowią istotny krok w rozwoju technologii optoelektronicznych i fotowoltaicznych nowej generacji, torując drogę do innowacyjnych i zrównoważonych rozwiązań przemysłowych.

Abstract (French)

Cette thèse de doctorat apporte une contribution significative aux domaines des sciences naturelles et de l'ingénierie et des sciences techniques dans les disciplines des sciences physiques et de l'ingénierie des matériaux en étudiant le potential des pérovskites et des complexes métallo-organiques dans les applications optoélectroniques et photovoltaïques.

La recherche s'est concentrée sur le développement et la caractérisation de matériaux sous forme de nanostructures et de couches minces, dans le but d'améliorer l'efficacité et la stabilité et d'accélérer le développement durable des cellules solaires et des dispositifs d'émission de lumière de la prochaine génération.

Les travaux présentés couvrent l'étude des propriétés optiques linéaires et non linéaires ainsi que les caractéristiques morphologiques des matériaux fonctionnels,

en utilisant des techniques expérimentales étayées par des calculs et des simulations théoriques.

Les films minces ont été fabriqués par dépôt physique en phase vapeur (PVD) et analysés à l'aide de techniques de caractérisation avancées, notamment la microscopie à force atomique (AFM), la microscopie électronique à balayage (SEM), la photoluminescence (PL), la spectroscopie infrarouge à transformée de Fourier (FTIR), la spectroscopie UV-Vis et la fluorescence des rayons X. Les matériaux pérovskites, en particulier $RbSn_{0,5}Ge_{0,5}I_3$ et $MAPbI_3$, présentent des propriétés exceptionnelles d'absorption de la lumière et un potentiel photovoltaïque significatif lorsqu'ils sont intégrés dans des cellules solaires.

En outre, des films minces de Znq_2, un complexe métal-organique dopé avec des molécules organiques (red-dye-DCM), ont été étudiés pour leurs propriétés structurelles, optiques linéaires et non linéaires, démontrant le transfert d'énergie par résonance de Förster, ce qui est crucial pour les applications optoélectroniques.

En outre, les calculs de la théorie de la fonctionnelle de la densité (DFT) ont fourni une analyse détaillée de la structure électronique de ces matériaux, contribuant à une meilleure compréhension des mécanismes impliqués et conduisant à une amélioration de la stabilité et de la performance dans les applications pratiques.

Ce travail a permis de découvrir, par le biais de recherches expérimentales et computationnelles, des matériaux prometteurs pour la fabrication de cellules solaires d'une épaisseur inférieure au micromètre, avec une efficacité comparable à celle des cellules solaires au silicium, tout en étant compatibles avec l'environnement. Les résultats obtenus dans le cadre de cette thèse constituent une avancée importante dans la construction des dispositifs photovoltaïques et optoélectroniques de la future génération, permettant des applications industrielles innovantes et durables.

PUBLICATIONS CONTRIBUTING TO THE DISSERTATION

I Generation of red light with intense photoluminescence assisted by Forster resonance energy transfer from Znq_2 and DCM thin films.

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DOI: 10.1007/s11356-022-23217-z.

II Optical and morphological properties of DCM thin films co-doped of Znq_2 by PVD: Theoretical and experimental investigations.

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IV Enhancing the efficiency and stability of Non_Toxic $RbSn_{0.5}Ge_{0.5}I_3$_Based perovskite solar cells through optimization.

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Optical Materials 157 (2024) 116045.

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VI Low-temperature influence on the properties and efficiency of thin-film perovskite solar cells fabricated by the PVco-D technique.

A. Zawadzka, A. Marjanowska, **A. Laouid**, K. Wisniewski, Y. El Kouari, Y. El Hani, P. Płóciennik.

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GENERAL INTRODUCTION

In recent years, the global need for eco-friendly and efficient energy solutions has driven remarkable progress in the area of materials engineering, particularly in the domain of advancing materials with tailored electronic and optical properties for use in optoelectronic and photovoltaic devices [1],[2]. Among these materials, nanostructures and thin films of metal-organic complexes and perovskites have been recognized as a potential solution because of their adjustable properties, which enable them to meet the growing requirements for high-performance, environmentally friendly devices [3],[4]. These materials have demonstrated exceptional potential not only in traditional applications, such as transistors and sensors, but also in advanced optoelectronic applications, notably organics light-emitting diodes (OLEDs), lasers, photodetectors, and solar cells. The exploration of nanostructures and thin films, which serve as the fundamental building blocks of numerous electronic and optoelectronic devices, has revealed a broad spectrum of characteristics, particularly high surface area, quantum confinement effects, and enhanced optical characteristics [5]. These properties can be precisely tailored by manipulating the dimensions and composition of nanostructures, preparing the ground for versatile applications across numerous fields.

