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The organic-inorganic solar cells device structure with different transport layers and compounds: The Guidelines for researchers

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Abstract

In current investigations the optoelectronic properties of perovskite structure-based (PSB) compounds are collected. The power conversion efficiency (PCE) dependency on device design and different transport layers are given in detail. The number of PSB compounds is taken into account as emerging materials for optoelectronic and spintronics applications. The electronic properties suggest that these PSB compounds have many properties starts from insulator to conductors and semiconductors. Furthermore, the best compounds for optoelectronic applications are suggested, which are organic-inorganic PSB ($AMPbX_3$ ($A=CH_3NH_3$, X=Cl, Br, I) compounds, best for optoelectronic applications especially for solar cells.

Keywords: Perovskite; Electronic; Optical; Solar cells; New research direction

1. Introduction

The electronic energy demand increases with ratio of increasing the world population. The energy demand can be solved by constructing dams, burning fuel or using renewable energy sources. The construction of dams requires more investments, more time and huge land to produce electric energy for supply. Also, the losses will be occurred when electric energy is supplied to customer through line as well as number of precautions are taken for carrying energy from dams to home/industries. Likewise burning fuels are limited in stock, not eco-friendly, noisy and costly. We need the electrical energy which should be very clean, ecofriendly, cost-effective as well as need less time for installation. The renewable energy is best that fulfills all the points but the material is quite is little expensive, which limits its production as well as commercialization.

The silicon based solar cells are available in market but it is not cost-effective, so it is far from an ordinary people. The new emerging materials for solar cells are suggested to be Perovskite, which shows remarkably outstanding power conversion efficiency (PCE) in solar cells. The details about PCE of PBS materials are available at national renewable energy laboratory (NREL) [1].

In this research we are focusing on the PSB compounds which are suggested best as alternative material instead of traditional semi-conductors. The PSB based solar cells has outstanding properties like absorption coefficient [2], high charge carrier mobility [3], ambipolar carrier-transport ability and tunable band gapes [4]. The properties are discussed and their scopes are given in detail for better understanding.

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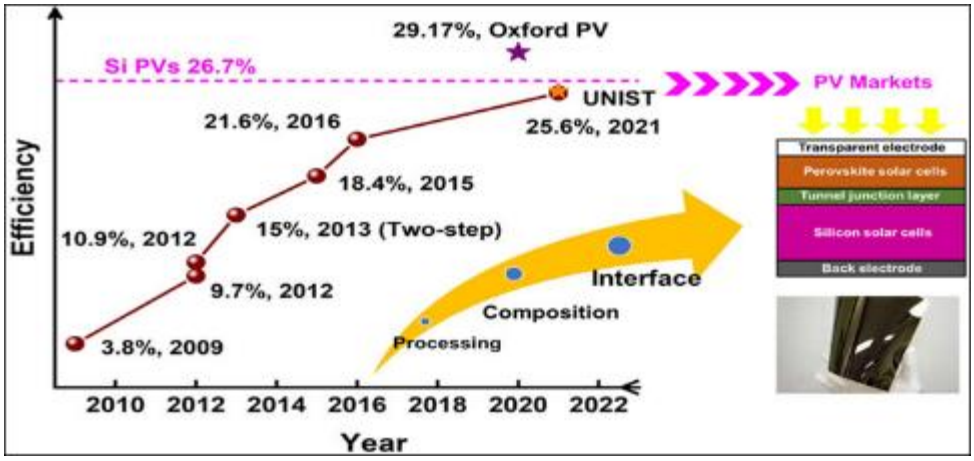


Figure 1 Worldwide efficiency chart of Perovskite structure-based solar cell available at National Renewable energy lab (NREL) [1]

