

Perovskite Material: A New Horizon in Renewable Energy Research; a Review

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Abstract:

Perovskite solar cells (PSCs) are the newest investigation field among various modern photovoltaic devices because of their incredibly high conversion efficiency (PCE). The PSC incorporates ABX₃ crystal structure known as perovskite structure as an active light-harvesting layer. Unlike silicon solar cells, PSCs are cheaper also may be manufactured using an easy wet chemical procedure. Various investigations are currently underway to enhance PSC's PCE to the limits of Shockley-Queisser. In addition, instability and short lifespan are other grave dangers to the PSC's commercialization. This review describes the material structure of perovskite, its applications, the properties of the best solar absorbers, the evolution of PSCs, the structure and mechanism of PSCs, challenges and future prospects.

Key Word: *Photovoltaic, Perovskite material, Perovskite solar cell, HTM, PCE.*

I. INTRODUCTION

For a variety of optoelectronic and photonic device applications, perovskite materials have proven to be the most effective and promising low-cost energy materials. Perovskite was thought to have originated from the calcium titanate (CaTiO₃) that Russian mineralogist Perovski discovered in 1839. Substances CaTiO₃ like compounds with similar crystal structure were referred to as perovskite materials (structure). The perovskite materials' chemical formula in general is ABX₃ [1], where X is the anion, usually an oxide or a halogen, and A and B are cations with A larger than B. [2] There is a great deal of interest in perovskite materials for optoelectronic and photovoltaic applications due to their distinctive physical characteristics, such as their high absorption coefficient, long-range ambipolar charge transport, low exciton-binding energy, high dielectric constant, and ferroelectric properties, among others.

The performance of perovskite-based optoelectronic and photovoltaic devices is significantly influenced by the perovskite film's quality (morphology, grain size, uniformity, coverage, etc.). [3] The development of perovskite thin films has advanced so quickly that perovskite-based solar device efficiency has increased. The bulk perovskite materials employed in these devices were primarily thin films, which were placed using a variety of strategies, including spin coating, sequential deposition, and thermal evaporation. Despite the devices demonstrated improved photovoltaic capabilities, the manufacturing process and device characterization must be done in a controlled (inert) atmosphere to prevent material degradation under ambient circumstances. The uniformity and purity of the thin films, as well as the purity of the materials, are essential for better device performance since the unavoidable creation of grain boundaries and defect states in these thin films led to a decline in device performance. New stable materials were synthesized along with enhanced device topologies in an effort to increase the effectiveness and environmental resilience of materials based on perovskites electronics.

The exploration of low-dimensional (LD) perovskite materials' characteristics for use in photonic and optoelectronic device applications has recently attracted more attention. [4] LD materials and nanocrystals are materials with a minimum of one dimension in the sub-nanometer (1-100 nm) range (NCs). The adjustable optical and electrical properties of LD perovskite materials, which are caused by quantum-sized effects, as well as they are mechanically flexible drawing more focus on optoelectronic devices and semiconductor materials. Perovskite quantum dots (QDs; zero-dimensional), perovskite nanorods or nanowires (NWs; one-dimensional), perovskite nanoplatelets, and perovskite nanosheets are some of the several morphologies of LD perovskites that have been created (two dimensional). The optoelectronic properties of LD perovskites clearly show the benefits of lowering the bulk perovskite materials' dimensionality. LD perovskites have already found extensive use in LEDs, photovoltaics, photodetectors, and laser applications due to their characteristics. [5] The preliminary findings of this study demonstrated the materials' potential for use in photonics and optoelectronics. With a full understanding of the material properties, there is still more to be advancement in the performance proficiency and stability of the device.