Thin Films and Nanostructures

Thin films are defined as layers of material with thicknesses varying from a few nanometers to many microns. Compared to bulk materials, thin film possesses a distinct range of electrical, optical, and mechanical attributes that are shaped by their reduced dimensions. Their reduced dimensionality and high surface-to-volume ratio make them a good candidate for all types of applications involving accurate control of material properties [6],[7]. For instance, in photovoltaics, thin films enable efficient light absorption and charge transport, while in optoelectronics, they facilitate the miniaturization and integration of components including light-emitting diodes (LEDs) as well as photodetectors [8]. The historical development of thin films dates back to the early 20th century, with the introduction of vacuum deposition techniques, and has since evolved to include advanced methods including physical and chemical vapor deposition, as well as atomic layer deposition [9]. These techniques allow for the accurate control of composition, morphology, and film thickness which are vital to improving device performance. Examples of thin films in nature, such as the iridescent layers on butterfly wings or the anti-reflective coatings on moth eyes, have inspired synthetic thin films with applications in anti-reflective coatings, optical filters, and semiconductor devices.

Nanostructured materials, characterized by features at the nanoscale (commonly varies from 1 to 100 nanometers), display properties that are fundamentally distinct compared to those of bulk materials [10],[11]. At this scale, materials display quantum confinement effects, resulting in size-dependent behavior of optical and electronic properties. This phenomenon arises because the dimensions of the nanostructures are comparable to the wavelength of electrons, leading to discrete energy levels and enhanced optoelectronic properties. Nanostructures can take various forms, including nanoparticles, nanowires, nanosheets, and quantum dots, each offering unique advantages for specific applications [12],[13]. For example, quantum dots, and nanoscale semiconductor particles exhibit tunable emission wavelengths depending on their size, which makes them ideal for use in display and bio-imaging applications. Similarly, nanowires and nanosheets provide high surface areas and efficient charge transport pathways, which are beneficial for energy storage devices and sensors. The combination of thin films and nanostructures paved the path for the progress of high-performance photovoltaic devices and optoelectronics. Thin films provide a platform for the integration of nanostructures, enabling the exploitation of their unique properties at the device level.

Metal-Organic Complexes

Metal-organic complexes are a class of coordination compounds that consist of metal centers bonded to organic ligands [14]. Particular attention has been paid to these materials in recent years because of their tunable optical, electronic, and morphological properties, which make them highly suitable for applications in serval domains such as optoelectronics, photovoltaics, catalysis, and sensing. Unlike conventional inorganic materials, metal-organic complexes provide the benefits of structural flexibility, processability, and the possibility of refining their properties by modifying both the metal center and the organic ligand [15].

Historically, metal-organic complexes were primarily explored for their catalytic properties and medicinal applications [15]. However, advancements in materials science and molecular engineering have led to their integration into state-of-the-art technologies including organics light-emitting diodes, hybrid perovskite, and dye-sensitized solar cells [16]. The ability to manipulate their electronic energy levels, charge transport behavior, and stability makes them highly promising candidates for next-generation energy conversion and photonic applications.

The fundamental architecture of metal-organic complexes is crucially defined by the coordination environment of the metal center and the properties of the organic ligands. The coordination number and geometry are determined by the electronic configuration of the central metal ion and the bonding characteristics of the ligands, resulting in commonly observed geometries such as octahedral, tetrahedral, square planar, and trigonal bipyramidal.

