



Copper oxide as inorganic hole transport material for lead halide perovskite based solar cells

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Received 19 May 2015; received in revised form 6 July 2015; accepted 24 July 2015

Communicated by: Associate Editor Takhir M. Razykov

Abstract

The use of inorganic layers as hole transport materials (HTM) has been suggested to enhance the resistance to degradation of methylammonium lead halide perovskite based solar cells. Few inorganic materials have been tested with limited success as they led to a lower power conversion efficiency (PCE) than the value obtained using spiro-OMETAD. In this work, we used wxAMPS and SCAPS software to compute the key characteristics of $\text{CH}_3\text{NH}_3\text{PbI}_3$ based solar cells with various HTM layers including spiro-OMETAD, NiO, CuI, CuSCN, and Cu_2O . The computations were carried out by considering defect free perovskite and HTM layers. The results show that solar cells containing Cu_2O as HTM outperform all other devices with organic or inorganic HTM hitherto tested. A power conversion efficiency exceeding 24% was obtained. These results indicate that there is a possibility to further increase the performance of perovskite based cells and reduce their cost by replacing the expensive and moisture sensitive spiro-OMETAD by copper oxide.

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Keywords: Perovskite solar cell; Hole transport material; Cu_2O ; Solar cells simulation; SCAPS

1. Introduction

Methylammonium lead halide perovskites ($\text{CH}_3\text{NH}_3\text{PbX}_3$, $\text{X} = \text{Cl}, \text{Br}, \text{I}$) have recently emerged as promising materials for optoelectronics. These materials are solution processable and made of earth abundant elements which made them materials of choice for the design of cost effective devices. Since the pioneering work of Miyasaka on Dye Sensitized cells in 2009 (Kojima et al., 2009), the use of perovskites as absorbing materials has enabled researchers to design solar cells with power conversion efficiency exceeding 15% (Burschka et al., 2013). Furthermore, lasers

made of perovskites show gains that exceed those of the best devices made of organic materials (Laquai, 2014).

However, there are few challenges that need to be addressed before perovskites dislodge silicon from its dominant position in photovoltaic industry: resistance to degradation, replacement of the expensive hole transport material (HTM) made of 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9',9'-spirobifluorene (spiro-OMETAD) and the substitution of lead by a non-toxic element. Intensive efforts are being deployed worldwide to tackle the above issues. Moisture and UV light were found responsible of the degradation of the lead halide perovskite based cells. Spiro-OMETAD HTM has been routinely used in organic photovoltaics (OPV) and organic optoelectronics. For that reason, it was suggested and used for perovskites based solar cells. However, it is known that spiro-OMETAD causes degradation in the devices

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performance and the field is still research active (Nogueira et al., 2004; Pudzych et al., 2006). There is some published work dedicated to the HTM layer and its effect on the stability of perovskite solar cells (PSC) (Malinauska et al., 2015; Badia et al., 2014; Nguyen et al., 2014). There is also a reasonable literature on the degradation of the performance of Dye Sensitized cell (DSC) due to the use of spiro-OMETAD (Bailie et al., 2014; O'Brien et al., 1998). It is reasonable to expect that the same conclusions apply to PSC as the reported issues are highly associated with the spiro-OMETAD itself. These issues are mainly related to the thermal stress effects (Malinauska et al., 2015; Bailie et al., 2014; O'Brien et al., 1998) and oxidization effects (Badia et al., 2014; Nguyen et al., 2014). Additionally, Snaith et al. reported recently TiO₂-free device that showed stability of the photocurrent over 1000 h of exposure to simulated sunlight (Leijtens et al., 2013). The loss of photocurrent was assigned by the authors to carrier recombination process at oxygen vacancy related sites on the surface of TiO₂.

Niu et al. reported that the insertion of thin layer of alumina improves the stability of the CH₃NH₃PbI₃ films when exposed to moisture and reduces the photo carrier recombination (Niu et al., 2014). The use of inorganic p-type materials as hole transport media offers the double advantage to reduce the cost of the cell and enhance its resistance to degradation. Few inorganic materials have been tested such as copper iodide (CuI) (Christians et al., 2014), copper thiocyanate (CuSCN) (Qin et al., 2014), and nickel oxide (Subbiah et al., 2014).