2. Literature review

In 1990s, Mitzi and coworkers used organic-inorganic perovskites (OIP) in transistors and diode with general chemical formula ABX_3, where A belongs to organic cations like, methyl-ammonium (MA-$CH_3NH_3)^+$ formamidine (FA-$CH_3CH_2NH_3)^+$, B belongs to inorganic cations like Tin Sn^+ and Lead Pb^+ and X indicates for inorganic anions Chloride Cl^-, Bromide Br^- and Iodide I^- [2-12]. In addition, the comparison of organic and inorganic semiconductors, the OIP materials exhibit unique electronic and optical properties. Furthermore, these OIP Materials has weak binding energy [13], high carrier diffusion length and diffusion velocity [14-17], high dielectric constant [18], consists large Bohr radius and outstanding light absorption capacity [19]. Due to these astonishing advantages, the OIP materials became suitable candidates for development of cost-effective and highly efficient solar cells. Usually, perovskite structure-based solar cells (PeSC) consist of three layers, the electron-transport layer (ETL), hole- transport layer (HTL) and perovskite layer which is sandwich between ETL and HTL When light falls, the absorption layer inserts electron and hole in ETL and HTL layers respectively. The generated electrons travelled thorough the external circuit and mesoporous film to cathode. While HTM restores oxidized perovskite and helps to reach ground state. Consequently, the extracted hole into HTM diffuses in counter electrode direction. Finally, hole and electron recombine and gives current. The thickness of absorber layer is very important and current depends on the size of that layer [20-22]. The charge transfer between ETL and HTL and energy levels are shown in fig 2 [23].

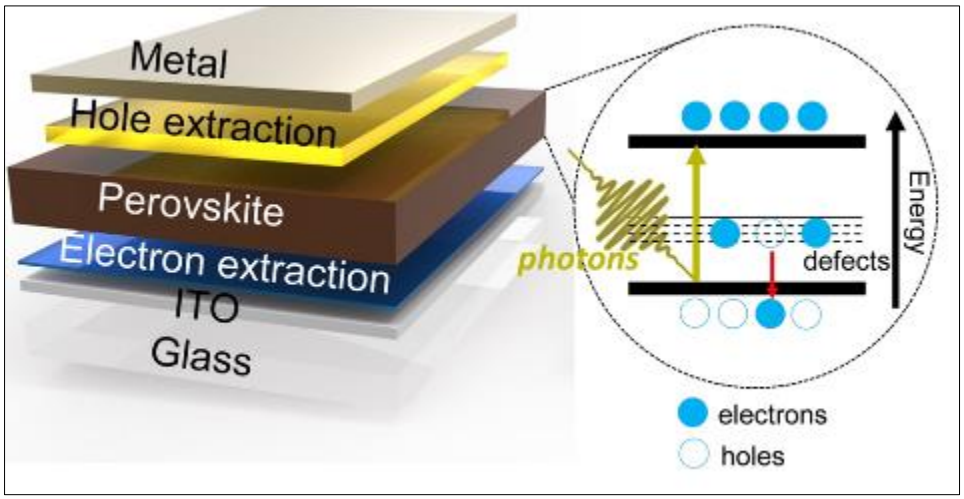


Figure 2 The charge-transfer process and energy levels of OIP solar cells [24]

Later two decades, in 2009, Miyasaka and coworkers used OIP material in solar cell applications [24]. They used methyl-ammonium lead halide $CH_3NH_3PbX_3$ as sensitizer in dye-sensitized solar cell (DSSC), which exhibit power conversion efficiency (PCE) 3.8%. Consequently, it opens the importance of OIP material in solar cell applications. Moreover, there

is abundant availability of precursor elements of OIP and very simple technique to prepares perovskite based solar cells like, the atmospheric solution-processing [25, 26], vacuum deposition [27, 28] etc., established.