II. STRUCTURE OF PEROVSKITES

Any substance with a crystal structure that matches the formula ABX_3 is referred to as a perovskite. Specifically, perovskite is composed of calcium titanium oxide, was the first one to be discovered with this formula ($CaTiO_3$). [6] 'A' and 'B' are two ions that are typically quite dissimilar in size, and X is an ion that forms a bond with both ions. Generally speaking, "A" atoms are larger than "B" atoms. The 6-fold coordination of the B cation is present and is encircled by an octahedron of anions in the ideal cubic structure. The A cation is in 12-fold cuboctahedra coordination. The A and B sites may be configured as $A_{x-1}A_{2x}$ and/or $B_{y-1}B_{2y}$ in other perovskite forms, and the X diverge from the ideal coordination arrangement as the ions in the A and B sites suffer oxidation state modifications. [7]

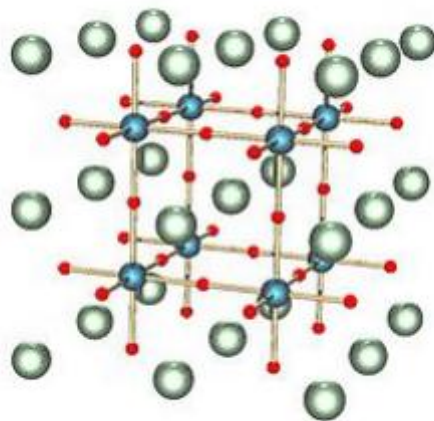


Fig. 1: Basic perovskite structure [7]

Perovskite structure with the chemical formula in general ABX_3 . The green spheres are the A atoms, the blue spheres are the B atoms (a smaller metal cation, such as Ti^{4+}), and the red spheres are the X atoms (often oxygens). In many perovskites, the consistency is reduced to orthorhombic, tetragonal, or trigonal, as opposed to the undistorted cubic structure seen in the image. [7]



Fig. 2: A calcium titanate perovskite mineral from Kusa, Russia. the Harvard Museum of Natural History was the location of this image.

The neutron diffraction data obtained spanning the temperature length of 296 to 1720 K were subjected to a Rietveld analysis to be able to refine the composition of the crystal calcium titanate perovskite $CaTiO_3$. [8]

Perovskites, among the most prevalent families of structures, are present in a huge variety of substances with varied properties, uses, and significance. [9] Perovskite is a naturally occurring compound that has this structure. Many oxides with the chemical formula ABO_3 adopt perovskite structures. A chemical compound known as an oxide is one whose chemical formula includes at least one oxygen atom in addition to another element. [10] A cubic structure, which is rarely seen, is the idealized shape. The most prevalent non-cubic variations are the orthorhombic and tetragonal phases. Although $CaTiO_3$ is the mineral for which the perovskite structure is named, it does not exist in an idealized form. Some examples of cubic perovskites are $SrTiO_3$ and $CaRbF_3$. A perovskite that may change shape depending on temperature is barium titanate, which can take on rhombohedral, orthorhombic, tetragonal, and cubic shapes. [11]

III. APPLICATIONS

Superconductivity, magneto resistance, ionic conductivity, and a wide range of dielectric characteristics are among the physical traits of perovskites that are of interest to materials research and are crucial in microelectronics and telecommunication. Due to their high light yield for radiation conversion, they are also of interest for scintillators. There are numerous varieties of distortions that might be produced by the optimal structure due to the adaptable nature of bond angles included in the perovskite framework. These include the octahedral tilting, cation displacements from the polyhedra at the centers of their coordination and octahedral distortions brought on by electronic variables (Jahn-Teller distortions). [12]

1. Lasers

Researchers proved perovskite can be used in produce laser light in 2008. Neodymium doped LaAlO_3 produced 1080 nm laser emission. [13] It was demonstrated in 2014 that optically pumped mixed methyl ammonium lead halide ($\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$) cells used to create VCSELs have a 70% efficiency in converting visible pump light to near-IR laser light. [14] [15]

2. Light-Emitting Diodes

Perovskites may make excellent light-emitting diode candidates because of their high photoluminescence quantum efficiencies (LEDs). [16] There is a lot of current research to address this issue, such as the incorporation of organic molecules [17] or potassium dopants [18] in perovskite LEDs, despite the fact that the stability of perovskite LEDs is not yet as excellent as III-V or organic LEDs.

