Modulate Organic-Metal Oxide Heterojunction via [1,6]Azafulleroid for Highly Efficient Organic Solar Cells

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Abstract: By creating an effective π-orbital hybridization between the fullerene cage and the aromatic anchor (addend), the azafulleroid interfacial modifiers exhibit enhanced electronic coupling to the underneath metal oxides. High power conversion efficiency of 10.3% can be achieved in organic solar cells using open-cage PCBM modified zinc oxide layer.

Introduction

The heterojunction between organic and inorganic semiconductor is one of the critical interfaces in the hybrid thin film electronic devices.[1-2] Across such interfaces with composition-distinct materials, the energy level alignment and charge extraction (or injection) need to be optimized in order to achieve good device performance. In fact, charge trapping and recombination due to the presence of physical and chemical defects often occur at these interfaces to deteriorate device performance. Therefore, approaches of tailoring these interfaces have been vigorously explored for device fabrication. Efficient charge extraction (or injection) from a semiconductor to a metal oxide electron transport layer (ETL) requires effective electronic coupling and minimized contact resistance between them that can be achieved through proper interfacial modifications.

Molecular Design and Electronic Structures

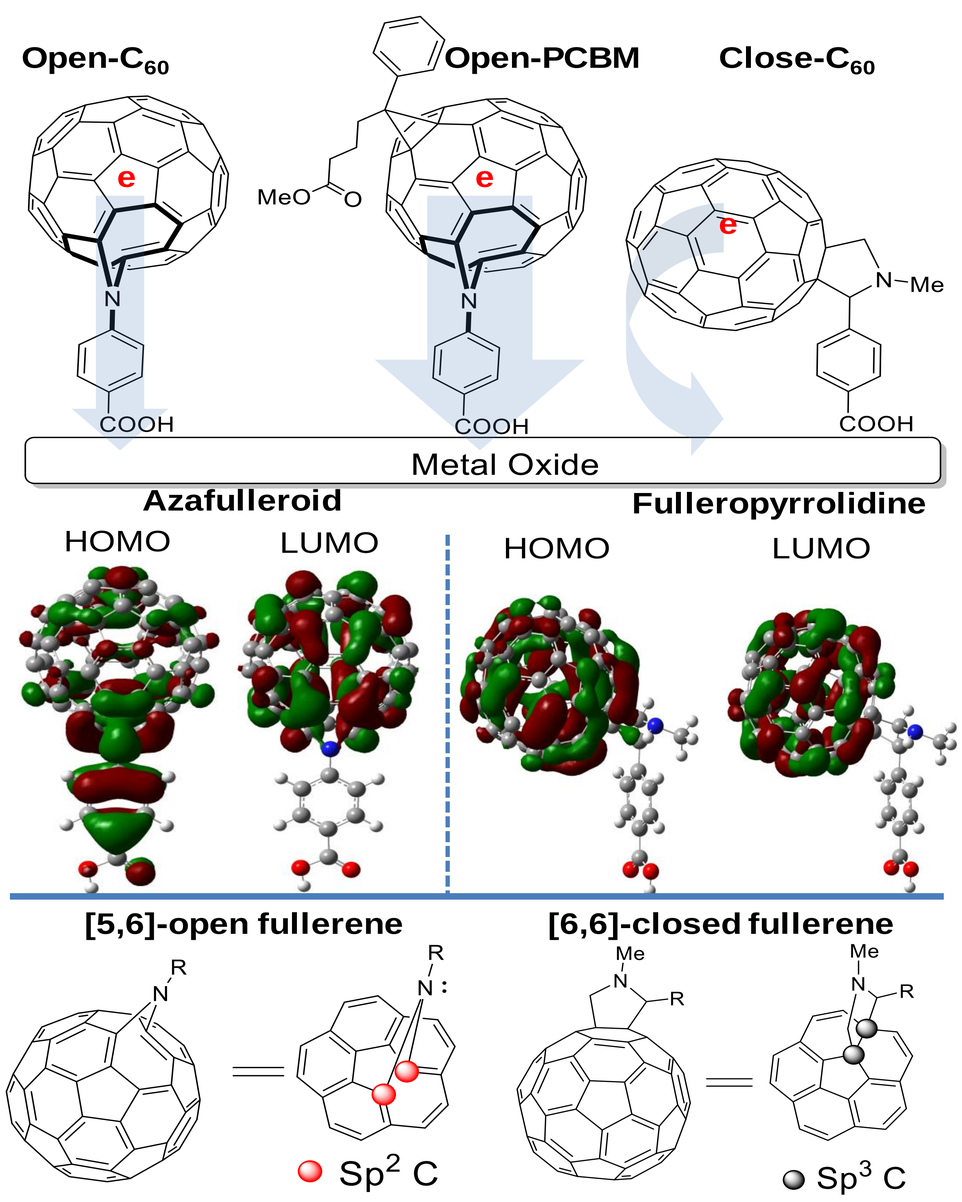


Figure 1. Schematic illustration of electron transport from fullerene interfacial modifier to ZnO (top), the modeled HOMO/LUMO (middle), and the structure difference of [5,6]-open fullerene and [6,6]-closed fullerene.

Material Properties

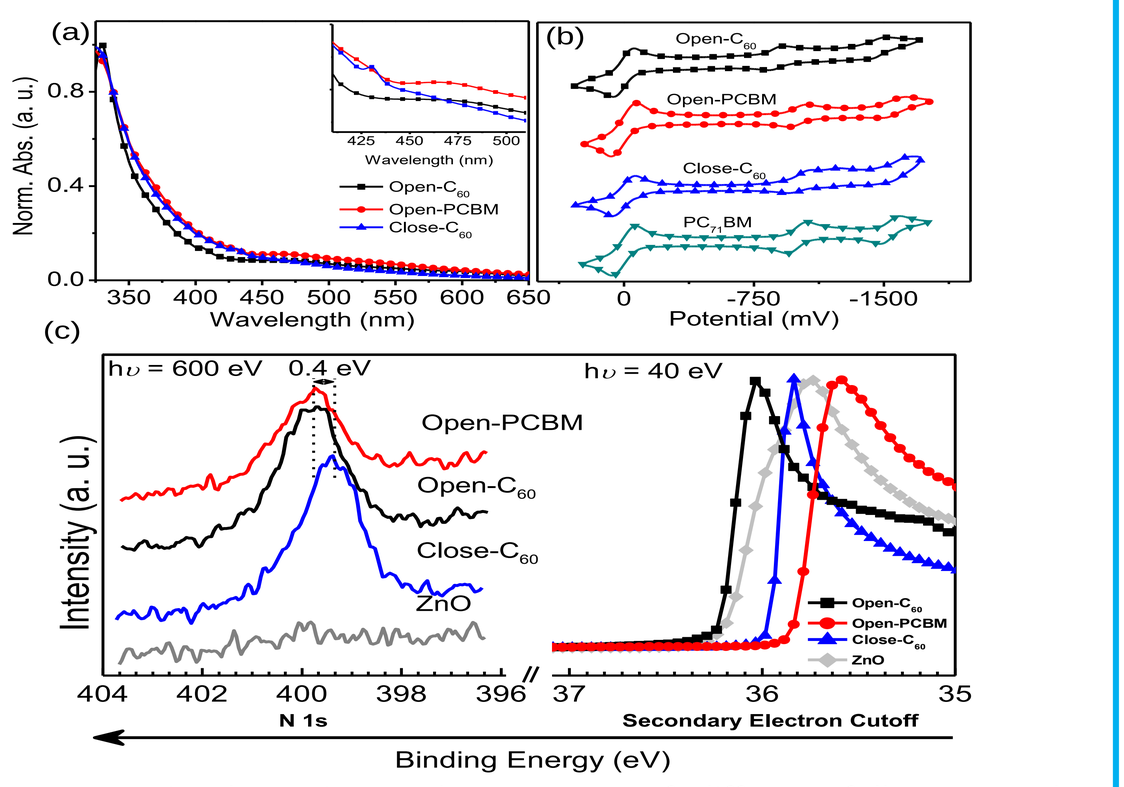
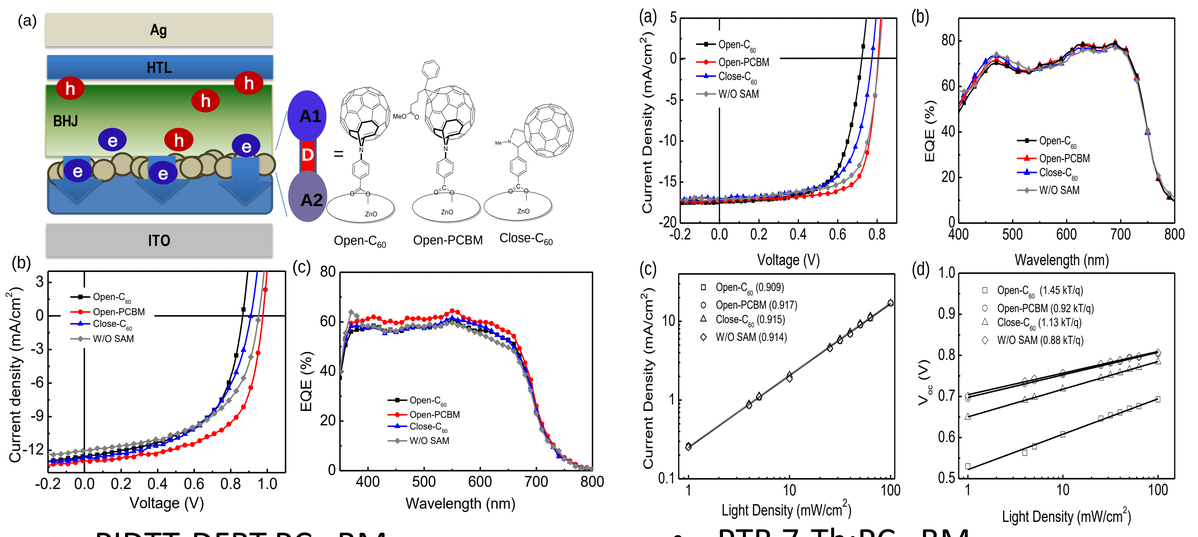