Ligands have a considerable influence on determining the optical and electronic properties of the complexes. They can be classified into different types, including neutral ligands (such as phenanthroline and bipyridine), anionic ligands (such as chloride and acetate), and π-conjugated ligands (such as porphyrins and phthalocyanines) [17]. The interaction between the metal center and the ligands results in characteristic electronic transitions, which govern the absorption and emission behavior of the complexes. The synthesis of metal-organic complexes follows well-established coordination chemistry principles, enabling meticulous control over their composition and structure. The most common synthetic method involves solution-based chemistry, where metal salts react with organic ligands in a carefully chosen solvent in rigorously controlled operating conditions. The choice of solvent, temperature, and ligand-to-metal ratio significantly impacted the stability and final properties of the complex. In addition to solution-based synthesis, several other methods are used for fabricating metal-organic complexes, particularly for thin-film applications. Electrochemical deposition allows for the controlled growth of metal-organic complexes on conductive surfaces, providing advantages in device fabrication. Solvothermal and hydrothermal synthesis techniques enable the production of highly crystalline metal-organic compounds with enhanced stability. For optoelectronic applications, physical vapor deposition and spin-coating techniques are used to create high-quality thin films with well-controlled morphology and thickness.

Metal-organic complexes exhibit unique electronic and optical properties that make them highly valuable for applications in light-harvesting and light-emitting devices [18]. The absorption spectra of these materials are predominantly influenced by ligand-to-metal charge transfer (LMCT), metal-to-ligand charge transfer (MLCT), and intraligand π-π* transitions. These transitions facilitate strong absorption of light in the near-infrared and the visible spectrum, and this makes these materials suitable for solar cells and photodetectors. In addition to their strong absorption characteristics, metal-organic complexes exhibit efficient charge transport behavior, which is affected by various factors including ligand conjugation, metal oxidation state, and crystal packing [19]. The ability to engineer these properties by selecting appropriate metal-ligand combinations allows for the design of materials with optimized charge mobility, which is essential for their incorporation into electronic and optoelectronic devices.

Despite their numerous advantages, metal-organic complexes face a number of issues that remain to be resolved before they can be widely implemented in commercial applications [20]. One of the primary concerns is long-term stability under working conditions. Many metal-organic complexes are liable to deteriorate when exposed to UV light, moisture, or elevated temperatures, limiting their long-term usability in devices. Researchers are actively working on improving the stability of these materials through ligand modifications and encapsulation strategies. Another challenge is the scalability and cost-effectiveness of fabricating metal-organic complexes for large-area applications [21]. While solution-processing techniques offer a promising route for cost-effective manufacturing, achieving uniform film deposition with high reproducibility remains a challenge. Advances in deposition techniques such as atomic layer deposition, molecular self-assembly, and physical vapor deposition could provide good pathways for scalable fabrication.

Toxicity concerns associated with certain metal-organic complexes, particularly those containing heavy metals such as lead and cadmium, have also raised environmental and health-related issues [22]. The search for non-toxic and earth-abundant metal complexes with comparable performance is an active area of research. Transition metals such as iron, copper, and cobalt are being examined as alternative options to traditional heavy metal-based complexes.

Perovskites

Perovskites have been recognized as a leading candidate material classes for optoelectronic and photovoltaic applications, as a result of their excellent optoelectronic properties, simple fabrication processes, and adjustable features. The original term "perovskite" is associated with a mineral having the chemical formula $CaTiO_3$, but in materials science, it has come to describe any material with the same crystal structure, defined by the general formula ABX_3 [23]. In this structure, A represents a monovalent cation, which can be either organic or inorganic, B is a divalent metal cation, and X is a halide anion. The versatility of this structure permits a broad spectrum of compositional modifications, allowing precise tuning of electronic, optical, and structural characteristics to suit specific applications. The perovskite framework is highly adaptable, to suit a wide range of cations and anions. This flexibility enables the tuning of key properties including bandgap, carrier mobility, and stability, turning this type of material suitable for several applications, including light-emitting diodes, photodetectors, solar cells, and lasers [24]. Perovskites can be grouped into three principal categories according to the nature of their composition [25]:

- Inorganic Perovskites: These materials consist entirely of inorganic components, such as $CsPbI_3$ (cesium lead iodide) or $CsSnBr_3$ (cesium tin bromide). Inorganic perovskites are renowned for their high stability and outstanding optoelectronic properties but often require high-temperature processing.