3. Photo Electrolysis

In a very effective and inexpensive splitting-water cell employing perovskite photovoltaic, researchers at EPFL in Lausanne, Switzerland, reported accomplishing water is electrolyzed at a 12.3% efficiency in September 2014. [19] [20]

4. Scintillators

In 1997, Lutetium Aluminum Perovskite doped with Cerium was found to have scintillation characteristics (LuAP:Ce) The great mass density of 8.4 g/cm³ in these crystals, which results in shortlengths of X- and gamma-ray absorption, is their primary characteristic. With a Cs^{137} radiation source, the scintillation light production and decay time are 11,400 photons/MeV and 17 ns, respectively. [21]

IV. PEROVSKITE AS SOLAR CELL

A perovskite solar cell particular kind a perovskite-structured substance is used as the light-harvesting active layer in solar cells, most frequently a lead or tin halide-based hybrid organic-inorganic substance. Perovskite substance are often easy to make and inexpensive to generate. They have inherent qualities which cause them particularly conceivable components for solid-state solar cells, including a wide absorption spectrum, quick charge separation, long transport distances for long carrier separation lifetime, electrons and holes, and more.



Fig. 3: Shows a conventional solar cell

Since then, perovskite solar cells' efficiency of converting sunlight into electricity has risen; the current laboratory record is 25.6 percent (as of April 2021).

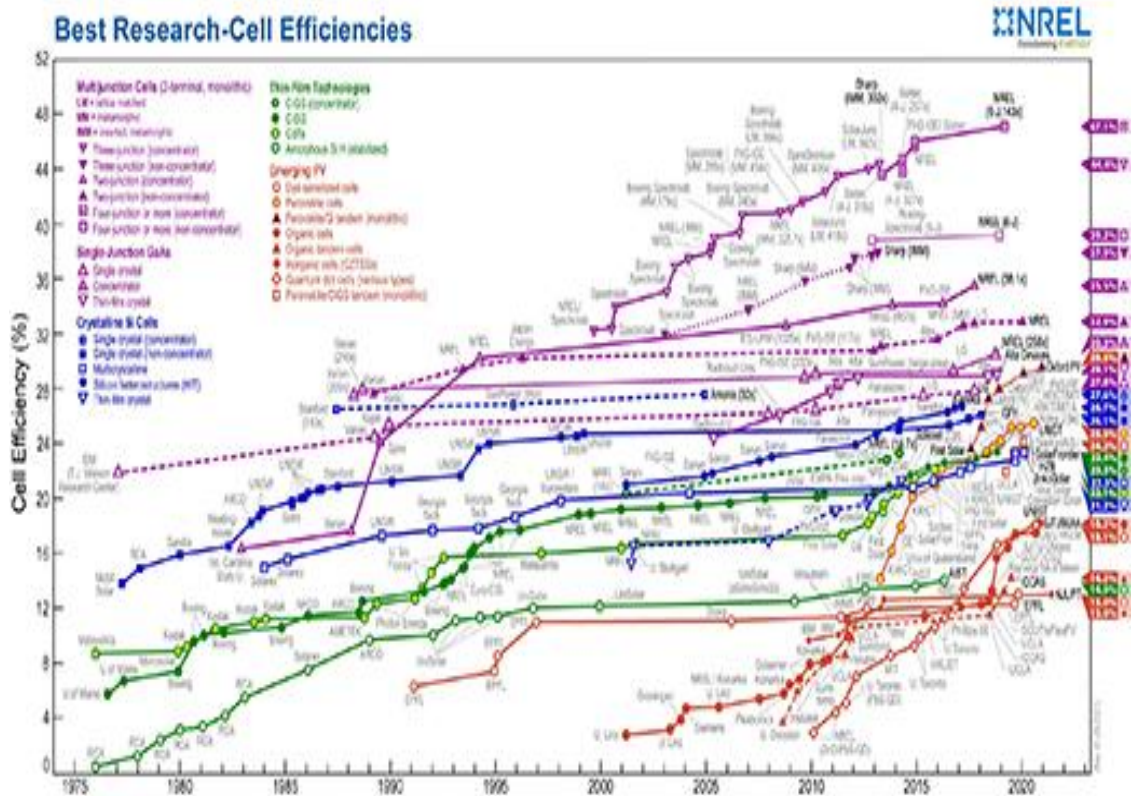


Fig.4: Solar cell efficiency. This state-of-the-art chart includes devices whose efficiency have been verified by independent, reputable test labs, such as NREL, AIST, JRC-ESTI, and Fraunhofer-ISE, and are reported on a consistent basis. [22]

Additionally, perovskite solar cells are being combined with traditional silicon solar cells by researchers. With better fabrication methods and more texturing, simulations show that nanotextured designs have a potential power conversion efficiency of above 29 percent.

