STABLE CARBON-BASED PEROVSKITE SOLAR CELLSUSING ADDITIVE ENGINEERING ON HALIDE PEROVSKITES

Jharna Sahane
Research Scholar (Physics) ISBM University Gariyaband Chhattisgarh
Dr. N K Swamy (Assistant Professor)
Research Supervisor, School of Science, ISBM University Gariyaband Chhattisgarh

---

Abstract

Perovskite solar cells (PSCs) have emerged as a transformative photovoltaic technology due to their high power conversion efficiency and low-cost fabrication. However, their long-term operational stability remains a major challenge, particularly due to the sensitivity of halide perovskite materials to moisture, heat, and light-induced degradation. In this study, we report the development of stable carbon-based perovskite solar cells through additive engineering of halide perovskite layers. The incorporation of functional additives into the perovskite precursor solution was employed to regulate crystal growth, passivate defects, and enhance film morphology. Carbon-based electrodes were utilized as a cost-effective and chemically stable alternative to conventional noble metal contacts, thereby improving device durability and reducing fabrication costs. Additives such as small organic molecules, polymers, and inorganic salts were systematically introduced to optimize crystallinity, reduce trap states, and improve charge transport properties. The modified perovskite films exhibited enhanced grain size, reduced pinholes, and improved surface uniformity, as confirmed by structural and morphological characterization techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM), and photoluminescence (PL) analysis. The fabricated devices demonstrated improved power conversion efficiency along with significantly enhanced thermal and environmental stability compared to control samples. Notably, the additive-engineered perovskite layers contributed to reduced non-radiative recombination and improved interfacial contact with the carbon electrode. Stability tests revealed sustained performance under ambient conditions, highlighting the effectiveness of additive engineering in mitigating degradation pathways. Overall, this study provides a promising strategy for enhancing the stability and performance of carbon-based perovskite solar cells. The findings offer valuable insights into material optimization and device engineering, paving the way for the development of durable, low-cost, and scalable photovoltaic technologies.

Keywords : *Carbon-Based, Perovskite Solar, Halide Perovskites*

Introduction

The global demand for clean and sustainable energy has driven significant advancements in photovoltaic technologies, with perovskite solar cells (PSCs) emerging as one of the most promising next-generation solutions. Since their inception, PSCs have witnessed a remarkable increase in power conversion efficiency, rising from below 4% to over 25% within a short span of time. This rapid progress is largely attributed to the exceptional optoelectronic properties of halide perovskite materials, including high absorption coefficients, tunable bandgaps, long charge carrier diffusion lengths, and low exciton binding energies. These characteristics make halide perovskites highly suitable for efficient light harvesting and charge transport. Despite these advantages, the commercialization of PSCs is hindered by their intrinsic instability under environmental stressors such as moisture, oxygen, heat, and prolonged light exposure. The degradation of perovskite materials leads to a rapid decline in device performance, posing a significant challenge for their practical application. In addition, the use of expensive and reactive noble metals like gold and silver as electrodes further limits the scalability and long-term stability of these devices. Consequently, there is a growing need to develop cost-effective, stable, and scalable alternatives for both materials and device architectures. Carbon-based perovskite solar cells have gained attention as a viable alternative due to the inherent advantages of carbon materials, including chemical inertness, hydrophobicity, thermal stability, and low cost. Carbon electrodes, such as graphite and carbon black, can replace conventional metal electrodes without compromising device functionality, while also enhancing resistance to environmental degradation. Moreover, carbon materials are compatible with scalable fabrication techniques such as screen printing, making them suitable for large-scale production. A critical strategy to address the stability issues of halide perovskites is additive engineering, which involves the incorporation of small quantities of functional additives into the perovskite precursor solution. These additives play a vital role in controlling crystallization kinetics, improving film morphology, passivating defects, and enhancing interfacial properties. By reducing trap states and suppressing non-radiative recombination, additive engineering significantly improves both the efficiency and stability of PSCs. Various types of additives, including organic molecules, polymers, alkali metal ions, and inorganic salts, have been explored to optimize perovskite film quality and device performance. The integration of additive-engineered perovskite layers with carbon-based electrodes represents a synergistic approach to overcoming the limitations of conventional PSCs. Improved crystallinity and reduced defect density contribute to enhanced charge transport, while the carbon electrode provides a stable and moisture-resistant interface. This combination not only enhances device efficiency but also significantly improves long-term operational stability under ambient conditions. Furthermore, understanding the relationship between additive chemistry, perovskite film formation, and device performance is essential for rational design and optimization. Advanced characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), UV–Vis spectroscopy, and photoluminescence (PL) analysis are commonly employed to investigate structural, optical, and electronic properties of the modified films. These insights enable the development of more robust and efficient solar cell architectures. In this context, the present study focuses on the development of stable carbon-based perovskite solar cells through additive engineering of halide perovskites. The objective is to enhance both efficiency and durability by optimizing material composition and device structure. This research contributes to the ongoing efforts to make perovskite solar technology more reliable, cost-effective, and suitable for real-world energy applications, thereby supporting the global transition toward sustainable energy solutions.

