

Core-expanded naphthalenediimide derivatives as non-fullerene electron transport materials for inverted perovskite solar cells

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ABSTRACT

Two core-expanded naphthalenediimide (NDI) derivatives NDI3HU-DTYM2 (**1**) and (DTYM-NDI-DTYA)₂ (**2**) with coplanar and twisted molecular backbones, respectively, were used as low-temperature solution-processed electron transport materials (ETMs) for CH₃NH₃PbI₃-based inverted planar perovskite solar cells (PSCs). The high electron mobility as well as low-lying lowest unoccupied molecular orbital (LUMO) energy levels and good film-formation ability on perovskite layers make **1** and **2** both promising ETMs for PSCs. The PSCs devices based on **1** show a power conversion efficiency (PCE) of 8.7%, while the PSCs devices based on **2** that has twisted molecular backbone exhibit a PCE value of up to 12.9%, a short-circuit current density (J_{sc}) value of 22.80 mA cm⁻² with negligible hysteresis, which is comparable to that of PCBM-based PSCs devices. Our results demonstrate that core-expanded NDI-based n-type organic semiconductors, especially those with twisted molecular backbones, have great potential for high-performance, low-cost, solution-processed non-fullerene ETMs in PSCs.

1. Introduction

As an emerging photovoltaic technology, perovskite solar cells (PSCs) that use hybrid organic-inorganic trihalide materials as the light absorber have attracted ever increasing attention and inspired much research interest over the past few years [1–17]. The use of perovskites affords several exceptional properties such as broad and tunable light absorption, balanced ambipolar charge transport, ultra-long charge carrier diffusion lengths and low exciton binding energy. With numerous efforts and extensive investigations, the power conversion efficiency (PCE) of PSCs has realized from initial 3.8% [18] to current a certified value of 22.7% [19]. The state-of-the-art planar PSCs were usually constructed into two device architectures, the n-i-p (regular) structure [10,11] with the electron transport material (ETM) at the front and the p-i-n (inverted) structure [9,14] with the hole transport material (HTM) at the front. Nowadays, the PSCs adopt the n-i-p architecture with PCE exceeding 20% were achieved by using either 2,2',7,7'-tetrakis [N,N-di (4-methoxyphenyl)amino]-9,9'-spirobifluorene (spiro-OMeTAD) or poly[bis(4-phenyl) (2,4,6-trimethylphenyl)amine] (PTAA) as the HTMs [20,21]. However, the widespread use of these HTMs was limited due to the costs, the solubility, as well as the scalability and the requirement of slow oxygen doping process. Very

recently, a great deal of efforts have been made to develop low-cost [22], ionic dopant-free HTMs [23,24]. In comparison with n-i-p architecture devices, devices with inverted structure have exhibited more superiority such as easy fabrication process, small hysteresis effect and high stability [25–27]. ETMs play a critical role in inverted structure devices, an ideal ETM layer possessed a suitable energy level and high electron mobility that guaranteed efficient hole-blocking and suppressed charge recombination, facilitated photo-generated electron injection and transport, reduced the energy loss to achieve high device performance [28]. Until now, the most commonly used ETM in p-i-n structure devices was (6,6)-phenyl-C₆₁-butyric acid methyl ester (PCBM) [29–32], other fullerene-based n-type materials such as fullerene (C₆₀), indene-C₆₀ bis-adduct (ICBA) and [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) were also employed as ETMs in p-i-n architecture, but unfortunately suffered from indecent performance [33,34]. Moreover, fullerene derivatives exhibited some drawbacks such as the high production cost, limited morphology stability as well as unfavourable chemical stability [35,36], which strongly restrict their further application in PSCs.

Because of the insufficient understanding of the interactions between organic ETMs and perovskite films, non-fullerene ETMs are still in a very beginning stage and only a few attempts have been made to

