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Exploring Halide Double Perovskites for Enhanced Efficiency in Photovoltaic Application

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Abstract

The investigation of halide double perovskites has gained significant attention in recent years due to their promising potential in photovoltaic applications. These materials, characterized by their unique structural, electronic, and optical properties, offer an alternative to traditional lead-based perovskites, addressing environmental and stability concerns. This study focuses on the structural, electronic, and optical properties of halide double perovskites, exploring their suitability for use in solar cells. By employing computational methods such as density functional theory (DFT), we analyze the crystal structure, band gap, and electronic transitions of these materials, aiming to understand how their intrinsic properties can be tuned for optimal photovoltaic performance. The results indicate that halide double perovskites exhibit excellent optical absorption in the visible spectrum, a desirable trait for efficient solar energy conversion. Additionally, the band gap of these materials can be fine-tuned through compositional changes, allowing for enhanced electronic performance. The stability of halide double perovskites, particularly in comparison to lead-based counterparts, is also highlighted as a key advantage for long-term use in photovoltaic devices. This research underscores the potential of halide double perovskites as a viable alternative for next-generation solar cells, offering a balance between high efficiency, environmental sustainability, and stability. The findings contribute to the growing body of knowledge on perovskite materials and pave the way for further experimental studies aimed at improving photovoltaic device performance using halide double perovskites. The significance of our study is to develop the halide double perovskites and their photovoltaic application.

Keywords: Solar cell; Bandgap; thermoelectric generator; Photovoltaic devices; Double perovskites

1. Introduction

Transitioning to renewable energy sources offers a viable solution to the rapidly depleting fossil fuel reserves. These sources, including solar, wind, hydroelectric, thermoelectric, and geothermal power, provide a sustainable alternative by harnessing natural processes that continually replenish energy supplies. Unlike conventional sources, renewable energy generation emits minimal greenhouse gases and pollutants, mitigating climate change and air pollution. Scientific research and technological innovations have propelled the efficiency and

cost-effectiveness of renewable energy technologies, making them increasingly competitive. Advancements in energy storage and grid integration further facilitate the reliable and scalable deployment of renewable energy systems.

Solar or photovoltaic (PV) energy directly converts sunlight into electricity using semiconductor materials within solar panels [1]. When photons from sunlight strike the surface of a PV cell, they excite electrons within the semiconductor material, creating an electric current. This direct conversion process makes PV systems highly efficient and reliable, with no moving parts and minimal maintenance requirements. PV technology encompasses a wide range of applications, from small-scale residential rooftop installations to large utility-scale solar farms. Additionally, advancements in PV technology have led to the development of a variety of solar cells, which are flexible and lightweight, expanding the possibilities for integration into various surfaces and environments [2, 3]. Our aim of ongoing research is to make better materials and designs to enhance performance and boost its applications, particularly in waste heat recovery and portable power generation [4, 5].

1.1 Solar Cell Evolution: From Crystalline Silicon to Perovskites

It traces back to the discovery of the photovoltaic effect, which is the phenomenon of generating electricity from sunlight [6]. The foundation of solar cell technology was laid in 1839 when French physicist Alexandre-Edmond Becquerel observed that certain materials produce small amounts of electric current when exposed to light [7]. This discovery laid the groundwork for subsequent developments in solar cell technology as discussed below and represented in Figure 1. The current state and annual advancements in different categories of solar cell research, as documented by the National Renewable Energy Laboratory (NREL), are depicted in Figure 2.



Disadvantages: costly, loss of photon energy



1.1.1 First Generation Solar Cells

Indeed, first-generation solar cells, primarily composed of crystalline silicon, have dominated the market since their development in the mid-20th century. Monocrystalline and polycrystalline silicon solar cells exemplify this generation. Monocrystalline silicon cells, with their single-crystal structure, boast higher efficiency, while polycrystalline silicon cells, made from multiple smaller crystals, offer affordability. These silicon-based solar cells, whether single-crystal (concentrator and non-concentrator) or polycrystalline, typically exhibit efficiencies ranging from 12% to 20%, with the highest certified laboratory efficiency reaching up to 27.6% [9]. However, challenges such as complex manufacturing processes, high production costs, and long energy payback times have hindered their widespread adoption. Despite the demand for increased efficiency, there's a growing need for alternative non-toxic material systems to address environmental concerns. Innovations in materials and manufacturing processes continue to drive advancements in first-generation solar cell technologies, aiming to enhance efficiency, reduce costs, and broaden their applicability in the renewable energy landscape.

