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SUPPLEMENTARY INFORMATION

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Next-generation organic photovoltaics based on non-fullerene acceptors

Pei Cheng[1], Gang Li[2*], Xiaowei Zhan[3*] and Yang Yang[1*]

[1]Department of Materials Science and Engineering, University of California, Los Angeles, CA, USA. [2]Department of Electronic and Information Engineering, Hong Kong Polytechnic University, Hong Kong, China. [3]Department of Materials Science and Engineering, College of Engineering, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Peking University, Beijing, China. *e-mail: gang.w.li@polyu.edu.hk; xwzhan@pku.edu.cn; yangy@ucla.edu

Supplementary information for

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Pei Cheng[1], Gang Li[2★], Xiaowei Zhan[3★] and Yang Yang[1★]

[1]Department of Materials Science and Engineering, University of California Los Angeles, CA 90095, USA.

[2]Department of Electronic and Information Engineering, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, P. R. China.

[3]Department of Materials Science and Engineering, College of Engineering, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Peking University, Beijing 100871, P. R. China.

★e-mail: yangy@ucla.edu, gang.w.li@polyu.edu.hk, xwzhan@pku.edu.cn

1. Abbreviations

Abbreviations	Full names
3D	Three-dimensional
A	Acceptor
AFM	Atomic force microscope
Ag	Silver
BHJ	Bulk heterojunction
Bis-PDI-T-EG	1,1’-bis(2-methoxyethoxyl)-7,7’-(2,5-thienyl) bis-PDI
BT	Benzothiadiazole
CT	Charge transfer
D	Donor
DFT	Density functional theory
DIO	1,8-diiodooctane
DPPEZnP-TBO	5,15-bis(2,5-bis(2-ethylhexyl)-3,6-dithienyl-2-yl-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione-5-yl-ethynyl)-10,20-bis(5-(2-butyloctyl)thienyl)porphyrin zinc(II)
DPPEZnP-TEH	5,15-bis(2,5-bis-(2-ethylhexyl)-3,6-dithienyl-2-yl-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione-5’-ylethynyl)-10,20-bis(5-(2-ethylhexyl)-thienyl)-porphyrin zinc(II)
DR3TSBDT	((5Z,5’E)-5,5’-((5’’,5’’’’’-(4,8-bis((2-ethylhexyl)thio)benzo[1,2-b:4,5-b’]dithiophene-2,6-diyl)bis(3,3’’-dioctyl-[2,2’:5’,2’’-terthiophene]-5’’,5-diyl))bis(methanylylidene))bis(3-ethyl-2-thioxothiazolidin-4-one)
EQE	External quantum efficiency
F	Fluorine
FF	Fill factor
FTPS	Fourier-transform photocurrent spectroscopy
GaAs	Gallium arsenide
GIWAXS	Grazing incident wide-angle X-ray diffraction
ICBA	Indene-C60 bisadduct
ICL	Interconnecting layer
IDT	Indacenodithiophene
IEIC	2,2’-((2Z,2’Z)-((5,5’-(4,4,9,9-tetrakis(4-hexylphenyl)-4,9-dihydro-s-indaceno[1,2-b:5,6-b’]dithiophene-2,7-diyl)bis(4-(2-ethylhexyl)thiophene-5,2-diyl))bis(methanylylidene))-bis(3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile
IEICO	2,2’-((2Z,2’Z)-((5,5’-(4,4,9,9-tetrakis(4-hexylphenyl)-4,9-dihydros-indaceno[1,2-b:5,6-b’]dithiophene-2,7-diyl)bis(4-((2-ethylhexyl)-oxy)thiophene-5,2-diyl))bis(methanylylidene))bis(3-oxo-2,3-dihydro-1H-indene-2,1-di

