Extended Abstracts of the 2020 International Conference on Solid State Devices and Materials, VIRTUAL conference, 2020, pp383-384

F-6-07 (Late News)

Small Molecule Materials as Hole Transporting Materials for Perovskite Solar Cells

LiangLe Wang[1], Md. Shahiduzzaman[2], Shoko Fukaya[1], Ersan Y. Muslih[3], Masahiro Nakano[3], Makoto Karakawa[2,3], Kohshin Takahashi[3], Koji Tomita[4], Jean Michel Nunzi[2,5] and Tetsuya Taima[1,2,3]

Kanazawa University
[1] Graduate School of Frontier Science Initiative, Kakuma, Kanazawa 920-1192, Japan
[2] Nanomaterials Research Institute, Kakuma, Kanazawa 920-1192, Japan
[3] Graduate School of Natural Science and Technology, Kakuma, Kanazawa 920-1192, Japan
[4] Tokai University
Department of Chemistry, School of Science, Kitakaname, Hiratsuka 259-1292, Japan
[5] Queen's University
Department of Physics, Engineering Physics and Astronomy, Kingston K7L-3N6, ON, Canada
Phone: +81-70-2616-5541 E-mail: bro.wang@outlook.com (L.W.); taima@se.kanazawa-u.ac.jp (T.T.)

Abstract

Molecular glass compounds are appealing building blocks with interesting optoelectronic properties for application in a variety of fields. Here, the synthesis, characterization and photovoltaic performance of series of novel molecular glass as hole transport materials (HTMs) with the different electron donor units triphenylamine (TPA) and dimethoxydiphenylamine (OMe-DPA) are presented. Our results show that the perovskite solar cells (PSCs) fabricated by the novel molecular HTM with OMe-DPA unit achieved a champion performance, while a circuit current (*Jsc*) of 15.87 mA/cm^2, an open-circuit voltage (*Voc*) of 0.91 V and a fill factor (FF) of 0.58, leading to a power conversion efficiency (PCE) of 8.35% at standard AM 1.5G solar illumination.

1. Introduction

Hybrid organic-inorganic metal halide perovskite solar cells (PSCs) are currently the fastest growing technology in the history of photovoltaics because of their advantages for optoelectronic devices, including strong optical absorption, adjustable bandgap, long diffusion lengths, and high carrier mobility. In just over a decade, the power conversion (PCE) of PSCs has rapidly increased, from the beginning 3.8% by Professor Miyasaka in 2009 [1] to the latest certification record of 25.2% [2], which is approaching the top values achieved for single-crystalline silicon solar cells. The hole transport layer (HTL) is essential for high-performance perovskite solar cells. At present, the most of hole transporting materials for perovskite solar cells that have been reported introduce additives to further improve the device performance. Spiro-OMeTAD is usually used as the best HTL material. However, this material has disadvantages with complex processes and high cost, which makes the development of new low-cost hole transport materials (HTMs) to be a very important issue.

Hence, in this work, we report a new type of hole transporting molecules (Fig. 1), molecular with triphenylamine (TPA) and methoxydiphenylamine (OMe-DPA), which name of TPA-glass and OMe-DPA-glass. Perovskite solar cells employing the investigated HTMs demonstrate champion PCE of 8.35%. Furthermore, these compounds do not require extensive and costly synthesis procedure and could be obtained using a simple method from readily available commercial starting materials.

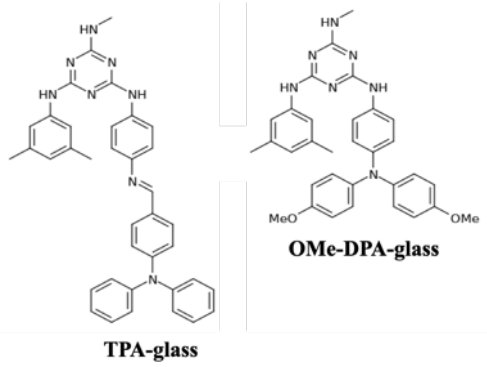

Fig. 1 Chemical structures of HTMs.

2. Experiment

The device is constructed by the structure of FTO/compact TiO_2/BK TiO_2 NPs/$MAPbI_3$/HTL/Au. Fluorine-doped tin oxide (FTO)-patterned glass substrates were treated by UV–ozone treatment for 20 min prior to use. Then, compact-TiO_2 was deposited on the FTO-glass by spin coating. (0.15 M for 1 time, and 0.3 M for 2 times. Anneal at 125 °C for 5 min, and then at 450 °C for 30 min.). Then the as-synthesized, pure-phase BK TiO_2 NPs colloidal suspension were deposited on the compact-TiO_2 by spin-coating at 2000 rpm for 30 s and annealed at 105 °C for 5 min, followed by baked at 180 °C for 60 min in a muffle furnace. Perovskite precursor solutions were prepared from 1 M PbI_2 and 1 M CH_3NH_3I in a mixed solvent of DMF and DMSO (4:1) and stirred at 70 °C for 60 min prior to spin-coating. The as-prepared precursor solution was spin-coated by 0rpm(10s), 1000rpm(10s), 5000rpm(20s). In the third step a 600 μL of chlorobenzene solution was dripped at just 10 s before the spin-coating stops. The samples were directly transferred to a hot plate at 100 °C for 60 min. For the hole transport layer (HTM), a TPA-glass and OMe-DPA-glass precursor solution was prepared by dissolving TPA-glass or OMe-DPA-glass (10mg) in 1 mL

chlorobenzene by vigorous stirring at 800 rpm at RT for 6 h. As prepared precursor solution was spin-coated on the perovskite layer at 4000 rpm for 30 s and obtained optimized thickness was around 90 nm. To complete the device, 100-nm thick gold (Au) electrode was thermally evaporated on top of the HTL.