Perovskite Solar Cells: An Overview

Perovskite solar cells (PSCs) represent a significant improvement in photovoltaic technology during the last decade. These devices use a class of minerals known as perovskites, characterized by a common crystal structure similar to calcium titanium oxide ($CaTiO_3$). Perovskite materials in solar cells are predominantly organic–inorganic hybrid halides, defined by the chemical formula ABX_3, where 'A' indicates a monovalent cation (such as methylammonium, formamidinium, or cesium), 'B' denotes a divalent metal cation (usually lead or tin), and 'X' represents a halide anion (iodide, bromide, or chloride). This unique structure provides exceptional optoelectronic properties that make perovskites very suitable for solar energy conversion. A key advantage of perovskite materials is their remarkable light absorption capability. Slender layers of perovskite can efficiently absorb a wide range of sunlight, enabling the creation of lightweight and adaptable solar systems.

Furthermore, perovskites have prolonged charge carrier diffusion lengths and low exciton binding energies, promoting the efficient separation and movement of electrons and holes inside the material. These properties improve power conversion efficiencies (PCEs), which have increased from around 3.8% in 2009 to over 25% in recent years, rivaling traditional silicon-based solar cells. The essential structure of a perovskite solar cell has many functional layers arranged in a specific order to enhance charge generation and extraction. The device typically consists of a transparent conductive oxide (TCO) layer, such as fluorine-doped tin oxide (FTO) or indium tin oxide (ITO), serving as the front electrode. The electron transport layer (ETL), often made of materials like titanium dioxide (TiO_2) or tin oxide (SnO_2), facilitates electron movement while preventing hole migration. The perovskite absorber layer is positioned above the electron transport layer and is essential for capturing sunlight and generating electron-hole pairs. The hole transport layer (HTL), positioned above the perovskite layer, often comprises organic materials such as Spiro-OMeTAD or inorganic options such nickel oxide (NiO). Ultimately, a back electrode, usually made of metals like gold or silver, completes the setup. Perovskite solar cells may be classified into many architectures based on their structural configuration, including mesoporous, planar, and inverted (p-i-n) structures. In mesoporous structures, a porous scaffold, often TiO_2, underpins the perovskite layer, hence enhancing charge separation and transport. Planar designs eliminate the mesoporous layer, optimizing production and enhancing compatibility with flexible substrates. The inverted design modifies the arrangement of electron and hole transport layers, often improving device stability and reducing hysteresis effects. Each architectural design has unique advantages and challenges, with ongoing research aimed at optimizing these structures for improved efficiency and resilience.

\Despite their remarkable efficacy, PSCs have several challenges that hinder their broad commercialization. A major worry is their instability in response to environmental factors such as moisture, oxygen, heat, and ultraviolet (UV) light. The organic components of hybrid perovskites demonstrate increased vulnerability to degradation, leading to rapid decline in device performance over time. The presence of lead in several high-performing perovskite compounds poses concerns about environmental safety and toxicity. Researchers are rigorously exploring lead-free alternatives, such as tin-based perovskites, despite their current lower efficiency and stability.

Carbon-Based Perovskite Solar Cells (C-PSCs)

To replace the costly noble metals used as back electrodes in traditional perovskite solar cells, carbon-based perovskite solar cells (C-PSCs) have recently gained popularity. The carbon materials used as the counter electrode in C-PSCs include graphene, carbon nanotubes (CNTs), graphite, and carbon black. These materials are ideal for improving the longevity and economic feasibility of perovskite solar cells because of their cheap cost, strong electrical conductivity, chemical stability, and hydrophobicity, among other benefits. Fixing the problem of stability over time is a major driving force behind using carbon electrodes instead of metal ones. Device deterioration may occur when conventional metal electrodes diffuse into the perovskite layer due to thermal or operational stress. Carbon, on the other hand, is chemically inert and hence improves the device's stability since it reacts less readily with perovskite components. Another important aspect in reducing environmental deterioration is the improved resistance to moisture intrusion that carbon electrodes provide owing to their hydrophobic characteristics.