Best Research-Cell Efficiencies



Figure 2: The top efficiencies achieved in various photovoltaic (PV) technologies, as documented by the National Renewable Energy Laboratory (NREL). Source: https://www.nrel.gov/pv/cell-efficiency.html

1.1.2 Second Generation Solar Cells

Second-generation solar cells, which emerged in the late 20th century, introduced thin-film technologies like cadmium telluride (CdTe), copper indium gallium solenoid (CIGS), and amorphous silicon (a-Si) [10, 11]. These cells offer flexibility, lightweight, and potentially lower manufacturing costs compared to traditional crystalline silicon (c-Si) cells. One instance of such a cell is the solar cell made of Cadmium Telluride (CdTe). Thin-film technology, designed to be approximately 100 times thinner than conventional crystalline silicon (c-Si), seeks to minimize production expenses and material consumption. Additionally, the thin film deposition process enables the production of flexible photovoltaic (PV) modules, potentially decreasing manufacturing expenses. Additionally, thin-film solar cells exhibit thicknesses ranging from nanometres to a few micrometres, facilitating lightweight and flexible designs. Furthermore, thin-film solar cells enable monolithic integration, allowing for a series of connections of cells during fabrication without the need for individual production steps, thus saving time and money.

1.1.3 Third Generation Solar Cells

Third-generation solar cells represent the latest advancements in solar cell technology, aiming to overcome the limitations of first and second-generation cells. These cells incorporate advanced materials and novel designs to enhance efficiency and performance. Some of these are discussed below:

A. Perovskite Solar Cells

Perovskite solar cells have attracted considerable interest because of their promising potential for high efficiency and cost-effective production. Perovskite materials exhibit excellent lightabsorbing properties and can be solution-processed, making them promising candidates for future solar cell technology. It is noteworthy that the highest certified efficiency of perovskite solar cells has reached approximately 26% [9].

B. Organic Photovoltaic Cells (OPVs)

Organic photovoltaic cells (OPVs) represent a burgeoning field within solar energy research, leveraging organic materials in their active layers to harness sunlight and convert it into electricity. What sets OPVs apart is their potential to offer solar panels that are not only cost-effective but also highly flexible and lightweight. This characteristic makes them particularly well-suited for specialized applications, such as powering portable electronics and integrating into wearable devices. While still undergoing development and refinement, OPVs hold significant promise for revolutionizing the landscape of solar energy utilization, offering innovative solutions for diverse energy needs [12, 13].

C. Dye-Sensitized Solar Cells (DSSCs) and Organic Solar Cells (OSCs)

Third-generation solar cells strive for cost-effective, large-scale production using earthabundant and environmentally friendly materials. While Dye-Sensitized Solar Cells (DSSCs) hold promise, they encounter obstacles such as rapid degradation and electrolyte leakage. Organic Solar Cells (OSCs), employing a two-component system, possess distinct advantages but suffer from degradation concerns and lower efficiency relative to established technologies. Despite challenges, DSSCs have achieved a noteworthy certified efficiency of 13%, underscoring their potential for advancement in solar energy technologies [9, 14, 15].

D. Quantum Dot-Based Solar Cells

Quantum dot-based solar cells represent a cutting-edge advancement in photovoltaic technology, offering several key benefits for next-generation solar cell applications. These cells capitalize on the unique properties of quantum dots, including their size and shape-dependent characteristics. Quantum dots exhibit high optical absorption cross-section, enabling efficient capture of sunlight across a broad spectrum. Additionally, their absorption range is tuneable, allowing for customization to match specific solar spectra. Furthermore,

quantum dot-based solar cells are fabricated via low-cost solution processes, making them economically viable. Notably, recent achievements have demonstrated a certified efficiency of 18.1%, highlighting their considerable potential for widespread adoption [9].