Within a very short period of time the breakthrough is accomplished, the PCE approached to 23.3%. [1] Also, the ETL plays a very dynamic role in OIP solar cells [29]. electron transport layer (ETL) in traditional OIP solar cells is thin-film of TiO_2 [30, 31], SnO_2 [32, 33], ZnO or their mesoporous systems [34, 35], which exhibit large grain boundaries with weak recombination effect at interface [36, 37]. Specifically, semiconductor ETL layer has natural defects due to trap assisted recombination and oxygen vacancies [38, 39]. To overcome these limitations, researchers suggested single crystalline material for ETL in OIP solar cells. In this regard, a thick or nano-sheet of transition metal dichalcogenides such as WS_2, TiS_2, MoS_2, [40, 41] etc. can be great candidates for ETL materials, because single crystalline nano sheet or atomic thick suggest to be defects free, which enhance the charge carrier transportation to the electrode [42-45]. Due to high transportation and low trap density MoS2 is widely used as ETL IN OIP solar cells [46]. Sometimes due to its ambipolar property it can be used as HTL [47]. So, in 2016 kim with coworkers used MoS_2 as HTL in perovskite solar cell which shows power conversion efficiency of 9.53% [48]. Similarly, Das and coworkers used MoS_2 thin film as HTL in p-i-n heterojunction planer perovskite and achieved PCE of 6.01% [49]. Later on, In 2020 Malek and coworkers prepared nanosheet of MoS_2 on Indium Tin Oxide (ITO) substrate [50]. They found that nanosheet homogeneity is depend on substrate temperature and ideal at 200 ℃. Additionally, they reported that MoS_2 nano-sheet layer as ETL enhances the performance, interfacial charge transfer capability and stability of PeSC. Furthermore, the PCE increases with decrease in ETL layer, especially MoS_2 nanosheet of 5-atomic thick exhibit open circuit-voltage (V_{oc}) of 0.56 V short-circuit current density (J_{sc}) of 16.24 $mAcm^{-2}$ fill-factor (FF) of 0.37 and power conversion efficiency of 3.36%.

Likewise, HTL layer plays a main role to enhance the performance of photovoltaic devices/solar cells. Also, it is investigated that dopants can improve HTL conductivity and minimize the recombination of charge carriers at HTL as well as at perovskites interface [51-53]. Surprisingly, the (Spiro-OMeTAD) is most studied and suitable HTL having special feather like high solubility, light weight, low cost, etc. However, the raw spiro-OMeTAD has poor PCE due to insufficient oxidation states. Normally, for attaining good performance in PeSC a high oxidation time is needed. For this purpose, Kim and his team engaged oxygen plasma [54]. But, under plasma conditions, the phase changes from PbI_3 to PbI_2, and resolved this by doping trivalent (p-type) dopants, which also enhanced the hole transport properties of Spiro-OMeTAD layer.

Until now, metal oxides, metal organic complexes and organic molecules are considered as effective active p-dopants. [56-58] But, the complex deposition methods and low solubility are limiting their usage optoelectronic applications. Furthermore, $FeCl_3$ and cobalt complexes can oxides spiro-OMeTAD and act as efficient p-dopants which enhanced conductivity and generate new holes [55-60]. Also, in PeSC acid additives can be used to shorten the aging time as well as to enhance oxidation process. [61] Recently researchers using acid additives for designing the hole transport layer and advancing the morphology of spiro-OMeTAD. For this purpose, Guan with coworkers reported that doping benzoic acid enhance the HTL layer hole transport capability and fastens the oxidation process [62].

Due to versatile nano-structure morphology high electron mobility and several making techniques ZnO is favorable material for photovoltaic applications [63, 64]. as we know that the performance of PeSC is depends on surface morphology and crystalline quality of Perovskite capping layer. So, the selection of appropriate solvent for making ZnO solution can modify surface morphology (i.e., surface roughness and grain size) of Perovskite accordingly to the solar cells performance. For this concern, Ahmadi et al [65]. used ultrasonic bath technique to synthesized ZnO nanoparticles by using three solvents, isopropyl-alcohol (IPA), ethanol and 2-methoxyethanol (2ME) for PeSC. Moreover, the investigations on device performance, structural and morphological suggest that ZnO layer using 2ME as solvent exhibit good properties among all solvents. Additionally, the PeSC prepared using methylammonium lead iodide MAPbI3 as absorber and 2ME-ZnO as ETL shows an outstanding power conversion efficiency of 22%. The astonishing results is due to larger grain size, low defect density at ZnO-$_2$ME/ $MAPbI_3$ and good surface coverage by methyl-ammonium lead iodide. Thus, the ZnO (as ETL) based solar cells are appropriate candidate for solar cells applications. Furthermore, ZnSnO (ZTO) can be suitable choice as ETL due to high transmittance nature in solar cells devices. Generally, in ZTO an oxygen-vacancies plays important in charge carrier transportation. On the other hand, these oxygen vacancies are responsible for major defects in ZTO layer. So, Miao et. Al investigated the oxygen vacancies of ZTO based solar cells by doping with silicon concentrations. For this purpose, they prepared films of Si-ZnSnO (SZTO) by RF-magnetron sputtering technology by varying Si content. As a consequence, due to silicon content the reduction in oxygen vacancies is caused in ZTO based solar cells, hence improved electronic mobility's. by using SZTO as ETL in perovskite solar cells, exhibit maximum PCE of 13.4%, V_{OC} of 1.04 V and J_{OC} of 21.6 $mAcm^{-2}$.