A hole transport material (HTM)-free design is often used to construct C-PSCs, which further simplifies device production and saves cost. Here, the carbon electrode serves as a collector of holes by coming into direct touch with the perovskite layer. Organic hole transport materials such as Spiro-OMeTAD are no longer necessary; these materials are unstable, costly, and vulnerable to moisture and dopant degradation, all of which may reduce their long-term effectiveness. Consequently, C-PSCs are sometimes called "fully printable" or "low-cost" solar cells since they can be made utilizing scalable processes like screen printing and doctor blading.

There are two primary structural forms of carbon-based perovskite solar cells (C-PSCs): those that are subjected to high temperature processing and those that are subjected to low temperature processing. Mesoporous scaffolds made of layers of elements like TiO_2, ZrO_2, and carbon are sintered at high temperatures (around 400-500°C) in high-temperature devices in a specific order. The next step is to introduce the perovskite precursor into this open architecture. Although they aren't compatible with flexible substrates because to the high processing temperature, these devices are quite stable and can be mass-produced. In contrast, low-temperature C-PSCs allow for the use of lightweight and flexible substrates by directly depositing carbon paste or ink onto the perovskite layer at comparatively lower temperatures.

Although C-PSCs have several benefits, their power conversion efficiencies are often lower than those of metal-electrode alternatives. This is mainly because the perovskite and carbon electrodes have a larger interfacial resistance and charge extraction efficiency is lower. But new developments in material optimization, additive integration, and interface engineering have made a world of difference to how well they work. Improved carbon formulations, surface passivation methods, and conductive additives have all contributed to better charge transfer and lower recombination losses. The fact that carbon-based electrodes may be manufactured under ambient circumstances is another great benefit. When processing C-PSCs, there is usually no performance loss even when processing in air, in contrast to traditional PSCs that need controlled settings (such glove boxes) to avoid deterioration during manufacture. Especially in contexts with limited resources, this quality lends credence to their commercialization and mass manufacturing possibilities. To address these performance issues, additive engineering has recently attracted a lot of attention in the realm of carbon-based PSCs. Perovskites may have their crystallinity, defect density, and interfacial contact with carbon electrodes improved by additives. Because of the significant gains in efficiency and stability brought about by this complementary strategy, C-PSCs are now a very appealing topic for researchers interested in photovoltaics. A scalable, stable, and inexpesive substitute for conventional perovskite solar cells is carbon-based perovskite solar cells. Efficacy and charge transfer over interfaces are still obstacles, but new developments in additive engineering and material design are helping to close the gap. Given their intrinsic benefits and increasing attention from researchers, C-PSCs have great promise for future use in cost-effective and environmentally friendly solar power systems.

Halide Perovskites: Composition and Properties

Perovskite solar cells rely on halide perovskites, the main functional material, to absorb light and generate charges. The typical chemical formula for these substances is ABX_3, where 'A' stands for a monovalent cation like methylammonium (MA^+), formamidinium (FA^+), or cesium (Cs^+), 'B' is a divalent metal cation like lead (Pb^{2+}) or tin (Sn^{2+}), and 'X' is a halide anion like iodide (I^-), bromide (Br^-), or chloride (Cl^-). Halide perovskites' exceptional optoelectronic capabilities are due to the three-dimensional crystal lattice that these ions generate when arranged in this way. The capacity of halide perovskites to absorb light is one of their most notable characteristics. These materials are able to effectively capture solar energy, even in thin sheets, due to their high absorption coefficients throughout the visible spectrum. This quality allows for the creation of solar cells that are both lightweight and flexible while also reducing the amount of material used. You may change the amount of halide ions or cations in halide perovskites to make them have different bandgaps. Substituting bromide for iodide raises the bandgap, which makes the material suitable to tandem solar cell uses. Halide perovskites also have long diffusion lengths and strong charge carrier mobility, which are important properties. Absorption of light causes electrons and holes to be created, which may then flow through the material for extended distances with little recombination losses. This improves the efficiency of charge collecting and helps perovskite solar cells achieve high power conversion efficiencies. At ambient temperature, electron-hole pairs may be easily separated into free charge carriers due to these materials' low exciton binding energy. The device performance is highly dependent on the shape and crystallinity of halide perovskite layers. Efficient charge transport with low recombination requires films that are uniform, large-grain, and defect-free. On the other hand, recombination centers created by defects like vacancies, interstitials, and grain boundaries may have a negative impact on stability and efficiency. This is why there is a strong emphasis on using methods like additive engineering and solvent engineering to manage the crystallization process.