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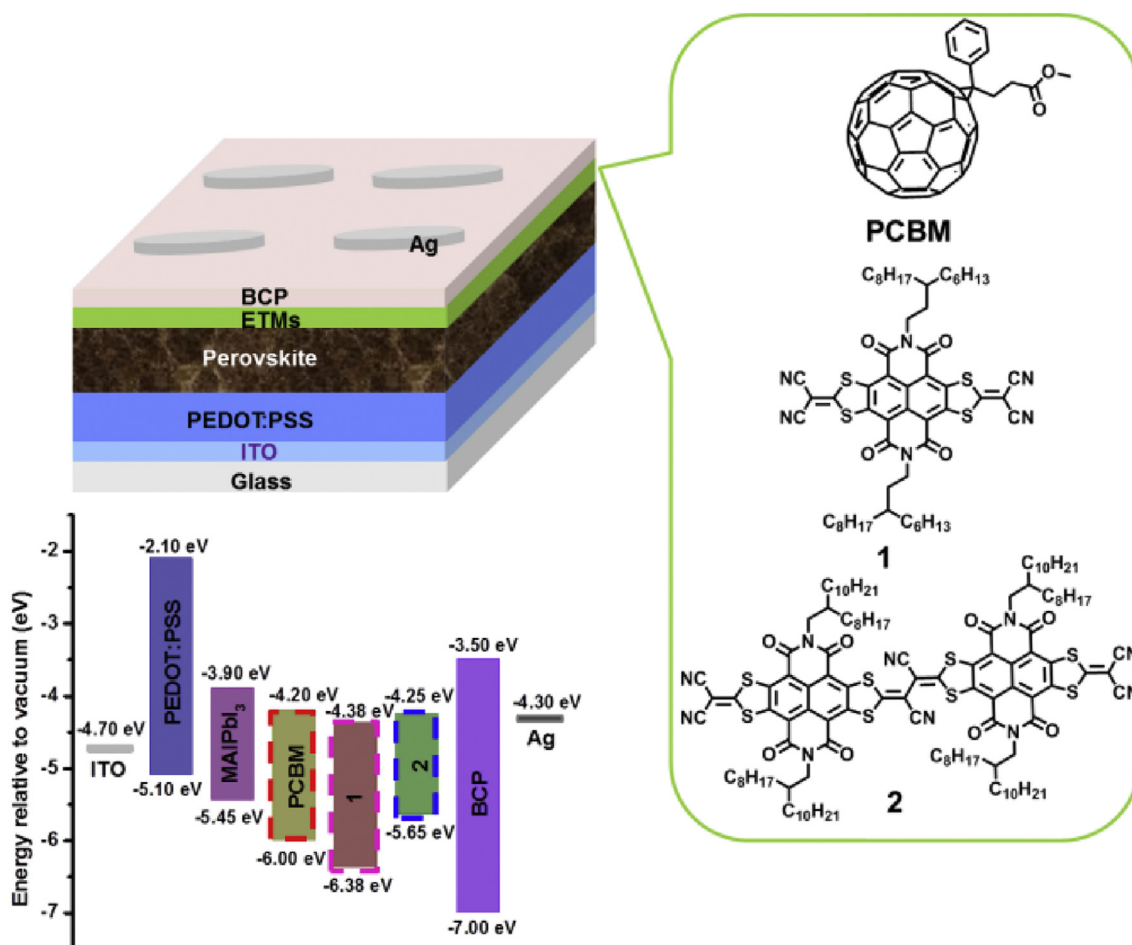


Fig. 1. Device configuration of inverted planar PSCs, the chemical structures of the ETMs and energy levels alignment of the materials used in this study.

use organic non-fullerene ETMs in PSCs [37–45], which is quite different from the fast developing non-fullerene acceptors in organic photovoltaics (OPVs) [46]. Fortunately, some non-fullerene ETMs show more attractive as a promising alternative to PCBM-based fullerene derivatives for PSCs [37–45]. It is well known that both HTMs and ETMs with low-cost and high efficiency features are the tickets to approach the practical application of low-temperature all-solution processed and large-scale PSCs. Therefore, besides the rapid developing HTMs, it is very urgent to develop high performance organic non-fullerene ETMs for PSCs. In recent years, we developed a series of core-expanded naphthalenediimide (NDI) derivatives [47–53], which are air-stable, solution-processed and high performance n-type semiconductors. Among them, two core-expanded NDI derivatives NDI3HU-DTYM2 (1) [49,50] and (DTYM-NDI-DTYA)₂ (2) [52] (Fig. 1) with planar and twisted molecular backbones, respectively, showed unipolar n-channel field effect characteristics with electron mobilities of up to $3.5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and $0.45 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, respectively. Herein compound 1 and 2 were employed as ETMs in $\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI₃)-based inverted planar PSCs. Thanks to the well-aligned low-lying lowest unoccupied molecular orbital (LUMO) energy level, high electron mobility and isotropic charge transport paths, a high PCE value of 12.9% with little hysteresis effect was achieved by 2-based PSCs devices, which can rival the device performance obtained from PCBM-based PSCs and outperform those based on 1 with planar molecular backbone. Our results provide a new insight to develop new high performance, low-cost, solution-processed non-fullerene ETMs for PSCs.

2. Experimental

2.1. Materials

$\text{CH}_3\text{NH}_3\text{I}$ (MAI) was synthesized by reacting 20 mL CH_3NH_2 (MA, 33 wt% in absolute ethanol, Energy Chemical, China) and 21 mL hydroiodic acid (HI, 55–58 wt% in water, Aladdin, China) in a 250 mL round-bottom flask under an ice bath with stirring for 4 h. The precipitate was recovered by evaporation off solvents at 50°C for 1 h. MAI was dissolved in ethanol, recrystallized from diethyl ether, and dried at 50°C in a vacuum oven for 24 h. 1.3 M MAPbI₃ solution (MAI:PbI₂ (99%, TCI, Japan) = 1:1 in a molar ratio) was stirred in a mixture of γ -butyrolactone (GBL, 99%, TCI, Japan) and dimethylsulphoxide (DMSO, 99.8%, J&K, China) (7:3 v/v) in a N_2 glovebox at room temperature overnight. Poly (3,4-ethylenedioxythiophene):poly (styrene-sulfonate) (PEDOT:PSS, CLEVIOS P VP Al 4083) aqueous solution was purchased from Heraeus, German. (6,6)-phenyl-C₆₁-butyric acid methyl ester (PCBM, 99.5%) was purchased from ADS, Canada. Bathocuproine (BCP, 99%) was purchased from TCI, Japan. Indium tin oxide-coated (ITO) glasses (sheet resistance $\leq 10 \Omega \text{ cm}^{-2}$) were purchased from Kaivo, China. Aluminum (Al 99.999%) was purchased from Cuibolin, China. Silver (Ag, 99.99%) was purchased from CNM, China. NDI3HU-DTYM2 derivative (1) [49,50], and (DTYM-NDI-DTYA)₂ (2) [52] were synthesized as previously reported.

2.2. Solar cell fabrication

ITO-coated glasses were cleaned consecutively in detergent, deionized water, acetone and isopropanol ultrasonic baths for 20 min,

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