

Star polymer donors

Jiamin Cao^{1, †}, Guangan Nie¹, Lixiu Zhang², and Liming Ding^{2, †}

¹Key Laboratory of Theoretical Organic Chemistry and Functional Molecule (MoE), School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan 411201, China

²Center for Excellence in Nanoscience (CAS), Key Laboratory of Nanosystem and Hierarchical Fabrication (CAS), National Center for Nanoscience and Technology, Beijing 100190, China

Citation: J M Cao, G A Nie, L X Zhang, and L M Ding, Star polymer donors[J]. *J. Semicond.*, 2022, 43(7), 070201. <https://doi.org/10.1088/1674-4926/43/7/070201>

Organic solar cells (OSCs) as a promising photovoltaic technology have attracted great attention due to its unique advantages, such as solution processing, low cost, lightweight and excellent mechanical flexibility^[1–5]. Conventional OSCs always employ fullerene derivatives, e.g. PC₆₁BM, PC₇₁BM and IC₇₀BA, as electron acceptors. Fullerene derivatives present weak absorption in the visible region, while polymer donors show excellent light-harvesting ability in the visible and even near-infrared (NIR) regions. Many medium- or low-bandgap polymer donors have been developed for complementary absorption, and the power conversion efficiencies (PCEs) for fullerene-based OSCs reach ~12%^[6, 7].

In 2015, a nonfullerene acceptor (NFA) ITIC was reported by Zhan *et al.*, bringing OSC to a new era. Many efficient NFAs have been developed, and the PCEs of solar cells have soared to ~19%^[1, 2]. NFAs always exhibit much low optical bandgap with strong absorption in 600–900 nm, so the development of wide-bandgap (WBG) polymer donors with good light-harvesting ability in 400–700 nm is desirable^[8–12]. The pairing of WBG polymer donors and low-bandgap (LBG) NFAs presents reduced voltage loss (V_{loss}), and the highest occupied molecular orbital (HOMO) offset between donor and acceptor can be very small, even close to zero^[2, 3].

BDTT is one of the best building blocks in constructing D-A conjugated polymers^[13]. The two-dimensional conjugated structure and weak electron-donating ability endow its copolymers with good hole mobilities and low HOMO energy levels. In 2015, Hou *et al.* reported PM6 (PBDB-TF), and its fullerene solar cells gave a 9.2% PCE (Fig. 1). PM6 offered over 18% PCE when blending with Y-series NFAs^[13]. PM6 works very well with most NFAs, and has become one of the best commercial polymer donors. In addition, the chlorinated derivative PM7 (PBDB-TCl) achieved over 17% PCE in PM7:Y6 cells^[14]. What's more, some donor or acceptor units as the third component were introduced into PM6. Efficient terpolymer donors were obtained by using random D-A copolymerization to tune the energy levels and absorption. Li *et al.* introduced an electron-withdrawing unit 2,5-bis(4-(2-ethylhexyl)thiophen-2-yl)pyrazine into PM6 backbone to get a D-A₁-D-A₂ type terpolymer PMZ-10. PMZ-10:Y6 solar cells

gave a PCE of 18.23%^[15].

In 2020, Ding *et al.* reported a milestone WBG polymer donor D18 based on DTBT unit with large molecular plane and strong electron-withdrawing capability^[1, 16]. D18:Y6 cells offered a PCE of 18.22%, with an open-circuit voltage (V_{oc}) of 0.859 V, a short-circuit current density (J_{sc}) of 27.70 mA/cm² and a FF of 76.6%, which was the first report on single-junction OSCs with over 18% efficiency^[1]. Then, the chlorinated analogue D18-Cl was reported. D18-Cl:N3 cells and D18-Cl:N3:PC₆₁BM cells delivered PCEs of 18.13% and 18.69%, respectively^[17, 18]. Later, D18-B and D18-Cl-B were also developed *via* side-chain engineering. D18-B:N3:PC₆₁BM and D18-Cl-B:N3:PC₆₁BM cells offered PCEs of 18.53% and 18.74%, respectively^[19]. D18 derivatives have been developed and present good performance^[20, 21].

