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Interfacial Investigation of Perovskite Opto-Electronic Materials and Devices

Seth Marder
GEORGIA TECH RESEARCH CORPORATION
505 10TH ST NW
ATLANTA, GA 30318-5775

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Seth Marder, Henry Snaith

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GEORGIA TECH RESEARCH CORPORATION
505 10TH ST NW
ATLANTA, GA 30318-5775 US

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14. ABSTRACT
During the no-cost extension period of this grant, remaining funds from a travel supplement were used to fund a month-long visit by a Georgia Tech graduate student to the University of Oxford. This provided the student with valuable training and experience in perovskite solar cell device work and enabled testing of interfacial materials developed at Georgia Tech in state-of-the-art devices. A crosslinkable p-dopable hole-transport material was found to be effective in perovskite solar cells; further work on this material is being carried out under our current award FA9550-18-1-0499. In addition further studies were carried out on a crosslinkable n-dopable fullerene electron-transport material developed at Georgia Tech; this work including both obtaining good efficiencies for n-i-p perovskite solar cells incorporating this material, and extending its use to p-i-n cells, in which even higher efficiencies were obtained.

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PI: Seth Marder, Georgia Institute of Technology
Co-PI: Henry Snaith, University of Oxford

Abstract:

During the no-cost extension period of this grant, remaining funds from a travel supplement were used to fund a month-long visit by a Georgia Tech graduate student to the University of Oxford. This provided the student with valuable training and experience in perovskite solar cell device work and enabled testing of interfacial materials developed at Georgia Tech in state-of-the-art devices. A crosslinkable p-dopable hole-transport material was found to be effective in perovskite solar cells; further work on this material is being carried out under our current award FA9550-18-1-0499. In addition further studies were carried out on a crosslinkable n-dopable fullerene electron-transport material developed at Georgia Tech; this work including both obtaining good efficiencies for n-i-p perovskite solar cells incorporating this material, and extending its use to p-i-n cells, in which even higher efficiencies were obtained.

Contents:

1. Research Progress

As described in our previous report, our plan for the no-cost extension period was to use the remaining funds of a travel award supplement. These were used to support a second month-long visit by Marie-Hélène Tremblay (MHT), a Georgia Tech (GT) graduate student working on the project to conduct experiments and training at the University of Oxford in Mar/Apr 2018. Marie-Hélène is primarily supported by a Canadian graduate fellowship.

During the visit MHT worked on device aspects of various sub-projects involving interfacial layers for perovskite solar cells that we have discussed in more detail in previous reports. In general, she gained more invaluable first-hand experience in perovskite processing and solar-cell fabrication that can be subsequently exploited back in Atlanta. Specifically, she worked on the processing and p-doping of hole-transport materials (HTMs) for so-called n-i-p perovskite solar cells, gaining the experience to reproducibly fabricate cells based on the spiro-OMeTAD HTM, p-doped using both the traditional cocktail of materials (including LiTFSI) and molybdenum-dithiolene p-dopants, which we have previously demonstrated as an earlier part of this program to be superior in terms of device stability (A. Pellaroque *et al.*, *ACS Energy Lett.*, **2**, 2044-2050 (2017)). This work served as a benchmark for the testing of photocrosslinkable HT polymers. Crosslinking of HTMs can potentially improve stability, allow for spatially controlled doping, and can potentially allow the same HTM to be used in both n-i-p and p-i-n architectures.

Preliminary measurements were made using the photocrosslinkable polymer shown in Fig. 1 and indicate that the crosslinked polymer can be p-doped in a similar way to spiro-OMeTAD and that the doped crosslinked HTM can be successfully used in devices. Further work on these systems, including device optimization and potentially including their extension to p-i-n cells, is currently being carried out under our new grant (FA9550-18-1-0499).

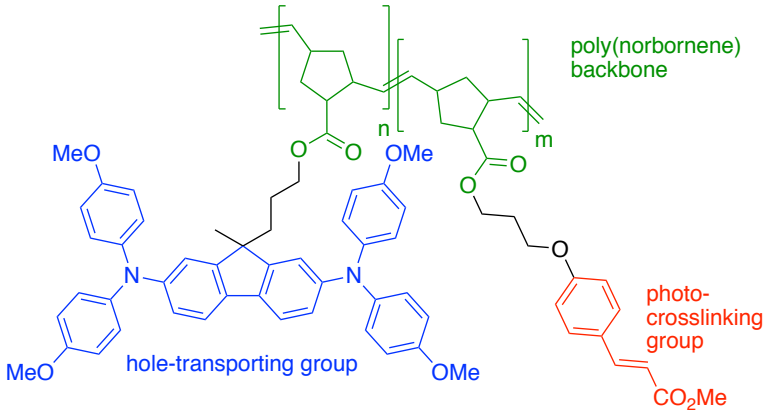

Fig 1. Chemical structure of a crosslinkable and p-dopable HTM.

MHT also worked on crosslinkable dopable *electron*-transport materials (ETM), specifically PCBCB (Figure 2), which we originally developed with ONR funding (N. Deb et al., *J. Mater.*

Chem. A, 2015, **3**, 21856-21863) and have, under this program, introduced to the perovskite solar cell field (K. Wojciechowski *et al., ACS Energy Lett.*, **1**, 648-653 (2016)). More recently we have been investigating the use of n-doped crosslinked PCBCB as a bottom ETM for n-i-p perovskite solar cells and have achieved power conversion efficiencies of up to 16%. One drawback of this approach is that the perovskite film quality on fullerene ETMs is not particularly high. Accordingly, MHT has worked to investigate the applicability of this ETM to p-i-n solar cells, in which higher quality films of the perovskite can be obtained on an organic HTM. These devices have proven to even more efficient (up to ca. 18%). Representative device data are shown in Figure 2 and show that the most important factor in the higher efficiency of the p-i-n devices is a higher fill factor.