E. Hybrid Solar Cells and Organo-Lead Perovskites (OLHPs)

Hybrid solar cells, consisting of donor organic semiconductors and acceptor quantum dots, exploit the advantages of both components. OLHPs, with the general formula ABX₃, offer great potential for low-cost photovoltaics technology. Despite outstanding performance, their commercial application is limited by fast degradation under standard conditions. Notably, perovskite solar cells demonstrated a breakthrough efficiency exceeding 10% [16-19].

1.2 Challenges in Photovoltaic Technology

Despite significant advancements from crystalline silicon to perovskites, challenges persist in the widespread adoption and improvement of PV devices. Ensuring the long-term stability and durability of PV materials remains a critical concern. Additionally, further cost reductions are necessary to accelerate market penetration and achieve grid parity in regions with varying solar resources. Continued research into materials optimization, manufacturing efficiency, and economies of scale is crucial to drive down the overall cost of solar energy. Perovskite solar cells hold immense promise for revolutionizing the solar energy landscape, with ongoing research focused on addressing stability issues, scalability, and commercialization challenges.

2. Thermoelectric Devices: Evolution and Opportunities

Recent data analysis indicates that a significant portion of the energy produced globally, approximately 66%, is lost as heat during various processes such as fossil fuel combustion or nuclear fission (see Figure 3) [20]. This waste heat presents an opportunity for global energy reclamation. Thermoelectric (TE) materials emerge as promising solutions for harnessing waste heat while minimizing environmental harm by converting it into usable electrical energy without carbon emissions. A thermoelectric material captures heat directly, converting it into electricity within a device known as a thermoelectric generator (TEG). Similar to photovoltaics (PVs), wind, and hydropower, TEGs offer sustainable, long-term power generation alternatives. These devices are environmentally friendly, featuring advantages such as solid-state design, high reliability, compactness, lightweight construction, absence of moving parts, zero greenhouse gas emissions, noise-free operation and versatility across temperature ranges, and the requirement of a convenient power source.

Thermoelectric devices, leveraging the principles of the Seebeck and Peltier effects [21-23], have emerged as a transformative technology with vast applications across multiple industries. A deeper understanding of these phenomena can be gained by referring to Figure 4 [24]. One of the major breakthroughs in thermoelectric technology involves the exploration and refinement of new materials that exhibit improved thermoelectric characteristics. Traditional materials like bismuth telluride (Bi₂Te₃) and lead chalcogenides (PbTe) have been the cornerstone of thermoelectric applications [25-27]. However, recent research efforts have focused on exploring new material classes and optimizing existing ones to improve efficiency and performance.

Nanostructuring has emerged as a promising strategy for improving thermoelectric properties by lowering thermal conductivity while maintaining electrical conductivity [28, 29]. By engineering nanostructures such as nanoparticles, nanowires and thin films, researchers have been able to significantly enhance the figure of merit (ZT) of thermoelectric materials [30]. Furthermore, strategic doping has been employed to optimize carrier concentration and mobility, thereby enhancing the electrical conductivity and Seebeck coefficient of thermoelectric materials [31, 32]. Advances in computational modelling and high-throughput screening have accelerated the discovery of promising thermoelectric candidates, enabling researchers to explore a vast design space and identify materials with superior performance. Exploration of new material classes, such as half-Heusler, skutterudites, perovskites, and complex oxide compounds, has expanded the range of thermoelectric materials available for various applications. These materials exhibit unique electronic band structures and phonon scattering mechanisms, offering opportunities for further optimization and performance enhancement.



Figure 3: Diverse waste energy sources and the conversion of waste heat into electricity using a thermoelectric generator [20].



Figure 4: Diagram showing the thermoelectric Seebeck and Peltier effects [24].