Hou *et al.* reported two dithieno[3,2-f:2',3'-h]quinoxaline (DTQx)-based polymer donors PBQx-TF and PBQx-TCl with fluorinated or chlorinated BDTT as the donor units^[22, 23]. 19.0% and 18.0% PCEs were achieved for PBQx-TF:F-BTA3:eC9-2Cl and PBQx-TCl:BTA3:BTP-eC9 cells, respectively. Very recently, Hou *et al.* developed a WBG polymer donor PB2F containing fluorinated BDTT and 1,3,4-thiadiazole units with a very deep HOMO level of -5.64 eV. PB2F:PM6:BTP-eC9 cells gave a PCE of 18.6%^[24].

The polymer donors mentioned above are based on BDTT donor unit, and they need complex syntheses. Li *et al.* reported a low-cost polymer donor PTQ10 with thiophene and 6,7-difluoro-2-(2-hexyldecyloxy)quinoxaline units, which was synthesized from commercial materials *via* a two-step synthesis (yield 87.4%). PTQ10:BTP-FTh:IDIC cells demonstrated a PCE of 19.05%^[2].

Currently, most efficient polymer donors are synthesized through multi-step reactions, exhibiting high cost. Cheap and high-performance polymer donors well matching those LBG NFAs are needed^[25–30]. We are expecting single-junction OSCs with >20% PCE.

Acknowledgements

J. Cao thanks the National Natural Science Foundation of China (21604021), Hunan Provincial Natural Science Foundation (2018JJ3141), and the Innovation Team of Huxiang High-level Talent Gathering Engineering (2021RC5028). L. Ding thanks the National Key Research and Development Program of China (2017YFA0206600), the National Natural Science Foundation of China (51922032 and 21961160720), and the

Correspondence to: J M Cao, jiamincao@hnust.edu.cn; L M Ding, ding@nanoctr.cn

Received 13 APRIL 2022.