The quest for good Inorganic hole transport material must be guided by the need for high carrier mobility and defect free interface with the absorbing layer to minimize carrier recombination. Computer simulation is a valuable tool that can provide useful information for the screening process of materials to be tested experimentally.

In this work, we calculate the key parameters of lead halide perovskite solar cell with the following configuration: Glass/FTO/TiO₂/CH₃NH₃PbI₃/HTM/Au, HTM being NiO, CuI, CuSCN, Spiro-OMETAD or Cu₂O. The computations were carried out using wx Analysis of Microelectronic and Photonic Structures (wxAMPS) and 1D-Solar Cell Capacitance Simulator (SCAPS) software.

2. Cu₂O properties

Cuprous oxide (Cu₂O) is a p-type semiconductor with a direct bandgap of ($E_g \sim 2.17$ eV) (Gou and Murphy, 2003; Wang et al., 2002; Liao et al., 2009; Scanlon et al., 2009; Hossain and Alharbi, 2013). The first attempt to use this material for PV application was done by national science foundation and joint centre for graduate studies in 1978 (Abdu and Musa, 2009). Since then various techniques were used to fabricate schottky junction, hetero-junction, and homo-junction devices using Cu₂O as a light harvester (Minami et al., 2014; McShane et al., 2010; Nishi et al., 2012). However, low device performance was observed due to low absorption in the long wavelength region because of high energy gap. Due to low electron affinity (3.2 eV) (Jeong et al., 2008) and very high hole mobility (256 cm² V⁻¹ s⁻¹) (Li et al., 2009), this p-type semiconductor has been suggested as a potential hole transport material in heterojunction based solar cells (Lee et al., 2013a). Cu₂O thin films can be prepared using various techniques including sputtering (Lee et al., 2013a,b; Li et al., 2011, 2012; Nakano et al., 2009; Siah et al., 2012; Malerba et al., 2012), copper oxidation (Biccari, 2009), and atomic Layer deposition (ALD) (Waechter et al., 2009; Lee et al., 2014). Unintentionally doped films are naturally p-type because of the native defects identified as negatively charged copper vacancies (V'_{Cu}) rather than interstitial oxygen (O'_i) (Scanlon et al., 2009; Biccari, 2009; Raebiger et al., 2007). Experimental work reported hole trapping level between 0.40 eV and 0.55 eV above the valence band (E_v). A native defect state has been investigated as well at 0.45 eV above the valence band assigned to copper vacancies (Scanlon et al., 2009). Nitrogen doping has been used to prepare samples containing density of holes as high as 10¹⁸ cm⁻³ (Lee et al., 2013a,b; Li et al., 2011, 2012; Nakano et al., 2009; Siah et al., 2012; Malerba et al., 2012; Biccari, 2009). We carried out our computations using materials parameters that were extracted from published studies. These values are reported in Table 1.

The energy levels alignment is an important factor that affects the performance of the cell. Photoelectrons are injected from the perovskite to TiO₂ and holes from perovskite to HTM. The extraction of photoelectrons at the

Table 1
Material properties of Cu₂O.

Material properties	p-Cu ₂ O
Dielectric permittivity	7.11 (Zhu et al., 2011)
Electron mobility (cm ² /V s)	2.000E+2 (Korzavyi and Johansson, 2011)
Hole mobility (cm ² /V s)	8.000E+1 (Matsumura et al., 1996)
Acceptor concentration (1/cm ³)	1.00E+18 (Lee et al., 2013a,b; Li et al., 2011, 2012; Nakano et al., 2009; Siah et al., 2012; Malerba et al., 2012)
Bandgap (eV)	2.17 (Hossain and Alharbi, 2013)
CB DOS (1/cm ³)	2.02E+17 (Zhu et al., 2011)
VB DOS(1/cm ³)	1.10E+19 (Zhu et al., 2011)
Affinity (eV)	3.20 (Hossain and Alharbi, 2013)
Defect level (above the edge of E _v)	0.45 eV (Paul et al., 2006)

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