	ylidene))dimalononitrile
INCN	2-(3-oxo-2,3-dihydroinden-1-ylidene)malononitrile
IR	Infrared
ITIC	3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone)-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2’,3’-d’]-s-indaceno[1,2-b:5,6-b’]-dithiophene
J_{SC}	Short circuit current density
LUMO	Lowest unoccupied molecular orbital
MoO_3	Molybdenum trioxide
NDI	Naphthalene diimide
NFA	Non-fullerene acceptor
NIR	Near-infrared
NREL	National renewable energy laboratory
OSC	Organic solar cell
P(NDI2HD-T)	Poly[[N,N’-bis(2-hexyldecyl)-naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5’-thiophene]
P3HT	Poly(3-hexylthiophene)
PBDB-T	Poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b’]dithiophene))-alt-(5,5-(1’,3’-di-2-thienyl-5’,7’-bis(2-ethylhexyl)benzo[1’,2’-c:4’,5’-c’]dithiophene-4,8-dione))]
PBDTTTPD	Poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b’]dithiophene-alt-1,3-bis(thiophen-2-yl)-5-(2-hexyldecyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione]
$PC_{61}BM$	[6,6]-Phenyl-C61-butyric-acid-methyl-ester
$PC_{71}BM$	[6,6]-Phenyl-C71-butyric-acid-methyl-ester
PCE	Power conversion efficiency
PDI	Perylene diimide
PDTP-DFBT	Poly[2,7-(5,5-bis-(3,7-dimethyloctyl)-5H-dithieno[3,2-b:2’,3’-d]pyran)-alt-4,7-(5,6-difl uoro-2,1,3-benzothia diazole)]
PEDOT: PSS	Poly(3,4-ethylenedioxylenethiophene)-polystylene sulfonic acid
PFN	Poly[(9,9-bis(3´-(N,N-dimethylamino)propyl)-2,7-fluorene)-alt-2,7-(9,9–dioctylfluorene)]
PL	Photoluminescence
PTB7	Poly[[4,8-bis[(2-ethylhexyl)oxy]benzo-[1,2-b:4,5-b0]dithiophene-2,6-diyl]-[3-fluoro-2-[(2-ethylhexyl)-carbonyl]-thieno-[3,4-b]thiophenediyl]]
PTB7-Th	Poly[[2,60-4,8-di(5-ethylhexylthienyl)benzo-[1,2-b;3,3-b]dithiophene]3-fluoro-2[(2-ethylhexyl)-carbonyl]thieno[3,4-b]thiophenediyl]
S-Q	Shockley–Quiesser

