Perovskite Solar Cells (PSCs): Definition, Structure, and Solar Cells Development

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Abstract:- Due to the unique advantages of perovskite solar cells (PSCs), this new class of PV technology has received much attention from both, scientific and industrial communities, which made this type of solar cell has been improved at an unprecedented rate. Although the obvious significance of PSCs, this technology has shown low stability in environmental conditions, and it is far to reach the stability standards of commercial types. This review article shows the contents of perovskite matter and its perfect photoelectric properties and discusses the process of converting photo energy to electric energy in which perovskite light absorbers are sandwiched between an electron transporting matter (ETM) and a hole transporting matter (HTM) and the relationships between them. It is important to explain the stability issues of PSCs so that, the main factors, which degrade the different layers and reduce the stability of PSCs, are highlighted. Moreover, the recent improvements in the principal parts of PSCs are summarized in this review article. This work has been done for a better understanding of this promising PV technology. Presides, it surveys significant solutions and suggestions of several studies in this field. Consequently, this review article is going to help researches to understand the structure of PSCs, and figure out how they can enhance the stability and efficiency of PSCs to achieve the required standards to be a commercial technology.

Keywords:- Perovskite, PSCs, Solar Cells, Semi-Conductor.

I. INTRODUCTION

The demand rising of energy, the lack of the energy sources like fossil fuel which is suffer from the depletion of reserves and the last sources can cause ecological problems, such as environmental pollution and crisis. Consequently, in the last few years, many studies have focused on clean power or green energy from renewable sources like the sun which is named the solar cells system. Solar cells and photovoltaic manufacturers have various advantages, such as being inexhaustible, and eco-friendly [1].

Solar cells from the first and second generations are excellent technology. But for some reason, they all make excessive use of an energy-intensive substance like silicone as well as rare and expensive elements. We have lots of it, but it is hard to find in the required purity. Some of them, like the Cadmium Telluride cells, are even poisonous. the third generation of PV technology contains new components which can produce economical and efficient devices. It includes dyesensitized solar cells, organic (polymer)-based solar cells, nanocrystalline films, active quantum dots, tandem or stacked multilayers of inorganics based on III-V materials, such as GaAs/GaInP, and etc. [2,3].

Recently, a promising candidate for (PV) device, which is called organic-inorganic hybrid perovskite solar cells, has shown excellent photovoltaic performance (the efficiency is 22.1%). In 2006 organometallic halide perovskite was employed as a sensitizer in dye-sensitized solar cells. In 2009, Miyasaka and co-workers tried to develop CH₃NH₃PbI₃ as a hard-wearing sensitizer. After that, some researchers suggested using solid hole transport materials (HTMs) instead of liquid electrolytes and nanocrystalline TiO₂ to prevent the rapid degradation of the perovskite layer. Since that time, thousands of researchers have attempted to improve perovskite solar cells. [4-6].

II. PEROVSKITE AND ITS WORKING PRINCIPLE

A. Perovskite Materials for Solar Cells.

The perovskite material has calcium titanate (CaTiO₃) as the main compound and it is derived from it. The molecular structure of perovskite is ABX_{3} . These Materials of perovskite have attracted wide attention because of the electromagnetic, thermal, and unique optical properties and the cubic lattice nested octahedral layered structures.

Perovskite materials, which are used in solar cells, are a type of organic-inorganic metal halide compound with the perovskite structure, in which Group A (methylammonium, CH3NH3+MA+, or formamidinium, CH(NH2)2+, FA+) is located in the vertex of the face-centered cubic lattice, the metal cation B (Pb2+, Sn2+, etc.), and halogen A stable three-dimensional network structure is formed by joining the metal-halogen octahedral particles together [7].

The following four characteristics describe the materials having such a structure. First of all, the substances have superior photoelectric characteristics, a reduced exciton binding energy, and high optical absorption coefficients (up to 104 cm1) [9]. Second, the light-absorbing layer made of perovskite has a high capacity to absorb solar energy [8]. Thirdly, the materials have a high dielectric constant, effectively transporting and collecting electrons and holes. [10]. Lastly, simultaneous transmission of electrons and holes is possible, with a transmission distance of up to 100 nm or even more than 1 micro m. [11–14].