©2022 Chinese Institute of Electronics

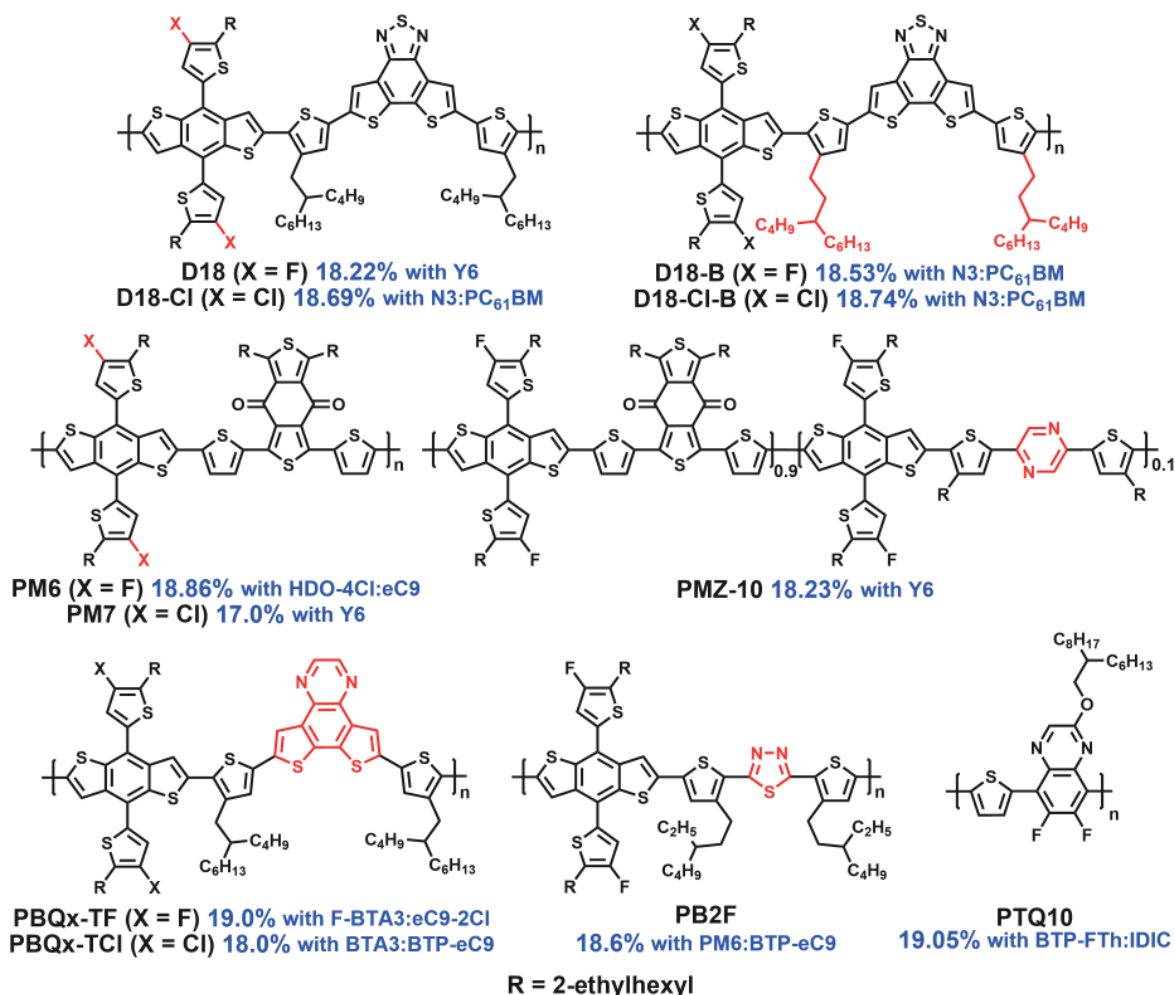


Fig. 1. (Color online) The chemical structures for representative polymer donors and the PCEs.

open research fund of Songshan Lake Materials Laboratory (2021SLABFK02) for financial support.

References

- [1] Liu Q, Jiang Y, Jin K, et al. 18% Efficiency organic solar cells. *Sci Bull*, 2020, 65, 272
- [2] Chong K, Xu X, Meng H, et al. Realizing 19.05% efficiency polymer solar cells by progressively improving charge extraction and suppressing charge recombination. *Adv Mater*, 2022, 34, 2109516
- [3] Zeng Y, Li D, Xiao Z, et al. Exploring the charge dynamics and energy loss in ternary organic solar cells with a fill factor exceeding 80%. *Adv Energy Mater*, 2021, 11, 2101338
- [4] Li D, Zeng Y, Chen Z, et al. Investigating the reason for high FF from ternary organic solar cells. *J Semicond*, 2021, 42, 090501
- [5] Luo Y, Chen X, Xiao Z, et al. A large-bandgap copolymer donor for efficient ternary organic solar cells. *Mater Chem Front*, 2021, 5, 6139
- [6] Duan C, Ding L. The new era for organic solar cells: non-fullerene small molecular acceptors. *Sci Bull*, 2020, 65, 1231
- [7] Cao J, Yi L, Ding L. The origin and evolution of Y6 structure. *J Semicond*, 2022, 43, 030202
- [8] Wang J, Gao Y, Xiao Z, et al. A wide-bandgap copolymer donor based on a phenanthridin-6(5H)-one unit. *Mater Chem Front*, 2019, 3, 2686
- [9] Wang T, Qin J, Xiao Z, et al. A 2.16 eV bandgap polymer donor gives 16% power conversion efficiency. *Sci Bull*, 2020, 65, 179
- [10] Xiong J, Xu J, Jiang Y, et al. Fused-ring bislactone building blocks for polymer donors. *Sci Bull*, 2020, 65, 1792
- [11] Jiang Y, Jin K, Chen X, et al. Post-sulphuration enhances the performance of a lactone polymer donor. *J Semicond*, 2021, 42, 070501
- [12] Ou Z, Qin J, Jin K, et al. Engineering of the alkyl chain branching point on a lactone polymer donor yields 17.81% efficiency. *J Mater Chem A*, 2022, 10, 3314
- [13] Zheng Z, Yao H, Ye L, et al. PBDB-T and its derivatives: A family of polymer donors enables over 17% efficiency in organic photovoltaics. *Mater Today*, 2020, 35, 115
- [14] Ma R, Liu T, Luo Z, et al. Improving open-circuit voltage by a chlorinated polymer donor endows binary organic solar cells efficiencies over 17%. *Sci China Chem*, 2020, 63, 325
- [15] Zhou L, Meng L, Zhang J, et al. Introducing low-cost pyrazine unit into terpolymer enables high-performance polymer solar cells with efficiency of 18.23%. *Adv Funct Mater*, 2022, 32, 2109271
- [16] Wang Z, Peng Z, Xiao Z, et al. Thermodynamic properties and molecular packing explain performance and processing procedures of three D18:NFA organic solar cells. *Adv Mater*, 2020, 32, 2005386
- [17] Qin J, Zhang L, Zuo C, et al. A chlorinated copolymer donor demonstrates a 18.13% power conversion efficiency. *J Semicond*, 2021, 42, 010501
- [18] Jin K, Xiao Z, Ding L. 18.69% PCE from organic solar cells. *J Semicond*, 2021, 42, 060502
- [19] Meng X, Jin K, Xiao Z, et al. Side chain engineering on D18 polymers yields 18.74% power conversion efficiency. *J Semicond*, 2021, 42, 100501

