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## Fullerenes with dipoles: boosting the efficiency of perovskite solar cells

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An unfortunate and fortunate discovery is that metal halide perovskites are not completely defect tolerant, while fullerenes, which are inexpensive and broadly applied in organic solar cells, have a considerable passivation effect toward the surface defects of perovskite materials [1]. The improvement of perovskite efficiency and stability in the last five years has shown the importance of passivating interfacial charge traps to reduce charge carrier recombination and to slow down the degradation of perovskites [2]. The ionic nature of perovskites produces at least two types of defects where opposite charges exist on the perovskite film surfaces, e.g., positively charged undercoordinated  $\text{Pb}^{2+}$ , negatively charged Pb–I anti-site defects ( $\text{PbI}^{3-}$ ), and undercoordinated halide ions. This characteristic makes the passivation more complicated than that in silicon solar cells, which requires extensive research to understand how to effectively passivate these defects. Based on the electrostatic interaction, organic compounds containing either a Lewis base or a Lewis acid moiety have been widely used to passivate charged defects, which has been described well in a recent review article Ref. [2].

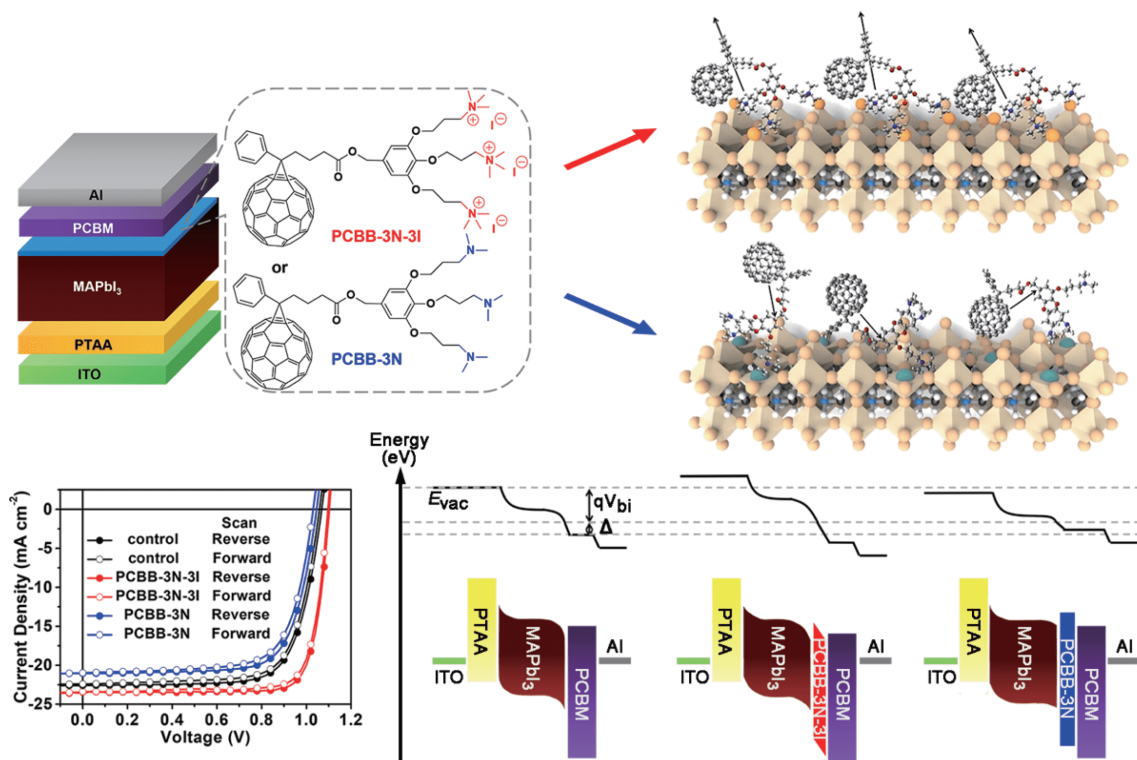
The search for an ideal passivation molecule has started many years ago. The rapid development of perovskite solar cell research requires additional functions from passivation molecules. In addition to the passivation function, charge passivation molecules should have other properties such as charge conduction, protection of perovskites films from degradation, tuning of metal electrode work function, and

doping of perovskites..