Further, TiO_2 as ETL in PeSC exhibit good power PCE over 20%. But it is unstable under ultraviolet radiations and decay faster in short current density (JSC) [67]. So, many researcher put their efforts to protect PeSC form UV-light by applying

interface layer between ETL and perovskite but device is effected by applying all techniques [68-72]. Thus, it is necessary to fabricate stable ETL material under UV radiation. For this reason, many stable materials under UV-radiation gained the attraction of researchers [73, 74]. Among all ETL material, $Mg_xZn_{1-x}O$ (MZO) exhibit good stability under UV-radiation, deeper conduction band and excellent electron mobility in PeSC [75, 76].

Recently, Han et al fabricated MZO based PeSC which shows outstanding stability in presence of UV- radiations [77]. Additionally, the MZO shows high charge carrier mobility as compared to TiO_2. Furthermore, the MZO-based PeSC device exhibit V_{oc} = 1.11V and PCE of 19.57%. Hence, MZO can be potential candidate as ETL in Perovskite solar cells.

Furthermore, Teimouri et. al lithium doped Li-TiO2 ETL layer by ultrasonic method which shows high conductivity. They reported, Li-doped TiO_2 decreased solar power loss and enhanced conductivity [78]. Recently, in 2020, Teseng et. al introduced new technique to for getting maximum PCE of PeSC by optimizing the interface, charge concentrations and morphology of $Cu_2O/MAPbI_3/SiO_2$ heterostructure. They fabricated using RF-magnetron sputtering technique, coated one side of $MAPbI_3$ using Cu_2O-HTL and other side using SiO_2-ETL targets. They reported maximum PCE of 18.4% and open circuit voltage V_{oc} of 1.12V using Cu_2O and SiO_2 as HTL and ETL respectively in PeSC [79].

3. Recently work on Perovskite compounds

A brief review is given about Electron transport material (ETL) and hole transport material (HTL) in device performance of Perovskite Solar cells. Many researchers focused on ETL and HTL and device designing to get high performance solar cells but perovskite compounds are less explored [5-79]. Actually, in perovskite solar cells (PeSC) the perovskite compounds are used as absorbers. There are numbers of perovskite compounds which can be potential candidates for PeSC technology.

The 2D and 3D organic-inorganic perovskites (OIP) $MAPbBr_3$ and $MAPbI_3$ ($MA=CH_3NH_3$) has been studied using symmetry analyses and density functional theory (DFT) calculations. Their electronic band structures are drafted in the form of valence band VB and conduction band CB with and without spin orbiting coupling. With spin orbiting coupling there is the conduction band splits to dominate band gape. The large spin orbiting coupling enhances the in CB hence reduced the band gap. So SOC enhances the conduction band of the compounds. The figure 2 shows the band structure with and without SOC.