If the materials are used in solar cell devices, their characteristics result in a high open-circuit voltage (Voc) and a short-circuit current density (Jsc).

B. Process of Transport and Structure of Perovskite.

The perovskite layer initially absorbs photons to create exciton when exposed to sunshine (electron-hole pairs). These excitons can create free carriers (free electrons and holes) to produce a current or can recombine into excitons due to the variations in the exciton binding energies of the perovskite materials. The CH3NH3PbI3 (MAPbI3) and other perovskite materials' low carrier recombination probability and enhanced carrier mobility result in a long carrier lifetime and diffusion distance. For MAPbI3, the carrier diffusion distance is at least 100 nm, and for MAPbI3-x Clx, it is greater than micro m. [11,12]. carriers' lifespan and diffusion distance. Then, an electron transport material (ETM) and a hole transport material respectively capture these liberated electrons and holes (HTM). From the perovskite material, electrons are transported to TiO2, which is utilized for the ETM layers, and are then collected by FTO (counter electrode). The holes are simultaneously moved to the HTM layer and gathered by the metal electrode. Finally, after connecting the FTO and metal electrode, the outside circuit produces a photocurrent. [1]. The pathways transport hole and electron in an HTM/perovskite/TiO2 cell are shown in Figure (1). Marchioro et al. believed that at the two heterojunction interfaces of TiO2/perovskite and Spiro-OMeTAD/perovskite, electron-hole pairs separated, then electrons were injected into TiO2. (Process (i) in Figure (1) and holes injected into HTM (process (ii)) to achieve charges transport [15]. At the same time, a series of behaviors that are detrimental to the cell's performance, such as exciton annihilation (process (iii)), photoluminescence, or nonradiative recombination, as well as reverse transmission of electrons and holes (process (iv) and (v)) and recombination at the TiO2/HTM interface (process (vi)) will also occur.



Fig 1 Schematic Diagram of Energy Levels and Transport Processes of Electrons and Holes in an HTM/ Perovskite/ Tio2 Cell.

In recent years, Different perovskite solar cell architectures, such as the mesoporous structure and the planar heterostructure shown in figure (2). Because of their porosity and significant specific surface area, mesoporous materials have received much study and utilization. The mesoporous metal oxide framework can be adhered to the perovskite absorber in this application to increase the photosensitive material's surface area that receives light and boost the device's effectiveness. [16]. The fundamental distinction between the planar structure and the mesoscopic structure is the removal of the porous metal oxide framework. The two layers and the perovskite materials form two interfaces (the electron transport layer and the hole transport layer). Consequently, the electron transport layer and the hole transport layer quickly and efficiently separate the electronhole pairs. The research on laminated perovskite solar cells with a planar heterojunction structure increases the flexibility of device optimization for the creation of highly effective laminated perovskite solar cells by advancing our understanding of the mechanisms of light absorption and electron-hole separation. [17].



Fig 2 Schematic Diagram and SEM Section Image of (A) Mesoscopic Architecture PSCs and (B) Planar Heterojunction Structure PSCs. [1].

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C. Stability of PSCs.

(Jason J. et.al) reported that Electroluminescence has an energy conversion efficiency of up to 21.6% and an external quantum efficiency of up to 17.2%. They perform as solar cells with a verified power conversion efficiency of 25.2%, or 80.5% of the bandgap's thermodynamic limit. [18]

There are various factors that affect the stability of PSCs. The most common negative factors are moisture and O_2 , UV light, and thermal effect [19]. These factors can affect the stability of the PSCs as follows:

• Moisture

There are a series of reactions that describe the degradation of perovskite according to XRD measurements before and after exposure to water.