When contrasted with conventional semiconductors, halide perovskites also show an impressive level of defect tolerance. This indicates that the material may keep its excellent electrical characteristics even when certain faults are present. The unusual property is a result of the electronic band structure, which is characterized by shallow defect states that do not trap charge carriers very well. Therefore, even with very basic manufacturing procedures, perovskite solar cells may attain high efficiency. These benefits aren't without their drawbacks, however; halide perovskites aren't without their stability issues. Moisture, oxygen, heat, and ultraviolet (UV) radiation are just a few of the environmental elements that may greatly affect these materials. The perovskite structure may degrade, ions can migrate, and the material can break down into its component parts when exposed to certain circumstances. Device performance might be negatively affected, for instance, when methyl ammonium lead iodide ($MAPbI_3$) breaks down into lead iodide (PbI_2). The long-term use of perovskite solar cells depends on fixing these stability problems.

The usage of lead, which is harmful to both humans and the environment, is another cause for worry when it comes to halide perovskites. Research on lead-free alternatives using elements like tin (Sn), germanium (Ge), and bismuth

(Bi) is continuing, even though lead-based perovskites provide the best efficiency at the moment. Still, these substitutes need more work before they can be considered serious contenders; they aren't always as stable or efficient. When designing halide perovskites, it is crucial to think about thermal and phase stability. At high enough temperatures, phase transitions may occur in some perovskite compositions, especially those that include methylammonium, which can cause structural instability. Alternatively, perovskites made entirely of inorganic elements, such cesium lead iodide ($CsPbI_t$), have higher thermal stability but could need very hot conditions to crystallize. To find a happy medium between stability and performance, scientists are investigating mixed-cation and mixed-halide compositions.

Solar cells aren't the only optoelectronic device that might benefit from halide perovskites; LEDs, photodetectors, and lasers are just a few other examples. Their strong photoluminescence quantum yield, simplicity of production, and adjustable optical characteristics make them materials with a broad variety of potential uses. The need of thoroughly comprehending their composition and characteristics is further underscored by their multifunctionality. Methods for improving halide perovskites' characteristics have recently emerged thanks to developments in additive engineering. The use of additives has the potential to increase film quality and decrease defect density by influencing nucleation and crystal formation. In addition to improving efficiency and stability, they may passivate grain boundaries and interfaces. Research into this method has grown in importance as a means of improving the efficiency of halide perovskite materials used in solar cells. The fast advancement of perovskite solar cells is supported by halide perovskites, a group of very promising materials. Their adjustable composition, cheap production cost, and outstanding optical and electrical characteristics make them perfect for next-generation solar systems. Nevertheless, ongoing research and innovation are necessary to tackle the issues of stability, toxicity, and scalability. Improving the efficiency and dependability of carbon-based perovskite solar cells and getting them commercialized requires a thorough understanding of halide perovskites' composition and characteristics.

Stability Issues in Perovskite Solar Cells

A key obstacle preventing perovskite solar cells (PSCs) from being commercialized is their long-term stability, even though power conversion efficiency has made tremendous improvement. Because of their inherent sensitivity to environmental and operational stress factors such moisture, oxygen, temperature, light exposure, and electrical bias, perovskite materials, particularly hybrid organic-inorganic halide perovskites, may cause stability difficulties. Chemical deterioration, structural instability, and a gradual decline in performance are all possible outcomes of these causes. Humidity is a major influence on the stability of PSCs. Perovskites based on halides, especially those containing methylammonium, are very receptive to water molecules and may form strong interactions with them. Through this interaction, the perovskite structure may undergo decomposition, releasing volatile organic components and its original components like lead iodide (PbI_2). Device efficiency drops dramatically as a consequence of the degradation process, which is often irreversible. Environmental protection is crucial for the lifespan of devices, since even low humidity levels may start deterioration. Perovskite deterioration, particularly when exposed to light, is accelerated by oxygen and other environmental factors. The perovskite lattice is vulnerable to superoxide species, which are formed when oxygen molecules combine with photo-generated electrons. As a result, the material degrades and the optoelectronic characteristics of the device degrade. One major issue with using it outside is the rate of breakdown, which is accelerated when oxygen and moisture are present. Concerns of thermal instability are equally substantial with PSCs.