- Hybrid Organic-Inorganic Perovskites: These materials combine organic cations (e.g., methylammonium, formamidinium) with inorganic metal halides (e.g., PbI_2, $SnBr_2$). Hybrid perovskites, such as $MAPbI_3$ and $FAPbI_3$ (formamidinium lead iodide), have achieved remarkable efficiencies in solar cells but suffer from stability issues caused by the volatile nature and instability of the organic cations.

The key features of perovskites include:

- High Absorption Coefficient: Perovskites exhibit strong light absorption across a broad spectrum, making them ideal for photovoltaic applications.
- Long Carrier Diffusion Lengths: The excellent charge transport properties of perovskites result in long carrier diffusion lengths, often exceeding 1 micrometer. This property is essential for efficient charge extraction not only in solar cells but also in many other devices.
- Tunable Bandgap: The bandgap of perovskites is possible to be controlled by varying the composition of the A, B, and X sites. For instance, replacing iodine (I) with bromine (Br) or chlorine (Cl) in the X site can increase the bandgap, while substituting lead (Pb) with tin (Sn) or germanium (Ge) in the B site can reduce it.
- Solution Processability: Perovskites can often be fabricated using cost-effective techniques based on a solution including spin-coating, inkjet printing, and dip coating. This renders them highly appealing for flexible electronic and large-scale manufacturing applications.
- Defect Tolerance: Perovskites exhibit a degree of defect tolerance, meaning that their performance is less sensitive to impurities and defects compared to traditional semiconductors. This property simplifies the fabrication process and reduces production costs.

Inorganic perovskites present several advantages over their hybrid organic-inorganic counterparts, particularly in terms of stability and durability [26]. One of the most notable benefits is their superior thermal stability, which ensures that their structural and electronic properties remain intact even under high-temperature conditions. This characteristic is crucial for photovoltaic applications, where prolonged exposure to sunlight and elevated temperatures can degrade material performance over time. Unlike hybrid perovskites, which contain organic components susceptible to thermal decomposition, inorganic perovskites maintain their integrity, making them more reliable for long-term use. Another key advantage of inorganic perovskites is their enhanced resistance to moisture. Hybrid perovskites often suffer from rapid degradation when exposed to humidity, leading to a decline in efficiency and device lifetime. Fully inorganic perovskites, such as $CsPbBr_3$ and $CsPbI_3$, exhibit significantly higher moisture tolerance, reducing the risk of performance loss due to environmental factors. This increased robustness makes them particularly promising for outdoor photovoltaic applications, where exposure to varying humidity levels is inevitable. Furthermore, the improved stability of inorganic perovskites contributes to the development of more reliable and commercially sustainable solar cells [27]. Their ability to withstand harsh environmental conditions without significant degradation enhances the longevity of photovoltaic devices, reducing maintenance costs and increasing energy yield over time. As research continues to refine the synthesis and processing of inorganic perovskites, they hold great potential for next-generation solar technologies, offering a path toward more durable and efficient renewable energy solutions.

Unlike other perovskites, hybrid perovskites (organic-inorganic) like methylammonium lead halides ($MAPbX_3$, where X = I, Br, Cl) have achieved notable efficiency gains. Their tunable bandgaps, high absorption coefficients, and excellent charge transport properties make them well-suited for optoelectronic applications. Hybrid perovskites, particularly those composed of organic and inorganic lead halides, have drawn considerable attention for their superior optoelectronic properties. These materials combine the advantages of both organic and inorganic components, leading to strong light absorption, extended carrier diffusion lengths, and adjustable band gaps. Their structural flexibility allows for compositional engineering, enabling researchers to optimize their stability and performance for photovoltaic and light-emitting applications. The fast evolution of solar cells based on hybrid perovskite has given rise to efficiencies exceeding 25%, making them strong contenders for next-generation photovoltaic technologies. Additionally, their solution-processability provides a cost-effective and scalable manufacturing process as compared to conventional solar cells based on silicon.

Despite their outstanding performance, hybrid perovskites are confronted with major challenges, mainly related to their environmental durability. The presence of volatile organic cations, particularly formamidinium (FA) and methylammonium (MA), results in a high sensitivity to moisture, leading to the risk of fast deterioration under humid conditions, oxygen, and thermal stress, leading to degradation and efficiency losses over time. Researchers have explored several strategies to enhance stability, including compositional modifications, encapsulation techniques, and the introduction of two-dimensional (2D) perovskite layers to improve moisture resistance. Another critical concern is the presence of lead, which raises environmental and toxicity issues, prompting efforts to develop lead-free alternatives. While these challenges remain, continuous progress in material engineering and device architectures is leading to more stable and efficient hybrid perovskite-based technologies.