 $\begin{array}{l} CH3NH3Pb13 \stackrel{H2O}{\longleftrightarrow} CH3NH3I(aq) + PbI2(s) \ (1) \\ CH3NH3I(aq) \Leftrightarrow CH3NH2(aq) + HI(aq) \ (2) \\ 4HI(aq) + O2 \iff 2I2(s) + 2H2O \ (3) \\ 2HI(aq) \stackrel{hv}{\Leftrightarrow} H2 \uparrow + I2(s) \ (4) \ [20]. \end{array}$

Yang et al. found that PSCs were degraded more rapidly at a higher level of relative humidity (RH) [21].

Christians et al. investigated the formation of hydrated perovskite (CH₃NH₃)₄PbI₆.2H₂O after exposing perovskite to moisture which decreases PSCs absorption. The evidence of the formation of this compound appeared from XRD measurements, which showed two strong peaks, 8.42° and 10.46° after exposure to 90% RH for 7 h. However, the hydrated perovskite was synthesized by researchers [22]. Moreover, spiro-OMeTAD, which is used as HTM, shows instability to moisture [23].

The most common solutions which were imposed by several studies to decrease the effects of moisture on PSCs are using blocking layer like (Al₂O₃) between perovskite film and HTL [24,25], preventing the degradation by moisture through exploiting the Hydrophobic properties of a carbon electrode and reducing the degradation of PSCs in moisture by using carbon electrode with ZrO_2 and TiO_2 [26].

• UV light

Through observing the low efficiency of PSCs, which follow the decrease in J_{sc} , the UV light influences the TiO₂ [27]. Using a UV filter on PSCs stops the degradation of PSCs under 1 sun AM 1.5 illumination. However, using a UV filter has disadvantages, such as increasing the cost of PSCs and decreasing the photovoltaic performance. It proves that PSCs get affected by UV light [23]. To solve the problem of instability which is caused by the susceptibility of TiO₂ to UV light, authors suggested finding the trap states, preventing the TiO₂ layer to be exposed to UV light, or using appropriate alternative ETM instead of TiO₂ [28].

• Temperature

Also, temperature plays a significant role in the stability of PSCs. Phillippe et al. found that by using X-ray photoelectron spectroscopy (PES), heating PSCs to 200°C under an ultra-high vacuum of $\sim 10^{-8}$ mbar caused converting the film to PbI₂ [29]. Other researchers found no formation of PbI₂ at 100°C for 30 min under vacuum (pressure value not quoted) [30].

Coning et al. proposed that $MAPbI_{3-X} CL_X$ is not stable itself because, under 85°C and inert conditions, it was decomposed. In Addition, the decomposing energy of $MAPbI_{3-X} CL_X$ per unit cell is close to the thermal energy of 85°C, which are (0.11ev-0.14ev), (0.093ev) consecutively [31].

 TiO_2 can be replaced by ZnO to avoid the required temperature fabrication of TiO2, but ZnO is less thermal stable in PSCs than TiO₂ [32,33]. Also, CNTs and graphene are other materials that can increase the resistance of PSCs toward temperature [34,35].

III. IMPROVEMENT IN THE PEROVSKITE SOLAR CELLS

D. Perovskite Light-Absorbing Layer

Light absorption and photoelectric conversion are crucial processes that include all of perovskite solar cells' components. The single ions that make up a perovskite (such as FAPbI3 and MAPbI3) are referred to as "simple perovskites" and have undergone much research. They occupy both the A-B- and X-sites. One way to increase photoelectric conversion efficiency is to optimize the contents and structures [7]. the band gap of perovskite should be tunned for light absorption efficiently. (Karmakar, A et. al) doping Cs2SbAgCl6 double perovskites with Cu2+ narrowed the band gap from $\sim 2.6 \text{ eV}$ to $\sim 1 \text{ eV}$. That means the excitation of the electrons of perovskite with a narrow band gap requires lower energy of the light and improves the absorption in the near-infrared region [36].

E. Electron Transport Layer

The primary function of the electron transport layer is to make an electron-selective contact with the perovskite lightabsorbing layer in order to increase photogenerated electron efficiency and prevent the hole from moving to the counter electrode, all of which serve to improve the carrier separation effect and lessen recombination. The perovskite active layer should be higher than its lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO). A photon must be able to travel through and be absorbed by the perovskite absorber with great transparency in the UV-Vis region [37].