Figure 2. UV-vis absorption and CV curves of different fullerene, and Photoemission spectroscopy of ITO/ZnO with and without modification.

Inverted OSCs with SAM Modified ZnO



- PIDTT-DFBT:$PC_{71}BM$
- PTB 7-Th:$PC_{71}BM$

Table 1. Photovoltaic properties of inverted devices using PTB7-Th:$PC_{71}BM$ BHJ

Device	Voc (V)	Jsc (mA/cm^2)	FF	PCE [a] (%)
W/O	0.81 (0.80±0.01)	17.10 (17.04±0.05)	0.69 (0.68±0.02)	9.51 (9.26)
Open-C_{60}	0.72 (0.71±0.01)	17.41 (17.36±0.06)	0.66 (0.64±0.02)	8.26 (7.99)
Open-PCBM	0.81(0.80±0.01)	17.32 (17.28±0.05)	0.74 (0.72±0.02)	10.30 (9.95)
Close-C_{60}	0.77 (0.76±0.01)	17.06 (17.02±0.06)	0.65 (0.64±0.01)	8.58 (8.39)

Conclusions: In conclusion, we have designed new aza[60]fulleroid derivatives as interfacial modifiers for engineering the contact between the organic BHJ and ZnO. By facilitating effective p-conjugation between fullerene and aromatic addends, the electronic coupling between fullerene and the underneath metal oxides (through conjugated anchors) could be enhanced. As a result, new interfacial modifiers with varied functionalities and energetics are found not only to be able to shift the WF of ZnO, but also mediate the electron extraction from BHJ to metal oxide ETL. The molecular design, synthesis, and experimental studies reported here provide valuable insights for designing new generation of functional materials for highly efficient organic electronics.

References:

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[3] Li, C.-Z. et al., *Mater. Horiz*. 2, **2015**, 414. [4] Li, C.-Z. et al., *Adv. Mater.,* **2013**, 25, 2457. [5] Li, C.-Z.et al., *Adv. Mater.,* **2013**, 25, 4425.
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