Photovoltaic and optoelectronic applications

Photovoltaic and optoelectronic technologies have revolutionized the way we harness and utilize light energy, playing a crucial role in modern energy generation, communication, and sensing applications [28],[29]. PV technology is primarily used in solar cells, where sunlight is converted into electrical energy through semiconductor materials with high charge carrier mobility and efficient light absorption. Optoelectronics covers a wider range of devices that can interact with light, including light-emitting diodes, lasers, photodetectors, and displays. These technologies have seen rapid advancements in recent decades, driven by the pressing need for sustainable and renewable energy solutions to address global energy challenges, high-performance optoelectronic components, and miniaturized, multifunctional devices for emerging applications.

The efficiency and performance of photovoltaic and optoelectronic devices are highly dependent on the materials used in their construction. Traditional semiconductor materials, particularly silicon, gallium arsenide (GaAs), and cadmium telluride (CdTe), have long been the foundation of these technologies due to their well-established fabrication processes and reliable performance. However, these materials come with limitations such as high production costs, rigid structures, and constraints in tunability. The demand for alternative materials that offer superior optoelectronic properties, cost-effectiveness, and ease of fabrication has led to the exploration of novel material classes that can overcome these limitations. Among the most promising emerging materials are perovskites and metal-organic compounds, which have demonstrated exceptional optoelectronic properties and versatility.

Perovskite solar cells have achieved remarkable progress, with PCEs exceeding 25% in single-junction devices and 30% in tandem configurations with silicon [30]. Perovskites are also widely used in photodetectors, light-emitting diodes, and lasers. Their tunable emission spectra and high photoluminescence quantum yields make them ideal for color-tunable LEDs and display technologies. Their high efficiency, combined with low fabrication costs, makes perovskites a promising replacement for traditional photovoltaics based on silicon. Recent advancements in 2D perovskites, lead-free alternatives (e.g., Sn, Ge-based perovskites), and interface engineering have addressed some of these issues, paving the way for more stable and environmentally friendly devices [31]. In photodetectors, perovskites offer high sensitivity and fast response times, enabling applications in imaging and sensing. Additionally, their nonlinear optical properties have been exploited for frequency conversion and ultrafast photonics.

Metal-organic compounds have also emerged as valuable materials in optoelectronics. Their molecular tunability, strong photoluminescence, and ability to form highly ordered structures make them particularly attractive for applications such as OLEDs, bioimaging, sensors, and photodetection. Metal-organic compounds are often used as charge transport layers, interfacial modifiers, or light absorbers in solar cells. For example, metal-organic compounds were employed in solar cells based on perovskite, as hole transport materials (HTMs), improving charge extraction and device stability [32],[33]. In photodetectors, metal-organic compounds offer high sensitivity and selectivity, enabling applications in environmental monitoring and biomedical imaging. Furthermore, their nonlinear optical properties have been explored for second-harmonic generation (SHG) and optical switching.

Research Objectives

The main objective of this dissertation is the fabrication, characterization, and optimization of thin films and nanomaterials based on perovskites and organometallic compounds for photovoltaic and optoelectronic applications. These materials exhibit remarkable optical and electronic properties, which can be adjusted by modification of their chemical composition and deposition conditions. The ultimate goal is to improve the performance and the durability of optoelectronic and photovoltaic devices by establishing correlations between the material's structure, its physical properties, and its energy conversion efficiency.

To achieve these objectives, a combined approach involving both experimental and theoretical methods has been adopted. Experimentally, thin films were fabricated using Physical Vapor Deposition and characterized through various morphological, linear, and nonlinear optical techniques. Additionally, numerical simulations were carried out using the SCAPS software to model the behavior of solar cells and assess their efficiency. Moreover, DFT simulations were developed to elucidate the electronic and structural characteristics of the deposited materials.