- [20] Li X, Xu J, Xiao Z, et al. Dithieno[3',2':3,4;2'',3'':5, 6]benzo[1,2-c][1,2,5]oxadiazole-based polymer donors with deep HOMO levels. *J Semicond*, 2021, 42, 060501
- [21] Sun A, Xu J, Zong G, et al. A wide-bandgap copolymer donor with a 5-methyl-4H-dithieno[3,2-e:2',3'-g]isoindole-4,6(5H)-dione unit. *J Semicond*, 2021, 42, 100502
- [22] Cui Y, Xu Y, Yao H, et al. Single-junction organic photovoltaic cell with 19% efficiency. *Adv Mater*, 2021, 33, 2102420
- [23] Xu Y, Cui Y, Yao H, et al. A new conjugated polymer that enables the integration of photovoltaic and light-emitting functions in one device. *Adv Mater*, 2021, 33, 2101090
- [24] Zhang T, An C, Bi P, et al. A thiadiazole-based conjugated polymer with ultradeep HOMO level and strong electroluminescence enables 18.6% efficiency in organic solar cell. *Adv Energy Mater*, 2021, 11, 2101705
- [25] Duan C, Ding L. The new era for organic solar cells: polymer donors. *Sci Bull*, 2020, 65, 1422
- [26] Qin J, Zhang L, Xiao Z, et al. Over 16% efficiency from thick-film organic solar cells. *Sci Bull*, 2020, 65, 1979
- [27] Xu J, Sun A, Xiao Z, et al. Efficient wide-bandgap copolymer donor with reduced synthesis cost. *J Mater Chem C*, 2021, 9, 16187
- [28] Yang X, Ding L. Organic semiconductors: commercialization and market. *J Semicond*, 2021, 42, 090201
- [29] Jin K, Ou Z, Zhang L, et al. A chlorinated lactone polymer donor featuring high performance and low cost. *J Semicond*, 2022, 43, 050501
- [30] Tong Y, Xiao Z, Du X, et al. Progress of the key materials for organic solar cells. *Sci China Chem*, 2020, 63, 758



Jiamin Cao got his PhD from National Center for Nanoscience and Technology in 2015 under the supervision of Professor Liming Ding. He was a visiting scholar in Ergang Wang Group at Chalmers University of Technology in 2018–2019. Now he is an associate professor in Hunan University of Science and Technology. His research focuses on organic optoelectronics.



Guangan Nie obtained his BS in 2021. Now he is a master student at Hunan University of Science and Technology. His research focuses on organic solar cells.



Lixiu Zhang got her BS degree from Soochow University in 2019. Now she is a PhD student at University of Chinese Academy of Sciences under the supervision of Prof. Liming Ding. Her research focuses on innovative materials and devices.



Liming Ding got his PhD from University of Science and Technology of China (was a joint student at Changchun Institute of Applied Chemistry, CAS). He started his research on OSCs and PLEDs in Olle Inganäs Lab in 1998. Later on, he worked at National Center for Polymer Research, Wright-Patterson Air Force Base and Argonne National Lab (USA). He joined Konarka as a Senior Scientist in 2008. In 2010, he joined National Center for Nanoscience and Technology as a full professor. His research focuses on innovative materials and devices. He is RSC Fellow, the nominator for Xplorer Prize, and the Associate Editor for Journal of Semiconductors.