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High performance of mixed halide perovskite solar cells: Role of halogen atom and plasmonic nanoparticles on the ideal current density of cell

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ABSTRACT

To be able to increase the efficiency of perovskite solar cells which is one of the most substantial challenges ahead in photovoltaic industry, the structural and optical properties of perovskite $CH_3NH_3PbI_{3-x}Br_x$ for values x = 1–3 have been studied employing density functional theory (DFT). Using the optical constants extracted from DFT calculations, the amount of light reflectance and ideal current density of a simulated single-junction perovskite solar cell have been investigated. The results of DFT calculations indicate that adding halogen bromide to $CH_3NH_3PbI_3$ compound causes the relocation of energy bands in band structure which its consequence is increasing the bandgap. In addition, the effect of increasing Br in this structure can be seen as a reduction in lattice constant, refractive index, extinction and absorption coefficient. As well, results of the simulation suggest a significant current density enhancement as much as 22% can be achieved by an optimized array of Platinum nanoparticles that is remarkable. This plan is able to be a prelude for accomplishment of solar cells with higher energy conversion efficiency.

1. Introduction

The efficiency enhancement of perovskite solar cells in short time frame in recent years, have been considered by researchers and scientists of photovoltaics industry and it seems to be a wonderful and practical matter for studying. The enhancement efficiency from about 3.8% in 2009 [1] to 22.1% in 2016 [2–4] for this matter has been reported which among the other generations of solar cells is unique and demonstrates the high potential for optoelectronic applications [5,6]. To exploit the solar cells more and better, first it is necessary that we have comprehensive information on the microscopic properties of absorbent layer. The results of experimental measurements show that due to temperature, pressure or external field changes [7,8] and variation of type and size in organic cation [9], phase transition [8,10] and consequently the structural properties would change [11]. The perovskite has a cubic phase in high temperatures [12], an orthorhombic one in low temperatures [13] and a tetragonal phase in moderate temperatures [14].

Berdiyorov et al. studied the effect of perovskite on electronic and structural properties of compounds and found that structures with more symmetry such as cubic phase were more desirable [11]. The bandgap of perovskite is not the same in different phases [11,15]. General structure of perovskite is ABX3 that A cation has basic and determinant role on the properties of perovskites and efficiency of perovskite solar cells. Also, it can be monovalent metal or an organic molecule. One of the most efficient solar cells that is related to methylammonium lead iodine ($CH_3NH_3PbI_3$) in which A is organic molecule (CH_3NH_3). Interestingly, the organic cation can rotate in structure and take different directions [16,17]. Rotation needs energy [7] so that it has a specific direction in orthorhombic phase [8,10]. But in high temperature and cubic phase due to increase of molecule energy, there is no barrier against movement and rotation of molecule and it is so fast that one cannot consider specific direction for it [10]. Movement and rotation of organic cation in perovskite compound is effective on the structural properties as bandgap of these structures [11,17] and causes the bandgap to convert from direct to indirect [17]. For this reason, we call them dynamical band gap semiconductors [17]. Changing direction of organic molecule causes direct bandgap at R point and shifts to Γ point as an indirect bandgap that shows valance band minimum and conduction band maximum dependent to rotation and space alignment of molecule. Long lifetime of charge carriers is also attributed to the dynamical band gap of the perovskites. This causes the molecules to move and prevent the carrier recombination that directly has a positive effect on the enhancement of efficiency [17].

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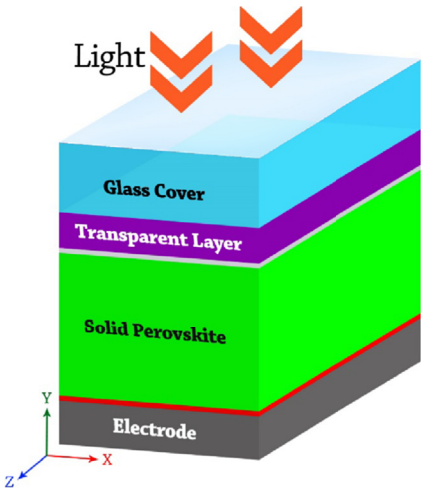


Scheme 1. Three-dimensional design of perovskite solar cell model.