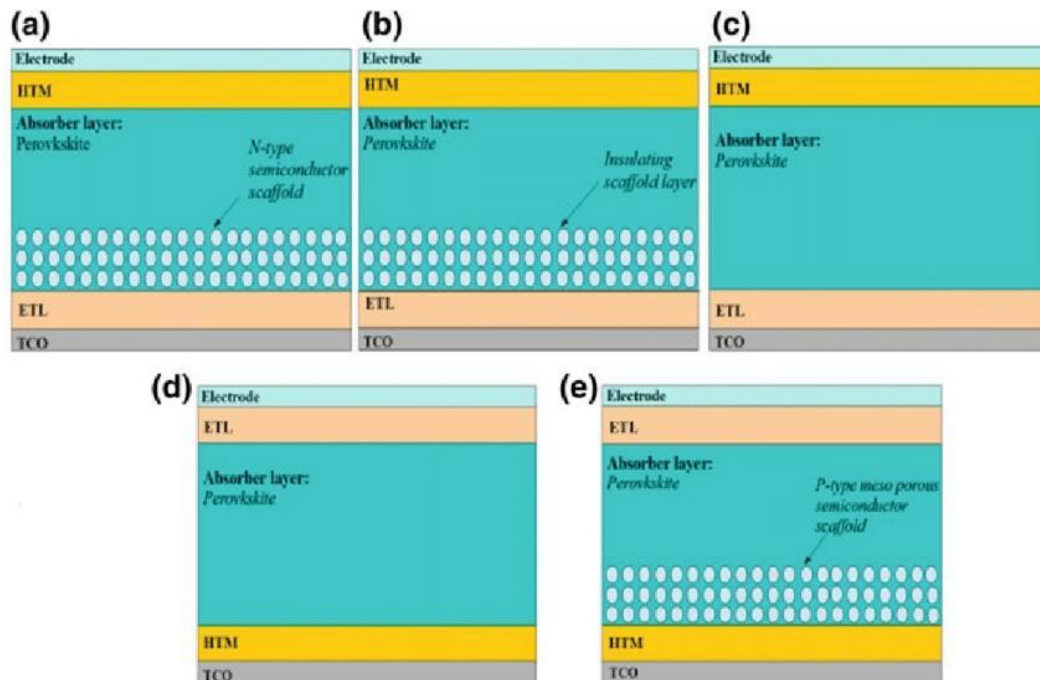


Fig.5: PSC is available in a variety of structures, including the following: regular, mesostructured, planar heterojunction, inverted planar heterojunction structure, and inverted p-type mesoporous structure.[23]

Perovskite solar cells and perovskite tandem solar cells could soon replace ordinary silicon solar cells as inexpensive, highly effective substitutes due to the exponential growth in efficiency.

V. $\text{Cs}_2\text{AgBiBr}_6$ ASSOLAR CELL

Slavney et al. published the first non-toxic, stable $\text{Cs}_2\text{AgBiBr}_6$ synthesis in 2016, and it shows potential for solar applications due to its extended 660 ns carrier lifetime and 1.95 eV indirect bandgap. [24] Since then, $\text{Cs}_2\text{AgBiBr}_6$ solar cells—whose shockley-queisser efficiency limit is 16%—have garnered a lot of attention from researchers. [25] Theoretically, the $\text{Cs}_2\text{AgBiBr}_6$ (200 nm) solar cells' spectroscopic limited maximum efficiency (SLME) is 7.92% due to their comparatively broad and indirect bandgap. [26] By carefully adjusting the valence band offset between the $\text{Cs}_2\text{AgBiBr}_6$ absorber (600 nm), a better 11.17 percent simulated power conversion efficiency can be attained.[27] More encouragingly, optimized devices with a structure of FTO/ZnOS/ $\text{Cs}_2\text{AgBi}_{0.75}\text{Sb}_{0.25}\text{Br}_6$ (400 nm)/ $\text{Cu}_2\text{O}/\text{Au}$ can generate a simulated 18.18 percent efficiency, emphasizing the great potential of $\text{Cs}_2\text{AgBiBr}_6$ -based lead-free solar cells. This is accomplished by choosing the right electron transport layer and HTL to avoid built-in voltage loss. [28] In order to demonstrate the viability of double perovskites for photovoltaic systems, the first $\text{Cs}_2\text{AgBiBr}_6$ solar cell (mesoporous structure, PCE = 2.43 percent) reportedly was in 2017 employing a spincoated $\text{Cs}_2\text{AgBiBr}_6$ film as the absorber. [29]