TiO_2	Titanium dioxide
V_{OC}	Open circuit voltage
ZnO	Zinc oxide

2. Chemical structures

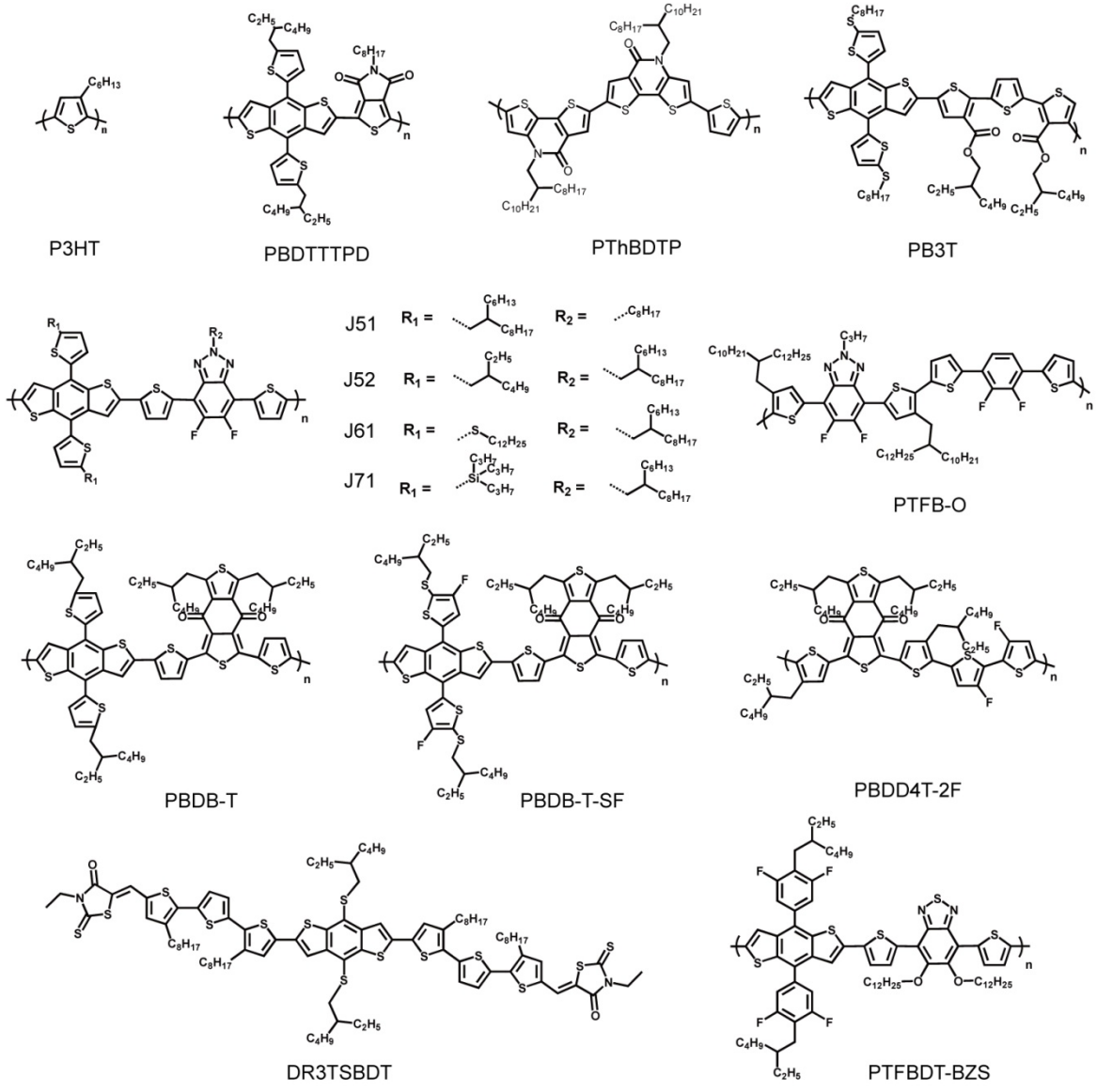

Figure S1 | Chemical structures of wide bandgap donor materials used in OPV.

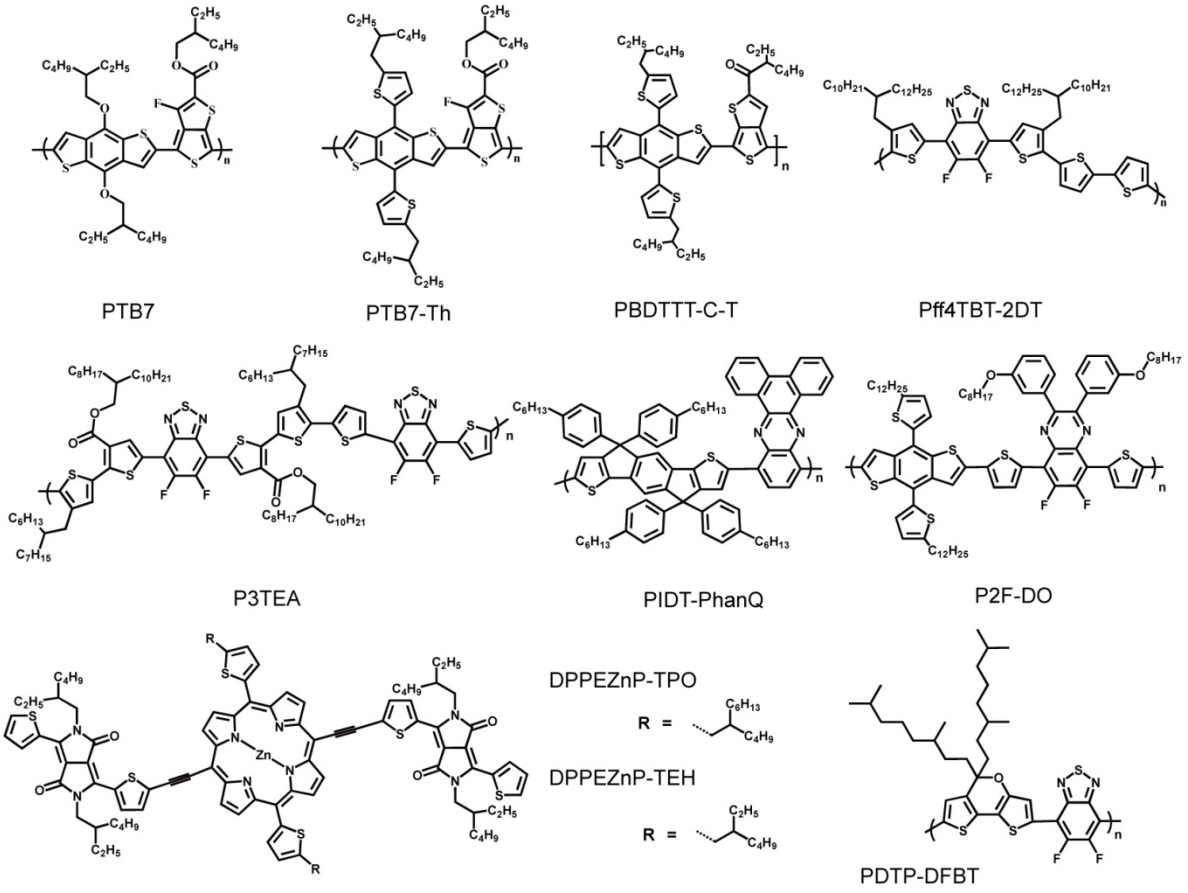

Figure S2 | Chemical structures of medium and narrow bandgap donor materials used in OPV.