2.1 Applications of Thermoelectric Devices

The versatility of thermoelectric devices has led to their adoption in a wide range of applications across various industries. One of the primary applications of thermoelectric technology is waste heat recovery, where thermoelectric generators (TEGs) are employed to convert waste heat from industrial processes, automotive exhausts, and power plants into electricity [33]. In the automotive industry, thermoelectric modules are integrated into exhaust systems to improve fuel efficiency and reduce emissions by converting waste heat into electricity to power onboard electronics or recharge batteries [34]. Similarly, thermoelectric devices find applications in aerospace systems, where they provide auxiliary power generation and thermal management solutions [35]. Thermoelectric coolers (TECs) are another prominent application of thermoelectric technology, offering precise temperature control and thermal management in electronic devices, refrigeration systems, and medical equipment [36]. TECs utilize the Peltier effect to create a temperature gradient across the device, enabling rapid heating or cooling of electronic components, sensors, and optical systems. Thermoelectric energy harvesting systems leverage ambient temperature gradients to generate electricity for remote power generation, wireless sensor networks, and IoT devices. These self-powered systems eliminate the need for batteries or external power sources, making them ideal for applications in remote or inaccessible locations.

2.2 Challenges and Future Directions

Despite the significant advancements and widespread applications of thermoelectric technology, several challenges persist, hindering its full-scale deployment and commercialization. One of the primary challenges is improving the efficiency of thermoelectric materials, particularly at high temperatures where traditional materials exhibit limited performance [37]. Cost reduction is another critical factor for the widespread adoption of thermoelectric devices across various applications. The high cost of thermoelectric materials and fabrication processes remains a barrier to large-scale commercialization, necessitating the development of cost-effective manufacturing techniques and scalable production methods [38]. Reliability and durability are also key challenges for thermoelectric devices, especially in harsh operating environments characterized by temperature fluctuations, mechanical stresses, and corrosive atmospheres. Improving the long-term stability and robustness of thermoelectric modules is essential to ensure their

performance and reliability in real-world applications [39]. Continued advancements in materials science and manufacturing techniques are essential to overcome existing challenges and unlock the full capabilities of thermoelectric technology. With ongoing research, thermoelectric devices are poised to play a significant role in addressing global energy challenges and driving sustainable technological advancements in the years to come.

3. Perovskites and Their Derivatives

Perovskites, with the CaTiO₃ prototype, were initially identified by Russian mineralogist Count Lev Aleksevich von Perovskite [40] and were aptly named in his honour. These materials have attracted considerable interest because of their versatile and multifunctional properties, making them a focal point of research across various scientific and technological fields. The ideal cubic structure of perovskites adheres to the stoichiometric formula ABX₃, wherein 'A' and 'B' represent cations, and 'X' denotes anions, which can encompass oxygen or halogen elements. Over time, the term "perovskite" has evolved to encompass a broader spectrum of synthesized materials that share the same crystal structure and stoichiometric ratio as CaTiO₃, adhering to the general formula ABX₃.



Figure 5: The Colour scheme for a variety of perovskite compounds.

3.1 Simple Perovskite Structure

The chemical composition ABX_3 typically describes simple perovskites in their idealized form, comprising cubes composed of three distinct chemical elements (A, B, X) in a 1:1:3 ratio. 'A' and 'B' represent metallic cations, which carry a positive charge, while 'X' denotes non-metallic anions, which bear a negative charge. 'A' primarily consists of alkaline earth elements with oxidation states of +2 or +3, whereas 'B' encompasses transition or rare earth cations with oxidation states of +4 or +3. Conversely, 'X' exists as an anion with an oxidation state of -2.

Perovskites fundamentally manifest as a three-dimensional array of corner-sharing oxygen octahedra, with 'A' site atoms positioned at the centre of each cube. The 'B'-site atoms occupy all eight corners, while 'X' atoms are situated at the midpoints of the cube edges. The basic structure of a simple perovskite adopts a simple cubic arrangement with the space group

 $Pm\overline{3}m$ (221), as depicted in Figure 6 [41]. In this arrangement, cation 'A' occupies the 4a position at coordinates (0, 0, 0); cation 'B' occupies the 4b position at coordinates (0.5, 0.5, 0.5), and anion X is situated at the face centre, occupying the (0.5, 0.5, 0) Wyckoff positions [41]. Initially, it was believed that perovskite structures only crystallized in cubic or pseudo-cubic forms. However, subsequent studies revealed that distortions within the cubic structure give rise to various phases, including tetragonal, orthorhombic, rhombohedra, and hexagonal structures. These distortions primarily stem from the tilting of the BO₆ octahedral and the displacement of cations at the 'A' positions.