In perovskite materials, phase transitions may be induced by high temperatures, especially in those that include organic cations such as methylammonium (MA^+). The efficiency of charge transport may be diminished and the crystal structure disrupted by these phase shifts. Furthermore, the material might become even more unstable due to the evaporation of volatile components caused by extended contact to heat. Thermal stability is an important metric for the practical deployment of solar cells since they are often exposed to high temperatures in real-world settings. Photostability, the degrading of perovskite materials under prolonged light exposure, is another critical concern. In instance, the perovskite layer and neighboring transport layers may be degraded by photo-induced processes initiated by ultraviolet (UV) light. Titanium dioxide (TiO_2), a popular electron transport material, may degrade when exposed to ultraviolet light, which lowers the device's efficiency. The need of using materials and layers that are resistant to ultraviolet radiation in PSC design is emphasized by this. Perovskite layer ion migration is another stability-affecting issue. Ions like iodide (I^-) or methylammonium (MA^+) may move across the crystal lattice when exposed to an electric field or light. As a result of this motion, current-voltage hysteresis, interface charge buildup, and defect creation occur. The movement of ions through a material may lead to permanent structural changes and a decline in device performance over time. In addition, it makes the system less stable while running continuously.

Degradation of the interface is another important problem with PSCs. Chemical reactions, defect formation, and energy mismatch often occur at interfaces between distinct layers, such as the charge transport and perovskite layers. Recombination losses and charge extraction efficiency may both be negatively impacted by interface quality. Under electrical or thermal stress, metal electrodes (such as gold or silver) may also diffuse into the perovskite layer, hastening the breakdown process even further. Also causing instability is the usage of organic hole transport materials (HTMs) like Spiro-OMeTAD. Dopants are used to improve the conductivity of certain materials; nevertheless, dopants may deteriorate when exposed to moisture. In addition, the device's stability is severely affected by ambient conditions due to the hygroscopic nature of these materials. As a result, there has been a surge in research on potential substitute methods, including electrodes made of carbon and HTM-free designs. To shield PSCs from the elements, encapsulation techniques have been developed; however, these methods increase the complexity and expense of device manufacture. Ion migration and thermal instability are fundamental degradation processes that cannot be entirely eliminated, even though encapsulation may greatly increase stability. As a result, studying how to make perovskite materials more stable inherently is still very important.

Oxide-Based Perovskite Materials

A big family of ABO3 structures are oxide-based perovskite materials. As a general rule, A cations are more significant than B cations and O anion in this kind of structure. The same chemical formula may take on many three-dimensional forms by varying the combinations of A, B, and O, all while maintaining charge neutrality. Because of its exceptional quality, ABO3 materials have been the subject of much research. In 1920, Goldschmidt provided an explanation about the deep chemistry of perovskites based on oxides.

Polyhedral packing, which is related to tolerance (t) and octahedral (μ) factors, was shown to be significantly affected by relative radii size, according to the research. The variables t and ν will be covered in more detail in the section that follows. A broad range of electronic characteristics, including capacitive, ferroelectric, piezoelectric, metallic, superconductive, catalytic, and magnetic, may be achieved under ambient conditions by adjusting the composition of oxide-based perovskite materials, which have a high bandgap. Ferroelectric and thermoelectric applications mostly make use of perovskite minerals like BaTiO3 and SrSnO3. These materials have recently undergone doping with rare earth ions, resulting in a novel class of phosphor materials.

Halide Based Perovskite Materials

When it comes to the chemical formula, ABX3, halide perovskites are quite similar to oxide perovskites. Here, X= I-, Cl-, and Br-and B is the divalent (inorganic) cation on the A cation of the ABX3 structure. There are two main categories of halide-based perovskites, however.

- Inorganic perovskite materials
- Organic-inorganic perovskite materials

Inorganic Halide Perovskite

The element A in these perovskite materials is an alkaline metal, such Cs+, Rb+, K+, Li+, etc., from the first group of the periodic table. The characteristics of inorganic halide perovskites are comparable to those of organic -Inorganic perovskites, with the exception that inorganic perovskites have better thermal stability.When it comes to perovskite quantum dot manufacturing, inorganic perovskite materials such as CsPI3, CsPbBr3, CsSnI3, and CsPbI3-xBrx are well-known. Of them, maintaining the stability of CsPbI3 perovskite materials under room temperature and humidity has proven to be the most difficult. Additionally, octahedral tilting and poorer symmetry are caused by the fact that Cs+ is smaller than (MA)+.The increased bandgap (1.73 eV) of CsPbI3 compared to CH3NH3PbI3 (1.57 eV) is mostly due to this.