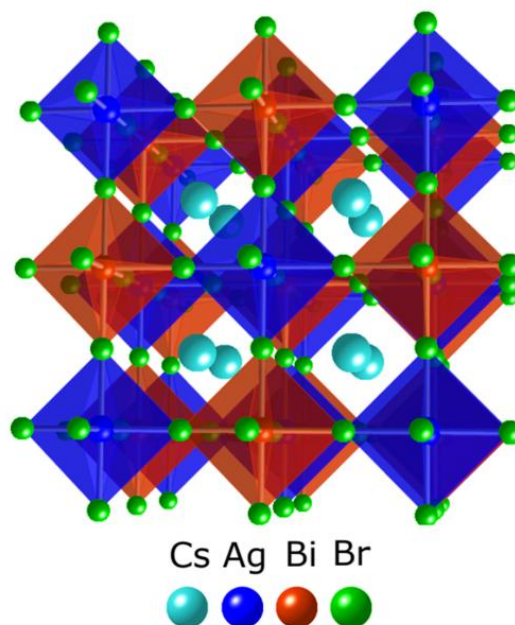


Fig. 6: $\text{Cs}_2\text{AgBiBr}_6$ perovskite structure for Pb free solar cell.

As $\text{Cs}_2\text{AgBiBr}_6$ solar cell technology advances, it is evident that the present PCE (below 3.11 percent) for single-junction or tandem solar cells is still far from satisfactory. The intrinsic qualities of the $\text{Cs}_2\text{AgBiBr}_6$ layer must also be taken into consideration if major advancements are to be realized. First, it is worthwhile to research the V_{OC} when looking for ways to enhance PCE more. In semiconductor solar cells, the distinction between divided quasi-Fermi levels of electrons and holes determines the possible V_{OC} . [30] The usual V_{OC} deficit ratio (V_{OC}/E_g) of $\text{Cs}_2\text{AgBiBr}_6$ solar cells is 0.56 (1.177 V / 2.12 V), which is lower than lead-based solar cells (0.69) and conventional amorphous silicon or GaAs thin-film solar cells but similar to organic solar cells (0.55). (0.80). [31] To strengthen the V_{OC} and lessen the loss of photon energy $\text{Cs}_2\text{AgBiBr}_6$ Understanding the limiting factors for solar cells is essential.

The relationship between the V_{OC} loss and the radiative limit ($V_{OC, rad}$) in $Cs_2AgBiBr_6$ solar cells is as follows:

$$\Delta V_{OC} = V_{OC,rad} - V_{OC} = - \frac{kT}{q} \ln(EQE_{EL})$$

$$V_{OC,rad} = \frac{kT}{q} \ln\left(\frac{J_{SC}}{J_{0,rad}} + 1\right)$$

$$EQE_{EL} = \frac{J_{0,rad}}{J_{0,rad} + J_{0,non-rad}}$$

Where, the thermal voltage is kT/q , EQE_{EL} is measured by measuring the electroluminescence of solar cells under injection current densities equal to J_{SC} , $J_{0, rad}$ is the saturation current density for radiative recombination, and $J_{0, non-rad}$ is the non-radiative recombination currents. EQE_{EL} is expressed as the ratio of radiative currents to total recombination currents. Therefore, the voltage losses brought on by non-radiative recombination in $Cs_2AgBiBr_6$ solar cells can be calculated using the radiative limit voltage or the whole cell EQE_{EL} . It is possible to determine the $V_{OC, rad}$, which stands for the thermodynamic voltage limit for $Cs_2AgBiBr_6$ solar cells, from the EQE by combining electroluminescence and Fourier transform photocurrent spectroscopy.