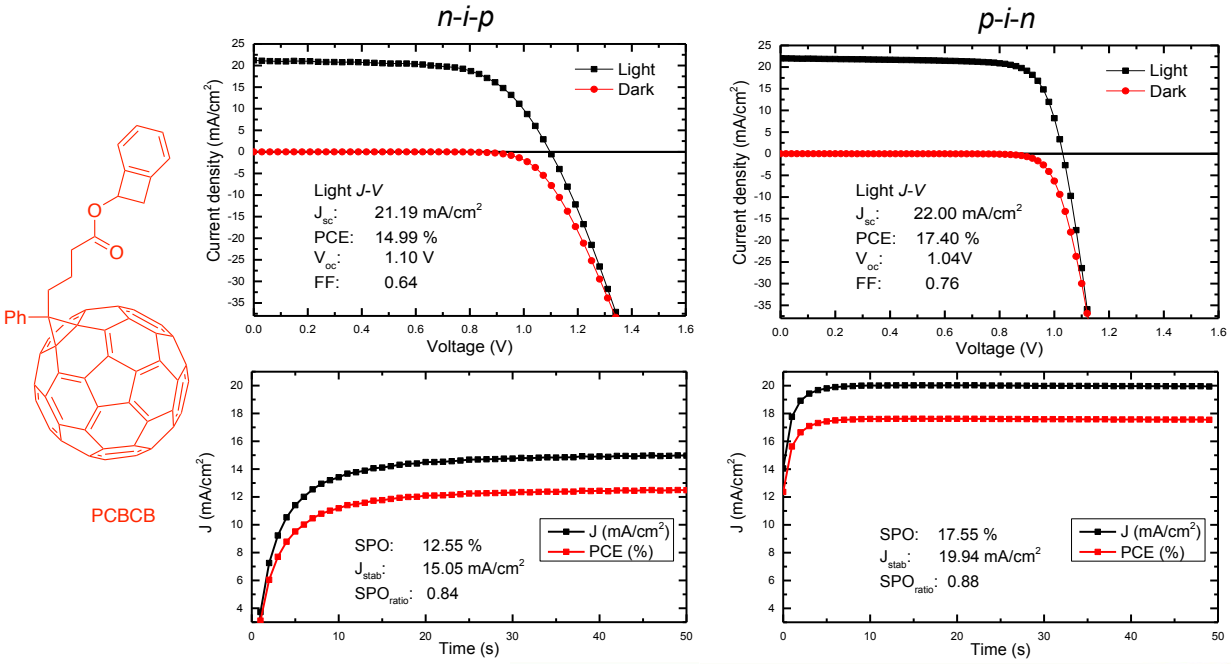

Fig 2. Left: Chemical structure of a crosslinkable ETM, PCBCB, and J-V characteristics. Yime-dependent photocurrent at the maximum power point for (left) n-i-p (n-doped PCBCB/[FA,Cs]Pb[I,Br]$_3$/p-doped spiro-OMeTAD) and (right) p-i-n (polyTPD/[FA,Cs]Pb[I,Br]$_3$/PCBCB) perovskite solar cells.

2. Statistical Information

3.1. Publications

3.1.1. Journal Articles

1. S. Song, R. Hill, K. Choi, K. Wojciechowksi, S. Barlow, J. Leisen, H. J. Snaith, S. R. Marder, T. Park, "Surface Modified Organic Electron Transport Layers for Stable and Reproducible Flexible Perovskite Solar Cells", *Nano Energy*, **49**, 324-332 (2018). (Reported in previous report, but now full citation available).

2. D. Luo, W. Yang, Z. Wang, A. Sadhanala, Q. Hu, R. Su, R. Shivanna, G. F. Trindade, J. F. Watts, Z. Xu, T. Liu, K. Chen, F. Ye, P. Wu, L. Zhao, J. Wu, Y. Tu, Y. Zhang, X. Yang, W. Zhang, R. H. Friend, Q. Gong, H. J. Snaith, Rui Zhu, "Enhanced Photovoltage for Inverted Planar Heterojunction Perovskite Solar Cells", *Science*, **360**, 1442-1446 (2018).

3. Z. Wang, Q. Lin, B. Wenger, M. G. Christoforo, Y.-H. Lin, M.-T. Klug, M. B. Johnston, L. M. Herz, H. J. Snaith, "High Irradiance Performance of Metal Halide Perovskites for Concentrator Photovoltaics", *Nat. Energy*, published online, DOI: 10.1038/s41560-018-0220-2.

4. F. Pulvirenti, B. Wegner, N. K. Noel, G. Mazzotta, R. Hill, J. B. Patel, L. M. Herz, M. B. Johnstion, M. K. Riede, H. J. Snaith, N. Koch, S. Barlow, S. R. Marder, "Modification of the Fluorinated Tin Oxide/Electron-Transporting Material Interface by a Strong Reductant and its Effect on Perovskite Solar Cell Efficiency", *Mol. Syst. Des. Eng.*, published online, DOI: 10.1039/c8me00031j.

3.1.2. Book Chapters

none in this period

3.2. Presentations

1. "Interface Chemistry for Organic Electronics and Opto-electronics", S. R. Marder, CIMTEC 2018 - 14th International Conference on Modern Materials / 8th Forum on New Materials, Perugia, Italy, June 10th-14th 2018.
2. "Redox-active molecules as electrical n-dopants for OLED transport materials," S. Barlow, SPIE Optics and Photonics 2018, San Diego, August 19th-23th 2018.

3.3. PhD Theses

none in this period

3.4 Patents

none in this period

3.5. Personnel Fully or Partially Supported

none in this period; no-cost extension period involved only use of travel funds