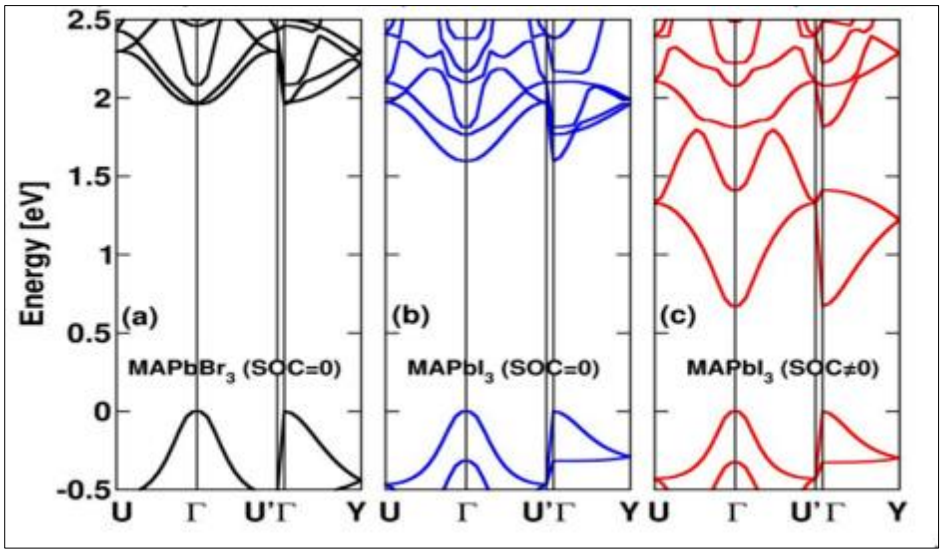


Figure 3 The band structures of OIP with and without Spin-orbiting coupling (SOP)

The calculated band gapes are 2.0 eV for $MAPbBr_3$ and 1.6 eV for $MAPbI_3$ using calculations in spin polarized manner. The downshift occurs in band gape when we used the calculation in spin polarized manner, which 0.7 eV for $MAPbI_3$. All two OIP compounds are found to be direct band gape semi-conductors in nature in both SOC and without SOC. [80]

Recently, Mehtab ur rehman et. al also investigated the electronic and optical properties of OIP compounds $AMPbX_3$ ($A=CH_3NH_3$, X=Cl, Br, I) using DFT approach. The electronic band gapes suggest that these are direct band gap semi-conductors in nature with band gape of 2.78eV, 2.36eV and 1.98eV for $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$

respectively. Furthermore, their density of states calculation suggests that VB and CB are mostly crowded due to halides and lead contents respectively. Electronic band gapes were calculated by using cubic path (ΓRXMΓ) in brillouin zone in generalized gradient approximation (GGA). The $CH_3NH_3PbI_3$ shown narrow band gap E_g as compared to all other structures.

The absorption coefficient and optical conductivity are also calculated using GGA are shown in figure 4 and the results are arranged in table 1 for maximum up-shift in absorption and optical conductivity. The optical conductivity and absorption coefficient are taken against energy in electron-volt (eV). The optical conductivity of $CH_3NH_3PbI_3$ is found to be very high as compared to $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ compounds. Overall, the $CH_3NH_3PbI_3$ compound is best then all others compounds due its narrow band gape, hence transfer more electrons. So, it is best alternative of traditional expensive silicon solar cells. [81]