VI. CELL STRUCTURE AND WORKING MECHANISM OF PEROVSKITE SOLAR CELL

Any existing solar cell's basic operation involves the absorption of energy from a light source, electron-hole separation, charge collection, and electron-hole recombination. Although the precise PSC operating principle still needs to be better appreciated. [32][33], explanations are the most straightforward and trustworthy. When a photon strikes the PSC surface, it has enough energy to be the absorber absorbed. Electricity to be created by the movement of the electron since the attraction between the electron and hole by the difference in electric fields created by the electrodes. The special benefits of perovskite materials, which have the capacity to transport electrons and holes, were demonstrated by a prior work that hypothetically examined the formation of a PSC without HTM [34]. However, the work function of the back contact with valence band energy (E_v absorber) determines how these cells are arranged. Another piece of literature [35] offers additional experimental support for this simulation. Although HTM-free PSC is conceivable, other academics have demonstrated that the presence of an HTM in PSC is crucial and can positively impact a number of outcomes, including PCE, FF, and V_{oc} . An HTM also reduces the cell's internal resistance and lengthens the electron lifetime, which encourages gathering electrons and indirectly prevents electron-hole recombination.

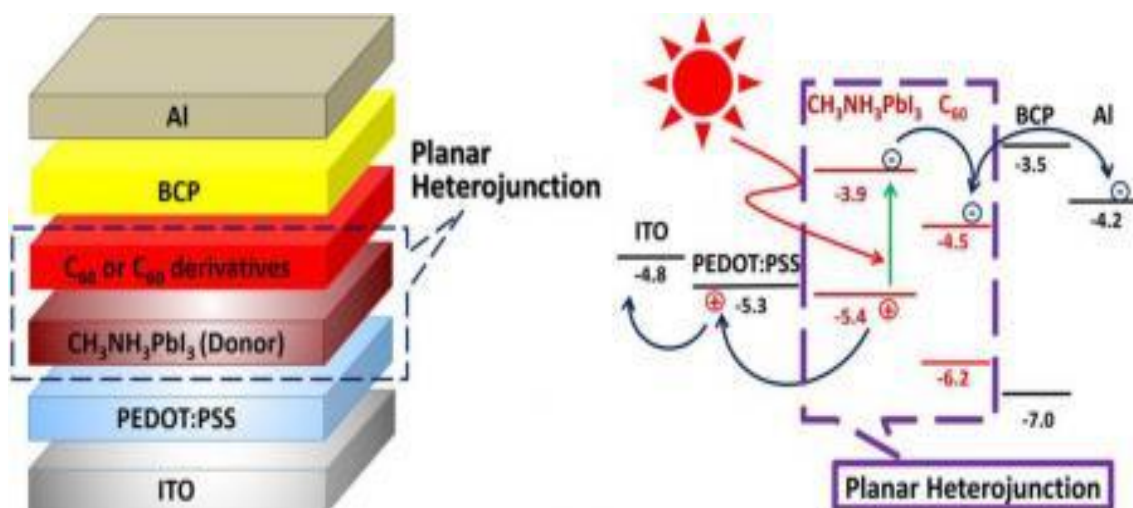


Fig. 7: PSC's cellular makeup and mechanism of action [36]

VII. MATERIALS AND STABILITY OF PEROVSKITE SOLAR CELL

Initially, organolead halide-based perovskite substance is utilized as a sensitizer in dye-sensitive solar cells (DSSC). Perovskite's general formula is AMX_3 , where A is the alkyl ammonia cation (for example, CH_3NH_3), M is the metal cation (for example, Pb^{2+}), and X is the halide anion (for example, Br^- , I^- , or Cl^-). According to earlier studies, the distance ratio between the metal cation-halide anion and the alkylammonia cation-halide anion determines how easily a material can be formed (A:X and M:X). This ratio is known as tolerance factor (TF) [37] and the formula is as below:

$$TF = (R_A + R_B) / [\sqrt{2}(R_B + R_X)]$$

When the molecular structure of a perovskite material is perfect cubical, $TF = 1$, the material is said to be ideal. When $TF < 1$, it is normal to expect distorted octahedral, which could affect the material's electronic properties. Thus, the best materials are found to be Formamidinium, $NH_2CH=NH^{2+}$ (1.90-2.20), Methylammonia, $CH_3NH_3^+$ (1.80), Ethylammonia, $CH_3CH_2NH_3^+$ (2.30), and Methylammonia, $CH_3NH_3^+$ (1.80). Small cation "A" with an ionic radius between 1.60 and 2.50 will result in the formation of perovskite. [38] The most used perovskite material nowadays is methylammonium lead halide ($CH_3NH_3PbX_3$, X=F, Cl, Br or I), which has adequate optical and electrical properties. [39] PbI_2 and $CH_3NH_3I_2$ are reacted in order to create this solar active layer. Considering that this reaction is reversible, the production of the perovskite layer itself occurs in one direction and, if reversed, the reaction decomposes to PbI_2 . The primary barrier to the commercialization of perovskite solar cells is the creation of water soluble PbI_2 during the degradation of perovskite material. In addition to humidity, other elements that might contribute to PSC deterioration include oxygen, temperature, UV radiation, and solution (perovskite compositions). [40-45] The following chemical reaction [46] describes the degrading effects of dampness on PSC:

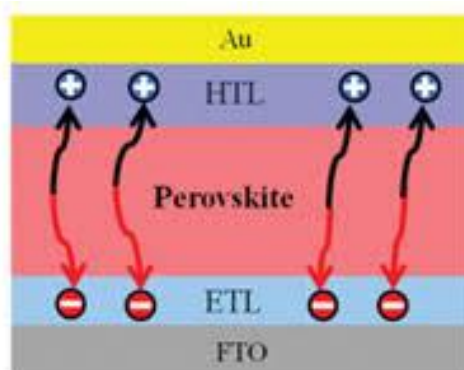
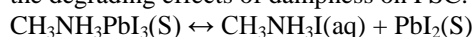


Fig.8: Schematic diagram of working principle for PSC [47]

Every other ETM is outperformed by cells using Cu_2O . Mesoporous perovskite solar cells based on reduced graphene oxide (rGO)/mesoporous (mp)- TiO_2 nanocomposite have also been introduced in a recent study [48]. According to the study, the improvement in electron transport characteristics and photon conversion efficiency is caused by a decrease in interface resistance. In a recent study, crystal crosslinking using alkylphosphonic (butylphosphonic) acid-ammonium chlorides enhanced the performance and stability issue of PSC (4-ABPACI). [49] This team modified the surface of methylammonium lead triiodide in the presence of alkylphosphonic acid-ammonium chlorides as the crosslink between neighboring grains through one-step solution processing, spin-coating (which, in the opinion of the authors, is the easiest and most advantageous way to fabricate PSC in which, if this method is proved successful in producing high-efficiency and high stability PSC would take this technology a wide step forward in the commercialization of PSC). In addition to boosting the cell's efficiency from 8.8 to 16.7%, 4-ABPACI also improves its resistance to moisture. When comparing Pristine and 4-ABPACI cells formed on mp- TiO_2 /FTO using XRD spectra before and after a moisture test, Pristine cells exhibit significantly more corrosion than 4-ABPACI cells. Other moisture barriers like carbon cathode or Al_2O_3 are also quite acceptable, although they could not be sufficient for widespread and long-term stability, necessitating the use of a more comprehensive stabilizer. Additionally, it has been demonstrated that the encapsulation approach can affect PSC's stability. The stability of PSC manufactured using encapsulation adapted from organic light emitting diode (OLED) technology was shown to be more stable under high humidity situations than the conventional UV curable epoxy resin approach when the two encapsulation techniques were compared. [50] According to what was said, the OLED approach employs a desiccant substance that collects any water that might seep through the epoxy resin sealant.