The charge transport layers are frequently used as a passivation layer. However, there are insulating molecules that have good passivation effect but cannot conduct current well. Thus, the passivation molecule layer needs to be very thin so that current could pass through the layer, which limits their capability in protecting perovskites. Out of many passivation molecules and functional groups, fullerene and its derivatives are still broadly applied in most efficient perovskite solar cells mainly because they can function as the 1) passivation, 2) electron transport, and 3) protection layers to improve the stability of the solar cells with the p–i–n structure. Both fullerene ( $\text{C}_{60}$ ) and its derivatives have shown excellent passivation properties. However, a potential issue with using the derivatives is the possible structure disorder that is induced by the energy disorder, which may lower the open-circuit voltage ( $V_{oc}$ ) due to the reduced upper limit of the quasi-Fermi level splitting [3]. Fullerene derivatives do not easily form a crystalline phase, compared to that of fullerene, unless additional steps are taken to promote their crystallinity.

Recently, Prof. Yaowen Li at Soochow University, Dr. Qi Chen at Suzhou Institute of Nano-Tech and Nano-Bionics, CAS and coworkers [4] have designed a new fullerene molecule that can solve all of the abovementioned issues. The authors synthesized PCBB-3N-3I, an iodide quaternized derivative of a fullerene derivative terminated with tris(dimethylamine) (PCBB-3N) (Figure 1), which exhibits high conductivity and strong molecular electric dipole moment.

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**Figure 1** Chemical structures of fullerenes with dipoles and their application in perovskite solar cells to achieve enhanced efficiency [4] (color online).

By treating perovskite with PCBB-3N-3I, the positively charged surface defects may act as anchor sites for iodide in PCBB-3N-3I via electrostatic interaction, which can be efficiently passivated and further provides a driving force for PCBB-3N-3I to be assembled with preferred orientation. This brings order to the fullerene derivatives, which should increase the quasi-Fermi level. The dipole of these molecules effectively reduces the work function of the metal and may facilitate charge collection. Consequently, the PCBB-3N-3I interlayer reconfigures the interfacial energy band structure, which results in larger open circuit voltage. Thus, inverted structure planar heterojunction perovskite solar cells exhibit enhanced PCE of 17.7%–21.1% as well as improved ambient stability of the solar cells (Figure 1). This is a considerable progress. Although it remains to be seen the cost and stability of these materials in operation condition. this study will in-

spire more designs from organic chemists to enlarge the library of fullerene derivatives that may address the abovementioned issues. The game is on now, and will be interesting to explore ideas on how to convert perovskite defective surfaces into wide bandgap and robust oxides that passivate the surface [5].

**Conflict of interest** The author declares no conflict of interest.

- 1 Shao Y, Xiao Z, Bi C, Yuan Y, Huang J. *Nat Commun*, 2014, 5: 5784
- 2 Chen B, Rudd PN, Yang S, Yuan Y, Huang J. *Chem Soc Rev*, 2019, 48: 3842–3867
- 3 Yang S, Dai J, Yu Z, Shao Y, Zhou Y, Xiao X, Zeng XC, Huang J. *J Am Chem Soc*, 2019, 141: 5781–5787
- 4 Zhang M, Chen Q, Xue R, Zhan Y, Wang C, Lai J, Yang J, Lin H, Yao J, Li Y, Chen L, Li Y. *Nat Commun*, 2019, 10: 4593
- 5 Yang S, Chen S, Mosconi E, Fang Y, Xiao X, Wang C, Zhou Y, Yu Z, Zhao J, Gao Y, De Angelis F, Huang J. *Science*, 2019, 365: 473–478