Organic-Inorganic Halide Perovskites

OIHPs are chemically defined as ABX3 (where X= I, Br, Cl, or a mixed halide). The organic component with the alkaline amine group occupies the A site here; examples of such groups are methyl ammonium (CH3NH3) +, formamidinium (FA), HC(NH2)2+, ethyl ammonium (PEA), etc. The term "hybrid perovskite material" describes the unusual blend of organic and inorganic elements found in perovskites. X represents a halide anion, whereas the B site includes divalent cations like Pb2+ or Sn2+.

Structural Properties of Organic-Inorganic Halide Perovskites

The cubic structure of perovskites is determined by octahedral and tolerance factors. Figure 1.5 shows that the electric characteristics of ABX3 perovskite materials are controlled by the B-X bond, which is mediated by inorganic materials, and not by the A cation. The ideal cubic symmetry of a perovskite material corresponds to 12-fold A cation coordination, 6-fold B cation coordination, and a BX6 octahedral corner. Of all the organic cations, MA ions are the most common A cations in hybrid perovskites. Because the t value is smaller at ambient temperature owing to the tiny size of MA, MAPbI3 possesses tetragonal symmetry instead of cubic symmetry. Substituting A cation with materials with large ionic radii, in the sequence RCs<RMA~RFA~REA, may reduce the band gap of MAPbI3, which is 1.51–1.55 eV. The data show that EA has the biggest ionic radii of any A site, yet its unusually large cation causes EAPbI3 to switch from a three-dimensional symmetrical crystal structure to a two-dimensional orthorhombic one, with a band gap of 2.2 eV. In contrast, FA is positioned between EA and MA, giving it more symmetry than MA and an advantageous energy gap of 1.43–1.48 eV for FAPbI3 perovskites.

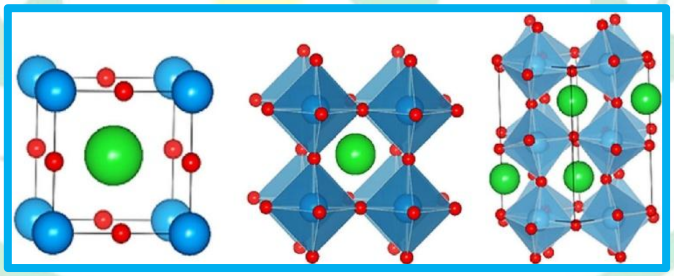
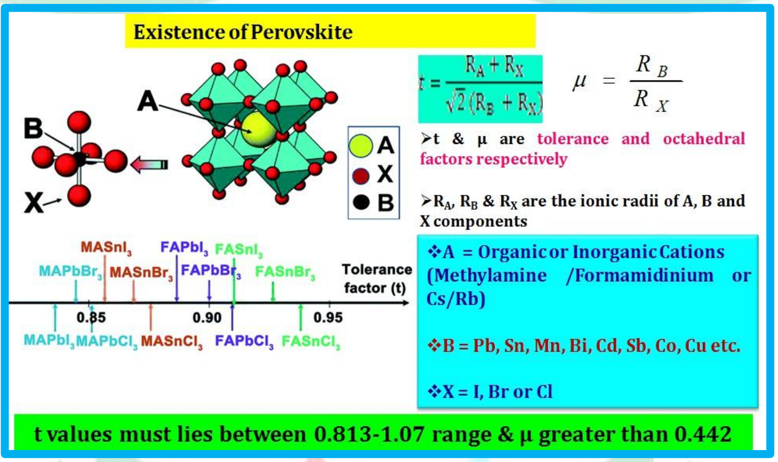


Figure 1. 1The ideal cubic perovskite unit cell (a) A cations (blue) occupy the lattice corners, B cations (green) occupy the interstitial site, and X anions (red) occupy lattice faces. (b) An alternative view depicting B cations assembled around X anions to form BX6 octahedral, as B X bonds are responsible for determining electrical properties. (c) Tilting of BX6 octahedral occurring from non-ideal size effects and other factors, inducing strain on the B X bonds.

❄♒♏ ☜⌧♓⬧⧫♏■♍♏ □♐ ⚐♏❒□❖⬧☚♓⧫♏ ⬧⧫❒◆♍⧫◆❒♏

The typical chemical formula for a perovskite structure may be either ABX3 or ABO3, depending on the content. When two cations and an anion (at the X site) are in charge neutrality, as stated in , we get N(A) + N(B)=3. N(X).