Thin Film Deposition by PVD:

The Physical Vapor Deposition method was employed in this study as it offers several key advantages for producing high-quality thin layers. A major advantage of PVD is that the thickness and composition of the deposited layers are highly controlled, ensuring high uniformity and reproducibility of material properties. Additionally, the process is carried out in a vacuum environment, significantly reducing contamination and leading to highly pure thin films. This purity is crucial for photovoltaic applications, where even minor impurities can degrade device performance.

Another major advantage of PVD is its flexibility in the choice of materials. It permits the manufacturing of different arrays of materials, including oxides, metals, and hybrid materials such as organometallic perovskites. Through the adjustment of deposition conditions, such as deposition rate, temperature, and pressure, the electronic and optical characteristics of thin films are optimized, which makes them more suitable for optoelectronic and photovoltaic applications.

Linear Optical Characterization:

The fabricated thin films were characterized using various linear optical techniques to study their interaction with light. Linear optics encompasses phenomena where the material's response is directly proportional to the intensity of the applied electromagnetic field. These studies are important for determining the material's ability to absorb, transmit, or reflect light, which is crucial for their implementation in photovoltaic and optoelectronic devices. Several characterization techniques were employed:

- UV-Vis Spectroscopy was employed to determine the absorption and transmission spectra of the films and determine their bandgap, a key parameter influencing the efficiency of solar cells.
- Photoluminescence (PL) Spectroscopy, which provided insights into the crystalline quality of the films and identified defects that could impact device performance.
- Fourier Transform Infrared Spectroscopy has been used to investigate molecular vibrations and identify chemical bonds in a material by measuring infrared absorption. It helps determine functional groups present in the material, making it useful for studying organic and hybrid perovskite materials.
- Decay Time (Photoluminescence Decay or Time-Resolved PL): provides information about the semiconductor carrier lifetime. This is crucial

for evaluating recombination dynamics, charge carrier mobility, and defect-related processes in photovoltaic materials.

These optical analyses were crucial for establishing correlations between deposition conditions and optical performance, allowing fine-tuning of material properties to optimize their photovoltaic and optoelectronic applications.

Morphological Characterization:

Thin films' morphology is crucial in determining their optical and electronic properties. To enquire about the structure and quality of the deposited materials, several morphological characterization techniques were employed:

- Atomic Force Microscopy was used to analyze the roughness of the surface and uniformity of the films at the nanometer scale, ensuring high homogeneity for device applications.
- Scanning Electron Microscopy provided detailed images of the film surface, revealing microstructural features and potential defects affecting performance.
- X-ray Fluorescence is a powerful non-destructive technique that was employed to accurately identify the elemental composition of thin films, providing valuable insights into their chemical composition. It helps quantify the presence of specific elements in perovskite and organometallic materials, ensuring accurate stoichiometry and detecting potential impurities.

These analyses helped establish relationships between deposition parameters, film morphology, and resulting optical and electronic properties, ensuring that the materials meet the requirements for high-performance photovoltaic and optoelectronic devices.

Nonlinear Optical Properties:

Nonlinear optics is a fundamental aspect of this research, particularly the examination of Second and Third Harmonic Generation. Unlike linear optical phenomena, nonlinear optical effects occur when the material's response to an electromagnetic field is non-linear to the field intensity.

- Second Harmonic Generation (SHG) is a process where two incident photons combine to generate a photon with double the frequency. This technique is highly sensitive to the crystalline structure of materials and is widely used to probe symmetry and detect structural defects in thin films.
- Third Harmonic Generation (THG) involves the conversion of three incident photons into a single photon with triple the original frequency. This phenomenon is particularly useful for studying electronic properties and quantum confinement effects in nanomaterials.

Analyzing these nonlinear optical properties provides deeper insights into light-matter interactions at high intensities, enabling the development of advanced technologies in telecommunications, laser systems, and nonlinear photonics.

Numerical Simulations: SCAPS and DFT Calculations

To complement the experimental studies, numerical simulations were carried out to simulate and optimize the performance of the investigated materials.

SCAPS (Solar Cell Capacitance Simulator) simulations were employed to analyze the energy conversion efficiency of solar cells, considering factors such as junction structure, optical absorption, and charge transport mechanisms. These simulations allowed the identification of optimal design parameters to maximize energy conversion efficiency.