Figure 6: The ideal cubic Pm-3m structure of an ABX₃ perovskite where X refers to the oxides and halogens [41].

3.2 Double Perovskite Structure

As previously discussed, the perovskite structure boasts remarkable compositional flexibility, allowing for the manipulation of 'A' and 'B' cations at various atomic sites, as well as the potential to increase the size of these cations. In the realm of double perovskites (DPs), the 'B'-site cations are precisely substituted with half of the 'B' cations, resulting in compounds known as double perovskites $A_2BB'X_6$ [42, 43]. Thus, double perovskites adhere to the general formula $A_2BB'X_6$, where 'A', 'B', and 'B' represent cations, while 'X' signifies an anion. These are of two types:

3.2.1 Oxide Double Perovskite Structure

In this type of structure, typically, the 'X' site is occupied by oxygen atoms; the 'A' site is occupied by alkaline earth or rare-earth metals, exhibiting a 12-fold coordination with oxygen atoms. Meanwhile, the 'B' and 'B'' sites are filled by transition or rare earth metals, featuring 6-fold coordination with oxygen anions and located within the octahedral centre. Notably, 'B' and 'B'' occupy alternative crystallographic sites, with the 'B'-type atom being surrounded only by 'B'' neighbours, and vice versa. This unique arrangement gives rise to ordered double perovskite structures, as illustrated in Figure 7 [44]. In terms of atomic positions within the structure, 'A' occupies the 8a position at coordinates (0.25, 0.25, 0.25), 'B' occupies the 4b position at coordinates (0.5, 0.5, 0.5), 'B'' occupies the (0, 0, 0) position, and 'O' occupies

the 24e position at coordinates (X, 0, 0) [45]. Additionally, in double perovskites, octahedral tilting occurs, leading to a reduction in symmetry, which can be quantified using the tolerance factor, considering the distance between the 'B' and 'B'' cations.

In compounds of the form $A_2BB'O_6$, the cations exhibit ordering in various directions, with the most common arrangement involving cations alternating in all directions, resembling a rock salt-type arrangement known as the elpasolite structure, named after the mineral K_2NaAlF_6 [46]. This distinctive combination of different B-site cations, including transition and inner transition metals in various oxidation states, results in a wide array of properties, making it a subject of significant interest and exploration.



Figure 7: (a) Perovskite and (b) Double Perovskite structure [44].

3.2.2 Halide Double Perovskite Structure

Halide perovskites trace their origins back to the 1800s following the discovery of elpasolite, a mineral composed of K_2NaAlF_6 . These perovskites, characterized by the general formula ABX₃, feature monovalent cations such as Methylammonium (MA+) and Formamidinium (FA+) at the 'A' position, divalent cations like Pb²⁺ at the 'B' position, and halide elements (commonly Cl, Br, I) denoted by 'X' [47, 48]. However, because of apprehensions about the stability of organic cations and the toxicity of lead, there's a pressing need for substitutions. Typically, the 'A' position is occupied by Cs, Li, Na, K, or Rb, while lead at the 'B' position is replaced by non-toxic, eco-friendly elements that offer structural and thermodynamic stability. In recent years, researchers have explored using 3d transition metal ions to replace lead, ensuring overall charge neutrality and stoichiometric stability [49]. Consequently, the interest in lead-free halide perovskites has grown due to their diverse applications in photovoltaics and has also been the subject of recent investigations into their transport properties.

3.3 Inverse Perovskite or Antiperovskite Structure

The antiperovskite structure is characterized by its ABX₃ crystal framework, where the positions of ions are inverted compared to traditional perovskites, featuring differently sized anions ('A' and 'B') and a cation ('X'). In this structure, the 'B' anions occupy the centre of a

six-fold coordinated octahedron, aligning within a cubic space group Pm-3m. The 'A' anions, on the other hand, engage in twelvefold coordination with the 'X' cations. This architecture is underpinned by a three-dimensional lattice comprised of BX_6 octahedra that share corners, a feature illustrated in Figure 8.



Figure 8: Perovskite structure to antiperovskite structure transformation [50].