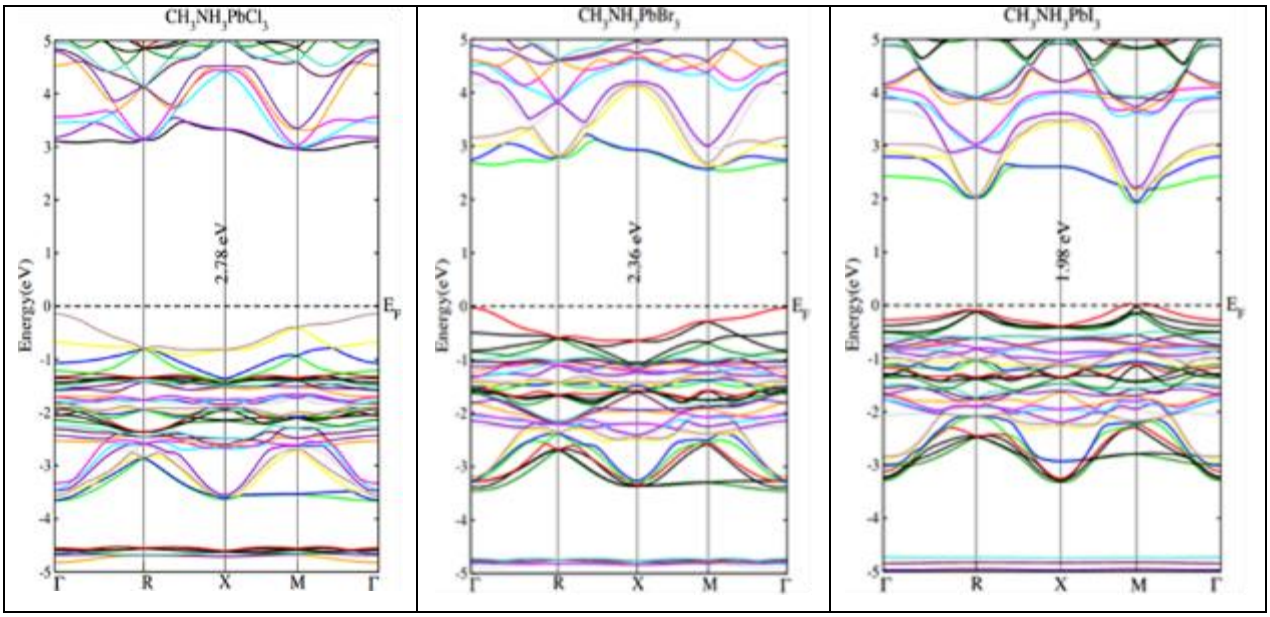
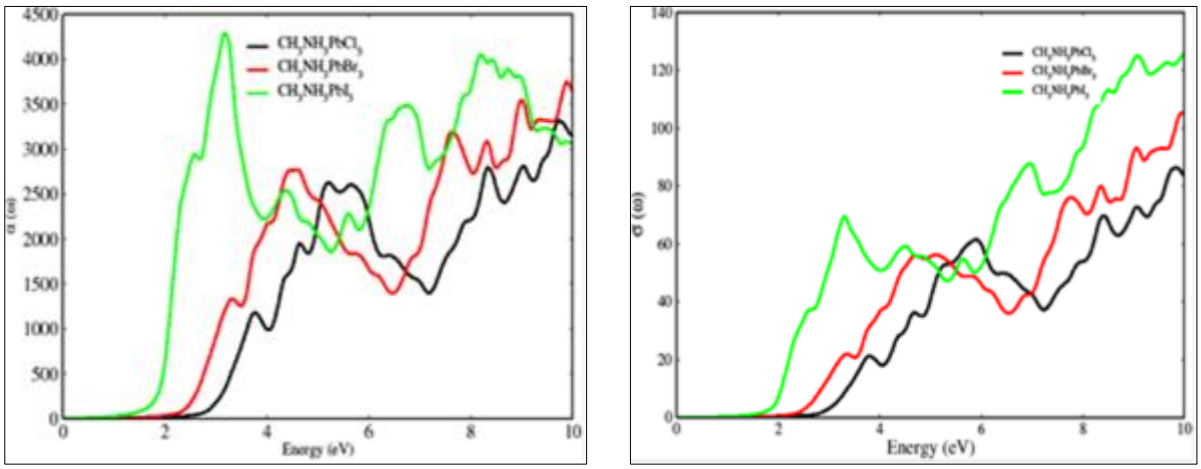


Figure 4 Band structure of $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ using GGA. [81]



(a) (b)

Figure 5 (a) Absorption coefficient and (b) optical conductivity of AMX_3

4. Conclusion

In the summary, we have collected the organic-inorganic perovskite structure-based solar cells progress from its origin. The device fabrication using different formation techniques with different HTL and ETL layers were studied, which affects the performance of solar cells PCE. The main compounds of perovskite $CH_3NH_3PbX_3$ Where (X=Cl, Br, I) are used in solar cells are key materials. Furthermore, we have discussed some electronic and optical properties of organic-inorganic compounds which are explored recently. These materials can be very effective candidates for solar cells technology. The compound $CH_3NH_3PbI_3$ shows outstanding performance because of narrow band gape, means can transfer more electrons, so it is suitable candidate for solar cells.

This research is a guideline for researcher to make more efforts on these device fabrications as well as to improve the PSB compounds properties. The research has mainly two directions of research; firstly, to make some more efforts for device fabrication using different techniques and secondly to work on PSB compounds because they are used as absorber in organic-inorganic perovskite solar cells.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare no conflict of interest.

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