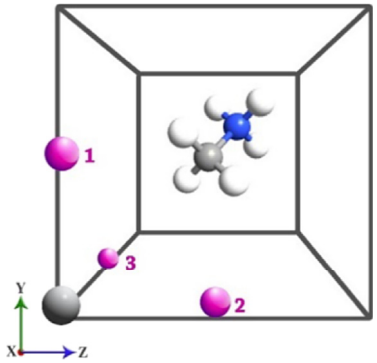
Table 1
Materials thickness for each layer.

Layer name	Material	Thickness (*nm*)
Glass cover	SiO_2	100
Transparent conductive oxide	ITO	80
Hole transport layer	PEDOT:PSS	15
Active layer	Perovskite	350
Electron transport layer	TiO_2	15
Metal contact	Aluminum	120

The unique features of perovskites that has become the source of focus for researchers at the moment are as follows: suitable bandgap about 1.5 eV [15] and significant light absorption, separation of carriers in perovskite and ability of transferring charge carriers in the absence of hole transport [18,19], long excitonic diffusion length [20] and high mobility of charge carriers [21–23]. Another feature of this matter is

Table 2
Ionic radius of halogens (anions).

Halogen	I	Br	Cl
Ionic radius(Å)	2.2	1.96	1.81



Scheme 2. Unit cell of cubic $CH_3NH_3PbI_3$.

suitable thermoelectric properties including ultra-low thermal conductivity [24]. Perovskite is employed for making of electronic devices such as diodes [25]. For efficient use of sunlight, we should make the solar cell with high efficiency, low cost and high stability. Although perovskite solar cells show high efficiency, high flexibility [26] and low manufacturing cost [27], they do not have desirable stability and there is an instability problem for them. One of the ways for improvement the stability of matter is doping it with other atoms. Adding Sn to Pb in $CH_3NH_3PbI_3$ compound or doping with Br and Cl halogens [15,28–34].

Jong et al. in their work showed that by adding Br to $CH_3NH_3PbI_3$ from 0 to 1, $CH_3NH_3Pb(I_{1-x}Br_x)_3$, the best state with proper efficiency and stability could be obtained for Br = 0.2 [34]. In the investigations done by Berdiyorov et al. in tetragonal phase, more transmission and better I-V curve was obtained for doped compound with one bromide halogen

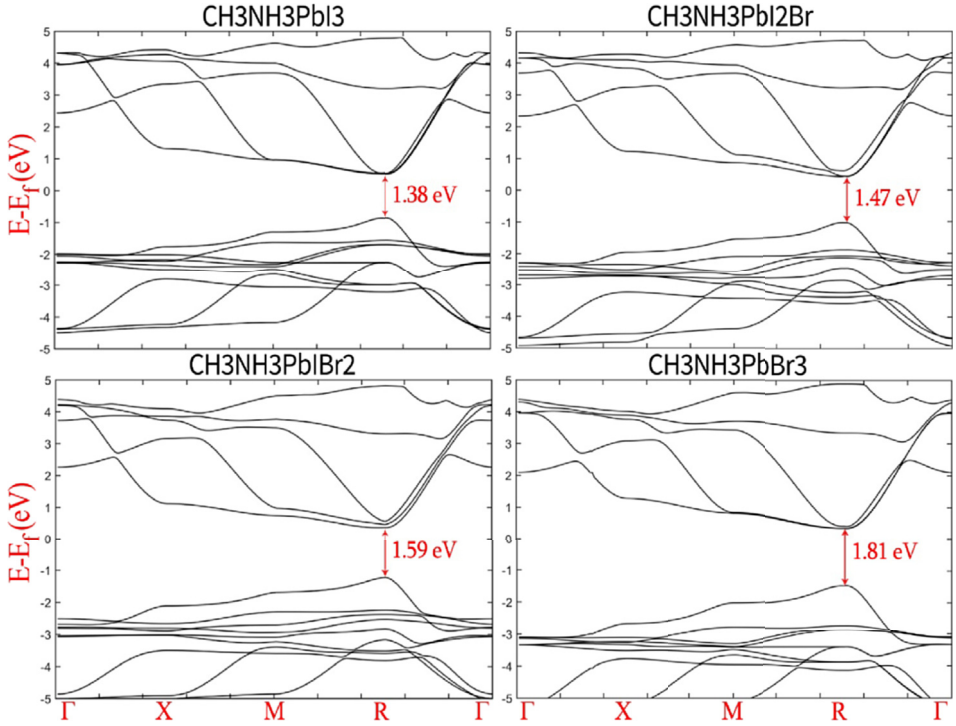


Fig. 1. Band structure of perovskite compounds.