The valence of the A and B components is represented by N, whereas X represents an anion. Since 1(MA) + 2(MB) = 3(I), the MAPbI3 perovskite, for instance, must adhere to the rule of thumb. It cannot be called a perovskite material unless it satisfies the condition of charge neutrality. Additionally, as seen in Figure 1.6, several characteristics pertaining to the structure's stability have been determined



.

Figure 1. 2Structure of halide perovskite material and variation in tolerance and octahedral with different perovskite material composition

The perovskite structure, which is part of the stability of the BX6octahedra, requires a material with an octahedral value that meets these parameters. Based on Goldschmidt's tolerance factor (t) and octahedral factor (μ), the perovskite structure has been calculated. One way to express tolerance and octahedral factors is as follows: t = (RA+RX) /√2 (RB+RX) and ν = RB/RX. Here, RA, RB, and RX are the effective ionic radii of A= [CH3NH3+], B= Pb2+ or Cd2+, and X=I-, Br-, or Cl- respective. According to, μ is frequently more than 0.442 for perovskite (hybrid) systems, while t values typically fall between 0.813 and 1.07. The variation in structure and deformation in hybrid perovskite materials is caused by the fact that t and μ values are dependent on A, B, and X values. The structure remains orthorhombic for smaller values of t, but it converts to cubic for larger values of t (like t=1). The tolerance and octahedral factors for several types of perovskite materials are shown in Fig.

⚐♏❒❑⬧❖⍓⧫♏ ✈◆♋■⧫◆❍ ♎❑⬧ ❖♏❒⬧◆⬧ ♍❑■❖♏■⧫⍓❑■♋● ✈♎⬧

Concerns about color purity, complex production methods, and poor PLQY have plagued nano-crystals and QDs for decades. Most traditional QDs relied on the notoriously difficult-to-control reaction temperature to adjust the visible emission colors. As a result, the visible range quantum yield is low in these instances. Alternatively, in

The emission color of perovskite quantum dots may be adjusted by adjusting the materials at room temperature or up to 70˚C. In addition to a narrow emission bandwidth and excellent color purity, modern PQDs boast high PLQY values (up to unity). Nanoparticles made of CdSe may undergo color changes as a result of variations in particle size, but they cannot undergo cation exchange (see to Fig. 1.8(a) for reference).

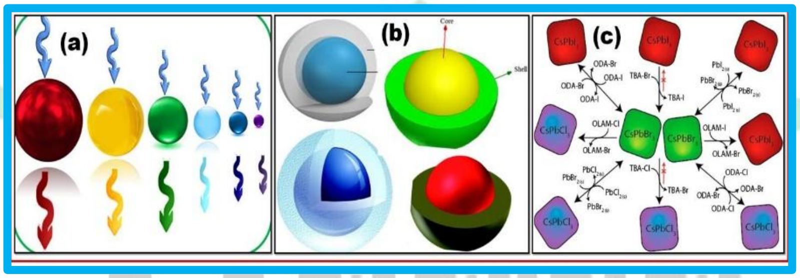


Figure 1. 3Traditional and perovskite quantum dots morphological structures (a) Metal chalcogenide (II-VI) and pnictide (InP) nano-particles (b) Metal chalcogenide and pnictide core/shell nanocrystals and (c) perovskite quantum dots

They created a core/shell structure for CdZnSe of InP to improve its optical characteristics and stability. The section on the outside is called a shell, while the part on the inside is called a core, as illustrated in Figure b. The creation of a core and a shell around nanoparticles protects the core material from environmental hazards including moisture, heat, and humidity. Many solution-processed techniques exist for synthesizing core/shell structures like this, and current research is concentrating on environmentally friendly ways to do so for nanomaterials. Although core/shell based nano-particles have a wider emission bandwidth (FWHM) than PQDs, they are stable and have a high PLQY. PQDs may have either a cubic or spherical shape, and their structure can be adjusted by changing the precursor concentration or the reaction temperature. The lead halide PQDs that are entirely inorganic are shown in Fig. 1.8c. Changing the halide components allows for the production of PQDs materials in green, blue, and red. Tabulated in Table 1.3 is a comparison of conversational QDs with perovskite QDs.