As an electron transport layer, TiO2, ZnO, and other ntype semiconductor materials are frequently utilized [38–41]. The following is the rationale behind the choice of materials for electron transport. First, it is advised to use n-type semiconductors with increased carrier mobility. Due to a very large band gap, the material should also be transparent to visible light. Thirdly, the material may be produced at low temperatures, and the preparation conditions should be gentle. Fourthly, the band structure should match the perovskite materials. Due to the advantages of TiO₂, such as long electron lifetimes, appropriate energy level, and easy fabrication, TiO₂ is the most common ETM. However, TiO₂ affect negatively on the efficiency and the stability of PSCs, due to its little electron mobility, electronic trap states, degradation by UV light, and the sintering of mesoporous TiO₂ requiring high temperature. So several studies suggested alternatives for ETMs with good electron mobility, low temperature for fabrication, and wide band-gap (eg ZnO, SnO, WO_X) [42-44]. Moreover, the ability of TiO₂ to extract employing plasmonic Au electrons increased by nanoparticlesUnder the CH3NH3PbI3-xClx layer, which exhibited (=16.2%), a TiOX-Au-TiOX layer was fixed [45]. The choice of frequently used electron transport materials is not the primary issue that restricts the power conversion efficiency of solar cells, as evidenced by the fact that the electron transport layer generated by various methods and architectures may reach high power conversion efficiency. [46].

F. Hole Transport layer

The primary function of the hole transport layer is to gather and move holes from the perovskite light-absorbing layer in order to work in tandem with the electron transport layer to facilitate the separation of the electron-hole pairs in the perovskite materials.

The most popular organic hole transport substance is spiro-OMeTAD, which has a variety of properties. Despite having a lower hole mobility than other organic hole transport materials, it exhibits strong penetration and matches the valence band energy of perovskite well [47]. Also, the difficulties of producing Spiro-OMeTAD cause an increase in the cost of PSCs. some studies recommended using inorganic HTMs to achieve good stability and low cost of PSCs [48]. Recently, CNTs have been intended as a promising HTLs alternative [4].

G. Solar Cells without the Hole Transport Layer

Recently, perovskite solar cells without the hole transport material have become an important research direction and such solar cells show great potential due to their advantages of simple structure, easy preparation process, and high stability [1]. In HTM-free perovskite solar cells, perovskite materials are used simultaneously as light absorbers and hole transport channels. The results obtained by Minemoto and Murata, who used a device simulation method, showed that the lack of hole transport layers did not affect the built-in electric field when the work function of metal electrodes was close to the maximum valence band of lightabsorbing materials [49].

IV. CONCLUSION

The advantages of green energy, which is generated from the sun, get many scientists' attention paid toward this clear energy. perovskite solar cells are the most promising and developed photovoltaic system in the last few years.

Perovskite matter has excellent photoelectric properties. The high ability of perovskite matter to absorb the light and convert it to current, compared to other types of solar cells, develop PSCs rapidly. Although the advantages of PSCs, the Several researches have attempted to increase the stability and the efficiency of PSCs. The structures and the contents of the perovskite layer have been attended to improve the efficiency and stability of PSCs. Moreover, the production and the structure of ETL affect the efficiency and the stability of PSCs, as well as the kind of ETM. Spiro-OMeTAD is the most common HTM, but due to its low stability toward moisture and the difficulty of preparation, that caused researches recommended alternatives such as inorganic HTM and CNTs. Moreover, perovskite solar cells without HTLs have shown good properties and stability.

We recommend focusing on both, the structure of PSCs layers and the appropriate additives, at the same time to increase the stability and the efficiency of PSCs. Moreover, it is important to find efficient alternative to avoid the poisonous effects of lead and to employ the excellent photoelectric properties and the low cost of perovskite layer with other stable solar cells to produce better solar cells.

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