3. Calculations

The calculation details are shown as below (Eq. 1 for tandem NFA OSCs with complementary absorption (for Fig 5b), and Eq. 2 for homo tandem NFA OSCs (for Fig 5d)):

Eq. 1:

$$PCE_{\ Tandem} = V_{OC\ Tandem} \times J_{SC\ Tandem} \times FF_{\ Tandem}$$

$$V_{OC\ Tandem} = E_{G\ \ Front\ cell} - W_{OC\ Front\ cell} + E_{G\ \ Rear\ cell} - W_{OC\ Rear\ cell}$$

$$J_{SC\ Tandem} = \min\left(F\left(E_{G\ \ Front\ cell}\right)\left(1\text{-}Mirror_{loss}\right), F\left(E_{G\ \ Rear\ cell}\right) \times 0.5\right)$$

Eq. 2:

$$PCE_{\ Tandem} = V_{OC\ Tandem} \times J_{SC\ Tandem} \times FF_{\ Tandem}$$

$$V_{OC\ Tandem} = 2 \times \left(E_{G\ \ Sub\ cell} - W_{OC\ Sub\ cell}\right)$$

$$J_{SC\ Tandem} = F\left(E_{G\ \ Sub\ cell}\right) \times 0.5 \times EQE_{Ave}/EQE^{*}$$

In these equations, E_G is the bandgap of OSCs; W_{OC} is the V_{OC} loss of OSCs; $Mirror_{loss}$ is induced by the absence of significant reflection at the interface between the front cell and ICL, this loss was recently estimated to be about 15 % in average[1].

As shown in Fig S4, F (E_G) is the fitting function of J_{SC} (as a function of E_G) with assumed EQE (EQE*) of tandem OSCs and AM 1.5G spectrum (1 sun). The EQE (EQE*) is assumed as 75% with all wavelengths; EQE_{Ave} in Eq. 2 is the assumed calculated total EQE (also as a constant value with all wavelengths) of homo tandem device.

The logic of $J_{SC\ Tandem}$ in Eq. 1: The minimum value of J_{SC} obtained from the absorption region of front cell or the half value of J_{SC} obtained from the absorption region of whole tandem device.

The logic of $J_{SC\ Tandem}$ in Eq. 2: The half value of J_{SC} obtained from the absorption region of sub cell.

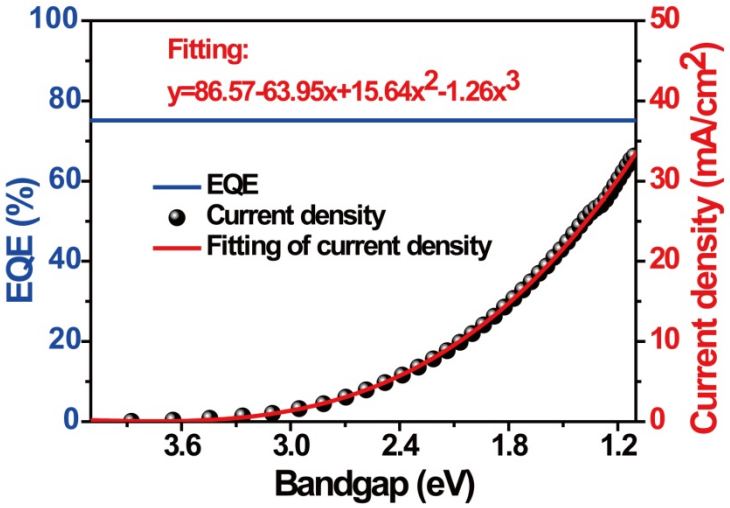

Figure S3 | Fitting of integral current density with different bandgaps, assume the average EQE is 75%.

Reference

1 Dennler, G. *et al.* Design rules for donors in bulk-heterojunction tandem solar cells—Towards 15 % energy-conversion efficiency. *Adv. Mater.* **20**, 579-583 (2008).