Table 1. 1A Comparison of Traditional and PQDs in Terms of Structure, Synthesis Methods, Optical Performance, and Applications

Properties	Metal Chalcogenide (II-VI) and InP Core	Metal Chalcogenides and Core-Shell	Perovskite Quantum Dots
Material Name	CdSe, ZnSe, InP	CdSe/CdS, CdSe/CdZnS, InP/ZnS	(Cs/FA/MA)PbX3 (X=Cl, Br, I)
Crystal Structure	Wurtzite, zinc-blende	Wurtzite, zinc-blende	Perovskite
Synthesis	An inert	High temperature, the	Facile synthesis, open
approach	atmosphere, high temperature	timetaken to process,	atmosphere synthesis, room temperature, less time consuming
Tunability	Only cation exchange	Only cation exchange	Cation exchange (both A & B sight) as well as anion exchange (X sight)

PLQY	Very Low (<10%)	Up to 95%	Up to 100%
Emission FWHM	25-30nm	30-40nm	10-20nm
Stability	stable	stable	Moderate
Oxidative & photo-stability	Moderate	High	High
Multi-exciton emission	Low Yield	High Yield	High Yield
Application	No commercial use	QD TV	Under R&D for PQDTV

REFERENCES

1. H. C. Yoon, H. Kang, S. Lee, J. H. Oh, H. Yang and Y. R. Do, ACS Appl. Mater. Interfaces, 2016, 8, 18189–18200.
2. Q. Chen, N. De Marco, Y. (Michael) Yang, T.-B. Song, C.-C. Chen, H. Zhao, Z. Hong, H. Zhou and Y. Yang, Nano Today, 2015, 10, 355–396.
3. C. K. Møller, Nature, 1958, 182, 1436.
4. D. Weber, Z. Naturforsch., 1978, 1443–1445.
5. R. K. Singh, S. R. Dash, R. Kumar, N. Jain and J. Singh, in AIP Conference Proceedings, 2018, vol. 1951.
6. D. B. Mitzi, Prog. Inorg. Chem., 2007, 1–121.
7. Kojima, K. Teshima, Y. Shirai and T. Miyasaka, J. Am. Chem. Soc., 2009, 131, 6050–6051.
8. H.-S. Kim, C.-R. Lee, J.-H. Im, K.-B. Lee, T. Moehl, A. Marchioro, S.-J. Moon,
9. R. Humphry-Baker, J.-H. Yum, J. E. Moser, M. Grätzel and N.-G. Park, Nat. Sci. Rep., 2012, 2, 591.
10. L. Etgar, P. Gao, Z. Xue, Q. Peng, A. K. Chandiran, B. Liu, M. K. Nazeeruddin and M. Grätzel, J. Am. Chem. Soc., 2012, 134, 17396–17399.
11. J.-Y. Jeng, Y.-F. Chiang, M.-H. Lee, S.-R. Peng, T.-F. Guo, P. Chen and T.-C. Wen, Adv. Mater., 2013, 25, 3727–3732.

12. J. H. Noh, S. H. Im, J. H. Heo, T. N. Mandal and S. I. Seok, Nano Lett., 2013, 13, 1764–1769.

13. M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami and H. J. Snaith, Science (80-.)., 2012, 338, 643–647.

14. K. Jena, A. Kulkarni and T. Miyasaka, Chem. Rev., 2019, 119, 3036–3103.

15. R. K. Singh, R. Kumar, N. Jain, S. R. Dash, J. Singh and A. Srivastava, J. Taiwan Inst. Chem. Eng., , DOI:https://doi.org/10.1016/j.jtice.2018.11.001.

16. S. Ponseca, T. J. Savenije, M. Abdellah, K. Zheng, A. Yartsev, T. Pascher, T. Harlang, P. Chabera, T. Pullerits, A. Stepanov, J.-P. Wolf and V. Sundström, J. Am. Chem. Soc., 2014, 136, 5189–5192.

17. J. Burschka, N. Pellet, S.-J. Moon, R. Humphry-Baker, P. Gao, M. K. Nazeeruddin and M. Grätzel, Nature, 2013, 499, 316–319.

18. S. Y. Yang, J. Seidel, S. J. Byrnes, P. Shafer, C.-H. Yang, M. D. Rossell, P. Yu, Y.-H. Chu, J. F. Scott, J. W. Ager, L. W. Martin and R. Ramesh, Nat. Nanotechnol., 2010, 5, 143–147.

19. L. Chao, Z. Wang, Y. Xia, Y. Chen and W. Huang, J. Energy Chem., 2018, 27, 1091–1100.

20. Y. Zhang, J. Liu, Z. Wang, Y. Xue, Q. Ou, L. Polavarapu, J. Zheng, X. Qi and Q. Bao, Chem. Commun., 2016, 52, 13637–13655.

21. F. Zhang, H. Zhong, C. Chen, X. Wu, X. Hu, H. Huang, J. Han, B. Zou and Y. Dong, ACS Nano, 2015, 9, 4533–4542.