This figure not only highlights the skeletal framework but also elucidates the transition from perovskite to antiperovskite structures. Exhibiting a wide array of intriguing characteristics, antiperovskites have captured the interest of researchers for their magnetic, ionic conductive, superconductive, and topological insulating properties. Moreover, they have been identified for their negative thermal expansion, superionic conductivity, and potential as host materials for photoluminescence, among other applications [51, 52].

4. Stability Factor

For solar cells to operate effectively, they must endure specific environmental and internal conditions without suffering degradation. These conditions include exposure to atmospheric elements such as moisture, light, oxygen, and water, as well as internal factors like thermal degradation attributable to the inherent properties of the materials used. Presently, the perovskite research community is primarily focused on addressing the challenge of long-term stability. The difficulty in predicting crystal structures based on chemical compositions remains a significant hurdle in the swift development of new materials [53].

The Goldschmidt tolerance factor, symbolized as "t", is pivotal in forecasting the stability of perovskite configurations via the equation:

$$t = (R_A + R_X) / \sqrt{2} (R_B + R_X),$$

where R_A , R_B , and R_X represent the ionic radii of the A, B, and X ions, respectively. This calculation aids in understanding the symmetry of the crystal structure of perovskites. A Goldschmidt tolerance factor (t) of 1 signifies an ideal cubic perovskite structure, whereas a value in the range of 0.9 < t < 1 suggests the occurrence of octahedral tilting, which reduces the crystal structure's symmetry.

Additionally, the octahedron factor, denoted as $\mu = RA/RX$, is used alongside the Goldschmidt tolerance factor to assess the likelihood of forming stable metal halide perovskite structures. If $\mu > 0.442$, the formation of a stable octahedral is probable [54]. Usually, the stability of the perovskite configuration remains intact within a tolerance factor (t) range of 0.71 to 1.12. A cubic phase prevails when t lies within 0.9 to 1.0. For values of t ranging from 0.71 to 0.9, the structure tends to be either orthorhombic or rhombohedra. In instances where t exceeds 1, a hexagonal configuration is favoured, whereas t values below 0.71 lead to the emergence of various other structural types [55]. The tolerance factor is not an adequate descriptor of stability for anti-perovskites, experimentally, their hygroscopic nature makes them challenging to synthesise and, as such, their preparation has been the subject of considerable debate in recent years.

Investigating the intriguing world of double perovskite structured materials, particularly their optical and thermoelectric characteristics, presents a promising research avenue. Given the scarcity of theoretical and experimental analyses concerning the lattice dynamics, along with the optical and thermoelectric features of the chosen materials, this study seeks to lay the groundwork for future experimental exploration into these compounds, potentially unlocking new applications. This research comprehensively examines the structural, electronic, optical, and thermoelectric properties of various HDPs. The methodology employed encompasses the first-principles FP-LAPW approach within the framework of DFT, complemented by the semi-classical Boltzmann theory, aiming to offer a comprehensive insight into these materials.

5. Conclusion

Halide double perovskites present a highly promising avenue for the development of nextgeneration photovoltaic devices due to their unique structural, electronic, and optical properties. This study has demonstrated that these materials offer several advantages over traditional lead-based perovskites, particularly in terms of environmental sustainability and long-term stability. The ability to fine-tune the bandgap of halide double perovskites through compositional modifications enhances their suitability for solar energy applications, enabling more efficient absorption and conversion of sunlight. Our investigation highlights the strong optical absorption capabilities of halide double perovskites in the visible spectrum, which is a key factor in maximizing the efficiency of solar cells. The electronic properties, such as band structure and charge carrier dynamics, also contribute significantly to their performance potential. Furthermore, the improved stability of these materials over lead-based perovskites addresses one of the major challenges facing perovskite-based solar cells, making them more viable for commercial and large-scale applications.

This study aims to investigate and analyse the fundamental physical properties of novel Halide double perovskite materials. Furthermore, given their potential utility in thermoelectric devices, exploring their thermoelectric properties is necessary. This study aims to thoroughly comprehend HDP materials' properties, thereby establishing a foundation for the advancement of sophisticated optoelectronic and thermoelectric applications.

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