DFT is particularly valuable in computational chemistry and materials science due to its versatility. It enables researchers to predict electronic properties, chemical reactivity, optical absorption spectra, and charge transport mechanisms. Additionally, time-dependent DFT extends the capabilities of standard DFT by allowing the study of excited-state properties, which is crucial for achieving optimal performance in specific applications, particularly in fields such as photovoltaics, optoelectronics, and photochemistry. Given its broad applicability, DFT has become an indispensable tool in both theoretical and experimental research.

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Co-authorship Statement

I hereby declare that I'm a co-author in the following articles:

Article . I: A. Laouid, A.A. Belghiti, K. Wisniewski, A. Hajjaji, B. Sahraoui, A. Zawadzka, Generation of red light with intense photoluminescence assisted by Forster resonance energy transfer from Znq2 and DCM thin films, Environ Sci Pollut Res (2022) 1–20. https://doi.org/10.1007/s11356-022-23217-z. My contribution to the work is 64 %.

Article . II: A. Laouid, A. Alaoui Belghiti, K. Wisniewski, J. Strzelecki, A. Karakas, A. Gozutok, Y. El kouari, A. Bouich, M. Tlemçani, P. Plociennik, A. Hajjaji, A. Zawadzka, Optical and morphological properties of DCM thin films co-doped of Znq2 by PVD: Theoretical and experimental investigations, Vacuum 222 (2024) 112997. https://doi.org/10.1016/j.vacuum.2024.112997. My contribution to the work is 50 %.

Article . III: A. Laouid, A. Alaoui Belghiti, K. Wisniewski, M. Boumhamdi, J. Strzelecki, P. Plociennik, A. Hajjaji, A. Zawadzka, A study of morphological, optical, and photoluminescence properties of ZnS thin films doped Mn and ca, Materials Chemistry and Physics (2024) 129270. https://doi.org/10.1016/j.matchemphys.2024.129270. My contribution to the work is 57 %.

Article . IV: Laouid A, Alaoui Belghiti A, Wisniewski K, Abouais A, Tlemcani M, Plociennik P, et al. Enhancing the efficiency and stability of Non_Toxic RbSn0.5Ge0.5I3_Based perovskite solar cells through optimization 2024. https://doi.org/10.1016/j.mseb.2024.117672. My contribution to the work is 62%.

Article . V: Laouid A, El Karout H, Alaoui Belghiti A, Wisniewski K, Plociennik P, El Kouari Y, et al. Control of second-and third-order nonlinear optical properties of DCM and Znq2 composites fabricated by the physical vapor co-deposition process. Optical Materials 2024;157:116045. https://doi.org/10.1016/j.optmat.2024.116045. My contribution to the work is 60 %.

Article . VI: A. Zawadzka, A. Marjanowska, A. Laouid, K. Wisniewski, Y. El Kouari, Y. El Hani, P. Płóciennik, Low-temperature influence on the properties and efficiency of thin-film perovskite solar cells fabricated by the PVco-D technique, Solar Energy Materials and Solar Cells 274 (2024) 112993. https://doi.org/10.1016/j.solmat.2024.112993. My contribution to the work is 6%.

As the primary author of Articles I, II, III, IV, and V included in this thesis, I, Amina Laouid, have played a fundamental role in every stage of the research and publication process. My contributions span from the initial conceptualization to the final manuscript preparation, ensuring the scientific rigor and coherence of each study. Throughout the research process, I was responsible for:

Conceptualization and Research Design – Developing the overarching research framework and defining key objectives.

Experimental Work and Material Fabrication – Synthesizing thin films using Physical Vapor Deposition and optimizing the fabrication process to achieve high-quality materials.

Material Characterization and Data Analysis – Conducting a comprehensive analysis of the optical, morphological, and structural properties of the fabricated thin films using advanced characterization techniques, including Atomic Force Microscopy, Photoluminescence, UV-Vis Spectroscopy, Fourier Transform Infrared Spectroscopy, and decay time.

Computational Modeling and Theoretical Investigations – Simulations by scaps to analyze and optimize solar cell performance by simulating key parameters like efficiency, charge transport, and recombination.

Manuscript Preparation and Scientific Writing – Drafting the original manuscripts, structuring the scientific arguments, interpreting the results, and refining the content through multiple review cycles to ensure clarity, precision, and adherence to high academic standards.