3. Results

To investigate the film-forming abilities of these two new molecular HTMs, we observed the morphology of HTL by scanning electron microscopic (SEM). The corresponding morphology is showed in Fig. 2a and Fig. 2b. It could be seen that perovskite/TPA-glass showed lots of pinholes, and perovskite/OMe-DPA-glass represents uniform microstructure, which means that perovskite/OMe-DPA-glass has better surface coverage than perovskite/ TPA-glass. It can be inferred that the perovskite/OMe-DPA-glass has better surface smooth nature, which will enhance the contact between the perovskite layer and the HTL, and prevent the direct contact between perovskite and the metal electrode, and prevent from a diffusion of the electrode into perovskite layer to improve stability of the device [3].

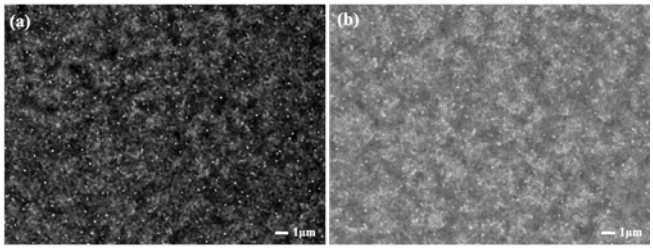

Fig. 2 SEM images of perovskite with a) TPA-glass, and b) OMe-DPA-glass.

Normalized UV-vis absorption spectra of these two new molecular HTMs in film are shown in Fig. 3. TPA-glass exhibit absorption maxima at 391 nm, while OMe-DPA-glass exhibit absorption maxima at 274 nm. It can be found that OMe-DPA-glass exhibit a blue shift of 117 nm of the absorption maxima, which is attributed to the structure containing DPA can provide a wider optical band gap [4].

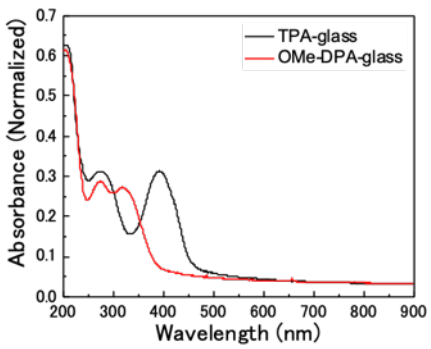

Fig. 3 Normalized UV-vis absorption spectra of different HTMs in film.

The current density versus voltage (*J-V*) characteristics at scan speeds of 0.05 V/s is presented in Fig. 4a. The parameters of reverse scan measurements from the opposing positive bias side to the negative bias side under AM 1.5G simulated solar lights are listed in Table 1. The device prepared with OMe-DPA-glass showed a *Jsc* of 15.87 mA/cm^2, Voc of 0.91 V, FF of 0.58, and PCE of 8.35% (Average of 7.80%). It is much higher than the device prepared with TPA-glass. The incident photon-to-current conversion efficiency (IPCE) curves and the integrated current density curves of PSCs with different HTLs are showed in Fig. 4b. The integrated current density values of PSCs with TPA-glass and OMe-DPA-glass are 9.41 and 14.46 mA/cm^2, respectively, which are almost in agreement with the *Jsc* value measured under the standard solar AM 1.5G.

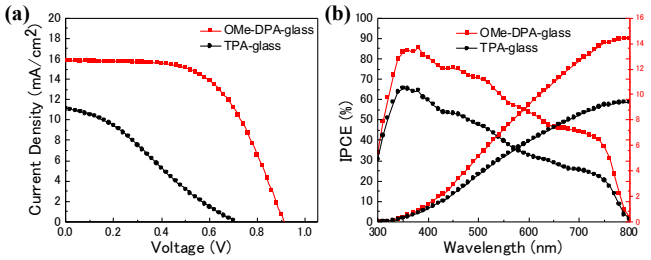

Fig. 4 a) *J-V* curves, and b) IPCE curves of the perovskite devices with different HTMs.

Table 1 Photovoltaic parameters of the PSCs with different HTMs.

	***Jsc* (mA/cm2) (Average)**	***Voc* (V) (Average)**	**FF (Average)**	**PCE (%) (Average)**
TPA-glass	11.14 (10.96±0.74)	0.71 (0.66±0.09)	0.29 (0.31±0.09)	2.27 (2.22±0.53)
OMe-DPA-glass	15.87 (14.76±0.79)	0.91 (0.88±0.03)	0.58 (0.60±0.04)	8.35 (7.80±0.59)

4. Conclusions

We successfully prepared a perovskite solar cell based on new molecular glass HTMs and obtained a maximum PCE of 8.35%. By comparing TPA-glass and OMe-DPA-glass, the effects of TPA and OMe-DPA units can be further analyzed.

Acknowledgements

This study was supported by the Grant-in-Aid for Scientific Research Grant Number 20H02838 for financial support.

References

[1] A. Kojima et al., J. Am. Chem. Soc. 131, 6050 (2009)

[2] NREL Best Research-cell Efficiencies [https://www.nrel.gov/pv/assets/pdfs/best-research-cell-efficiencies.20200406.pdf]

[3] L. Zhao et al. ACS Energy Letters. 1, 595 (2016)

[4] J. Urieta-Mora et al. Chemical Society Reviews. 47, 8541 (2018)