VIII. CHALLENGES AND FUTURE PROSPECTS

Lead-free double perovskite $\text{Cs}_2\text{AgBiBr}_6$ drew attention growing research interest concentrating on its basic material characteristics in recent years and a variety of applications, including photovoltaic conversion, light/X-ray detection, ferroelectricity, and magnetism, among others. This is due to the material's high structure-property diversity, high stability, and nontoxicity. As we advance, there are still obstacles that must be conquered.

- 1) $\text{Cs}_2\text{AgBiBr}_6$'s bandgap tunability is still a significant problem that calls for additional study. Ag or Bi element replacement attempts, which each have trade-offs, have not yet successfully overcome this issue. Low-dimensional derivatives of $\text{Cs}_2\text{AgBiBr}_6$ also provide the opportunity to switch the optoelectronic qualities from an indirect to a direct bandgap. We should also point out that even though $\text{Cs}_2\text{AgBiBr}_6$'s indirect bandgap feature is not favored, it is advantageous for long minority carrier diffusion lengths and consequently low carrier recombination rates, which are crucial elements in defining optoelectronic applications.
- 2) The carrier scattering, charge carrier mobility, and electron-hole recombination are all greatly impacted by strong electron-phonon coupling, which is a major worry for $\text{Cs}_2\text{AgBiBr}_6$ double perovskite. To fully comprehend the modification of the electron-phonon coupling in $\text{Cs}_2\text{AgBiBr}_6$, more research is required. The reduction of the electron-phonon coupling in $\text{Cs}_2\text{AgBiBr}_6$ may be accomplished using a number of techniques, including as doping and alloying in conjunction with hetero-junction structures, dielectric confinement, and bond length compression (by chemical/mechanical pressure). Higher current densities from solar cells and photo-detectors should come from a successful decrease, increasing their responsiveness and efficiency.
- 3) It is important to suppress the $\text{Cs}_2\text{AgBiBr}_6$ flaws carefully. Defect generation is more likely to occur in $\text{Cs}_2\text{AgBiBr}_6$, particularly deep level flaws. It is possible to decrease voltage losses and boost current density across numerous devices by reducing defect recombination.

IX. CONCLUSION

In conclusion, this review focuses on perovskite structures, widespread applications, perovskite solar cells, the material stability of Pb-based perovskite, and a different material that can be used in photovoltaic solar cells in place of Pb-based perovskite. Researchers frequently choose to either improve the manufacturing process or simply switch out the Pb-based perovskite for an alternate material in an effort to minimize the material instability of this type of perovskite. Despite the fact that many materials have been suggested, the majority of them either still exhibit some degree of stability or have a low performance efficiency by nature. Creating an appropriate encapsulation method might be important for improving perovskite resistance to moisture. Higher performance efficiency may also result from material choice at the ETM and HTM. The work is still in its early stages even though the performance efficiency of Pb-alternative perovskite is still quite poor. Due to the readily available, less toxic perovskite with high stability, progress at this study is anticipated. Research output is anticipated to help achieve this goal, which could turn perovskite solar cells into completely eco-friendly, highly reliable, and reasonably priced photovoltaic solar cells. It is clear that $\text{Cs}_2\text{AgBiBr}_6$ offers a promising prospect for numerous single/multifunctional applications other from solar cells, including photodetectors, X-ray detectors, ferroelectric data storage, magnetic spintronics, light emission, photocatalysis, etc. This makes it evident that there is still a huge potential for developing new devices based on the lead-free double perovskite $\text{Cs}_2\text{AgBiBr}_6$ material system. The performance of these various applications will therefore be improved by continuing research into the rational design and manipulation of materials and devices, allowing for the widespread commercialization of next-generation, non-toxic, stable, and effective perovskite-based electronics. Despite the fact that $\text{Cs}_2\text{AgBiBr}_6$ has demonstrated its versatility in a variety of applications, there is still a significant room for performance improvement. There is a belief that the wide and indirect bandgap will preclude photovoltaic uses, but we are hopeful that the approaches outlined above will enable a major improvement in efficiency, particularly the current density, in the near future. In fact, the large bandgap of $\text{Cs}_2\text{AgBiBr}_6$ might even open up new possibilities for promising tandem or semi-transparent photovoltaics.

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