In addition to conducting experiments and theoretical analyses, I was actively involved in the critical revision of each manuscript, ensuring the integrity and coherence of the findings presented.

In Article VI, where I contributed as a co-author, my role was particularly focused on SCAPS simulations, playing a key part in the Investigation, Formal Analysis, and Conceptualization of the study. I conducted numerical simulations to evaluate the electrical performance of the solar cells, analyzing key parameters to optimize device efficiency. My responsibilities included interpreting simulation data, assessing the impact of material properties, and refining structural configurations to enhance performance.

Amina LAOUID

(Signature)

CONCLUSION AND FUTURE WORK

The research illustrated in this thesis delivers valuable insights into the fabrication, characterization, and optimization of optoelectronic and photovoltaic applications of thin-film materials. Using a combination of experimental and theoretical studies, this research has established the capability of different organic and inorganic thin films in the improvement of device performance and advancing material science.

The first paper of this research concentrated on structural features of the optical properties of DCM and Znq_2 thin films of different compositions prepared via PVD. In the analysis, it is observed how the content of Znq_2 affects the optical as well as the morphological features of the coated layers. Spectra measured via UV-Vis as well as FTIR can explicitly verify the high purity of the samples, whereas theoretical calculations via DFT were useful in interpreting their electronic structures. The research findings highlight the significance of molecular interaction as well as energy level in controlling the suitability of these materials for optoelectronic applications.

An investigation of photoluminescence features of the DCM-Znq_2 films in this study demonstrates the effective transfer of energy between Znq_2 and DCM. Shift in peak position as well as augmentation in photoluminescence is evident in support of the applications of these materials in luminescence applications. Low-temperature PL studies in addition showed the temperature dependency of these films, stressing their applications in temperature-sensitive devices in optoelectronics.

In this study, the nonlinear optical features of the DCM-Znq_2 thin films were studied in addition, showing efficient generation of the second and third harmonics with optimal doping content. Nonlinear optical responses observed indentified these materials as prominent candidates for photonics applications like frequency conversion as well as optical processing of signals.

In the fourth article, the optical, photoluminescent, as well as the morphological, properties of Mn and Ca doped ZnS thin films were studied. It was found that Ca doping decreased the optical bandgap while Mn doping incorporated important luminescent features. These studies indicate that ZnS can be optimized through tailored doping for specific optoelectronic applications, making it suitable for future photonic applications.

In the fifth article, SCAPS-1D simulation is used to enhance the performance of $RbSn_{0.5}Ge_{0.5}I_3$ lead-free perovskite solar cells. Optimizing some of the important parameters like hole transport layer, electron transport layer, as well as doping concentrations, the power conversion efficiency of 24.28% could be achieved through the simulation. This research helps in the development of efficient and stable lead-free perovskite solar cells in line with the drive for sustainable technologies replacing conventional photovoltaics.

The sixth article successfully studies the development of a hybrid perovskite solar cell designed for operation under reduced temperature and pressure, with a thickness of less than 1 µm. Using the physical vapor co-deposition technique, a thin hybrid perovskite layer was created, and its behavior was analyzed over a temperature range of 10 K to 320 K. The results showed an efficiency of around 18.5%, with strong agreement between experimental data and SCAPS-1D simulations. Stability tests over six months confirmed the technique's positive impact on the cell's durability. These findings suggest that the developed perovskite solar cell is well-suited for space applications.

Perspectives

Building on the findings of this dissertation, future research will focus on further optimizing the fabrication and characterization of thin films to improve their optoelectronic and photovoltaic performance. The following perspectives can be considered:

- Integration of Perovskites in Functional Devices: Ongoing work on the development and characterization of perovskites as thin films will be extended to their integration into complete solar cells. The electrical and optical properties of these materials will be further optimized to enhance their efficiency and long-term stability.

- Experimental Validation of Simulated Perovskite Solar Cells: The SCAPS simulations have provided valuable insights into the performance of perovskite solar cells. Future work will involve the fabrication and experimental testing of these devices to validate the theoretical predictions and improve stability.

In conclusion, this dissertation has demonstrated the potential of organic and inorganic thin films in advancing optoelectronic and photovoltaic technologies. The combination of experimental and theoretical approaches has provided a comprehensive understanding of these materials, paving the way for future developments in sustainable energy and photonic applications.