Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Iformation

UV Organic Photodetector Employing Dithienylethene as a Photochromic tuner

Jianing Wang, [a‡] *Xiaopeng Zhang,* [b‡] *Minming Yan,* [*b] *Tianhe Xu,* [b] *Hong Xu,* [b] *Hong Chen,* [b] *Hao Yan,* [b] *Chaoyi Yan,*[b] *Wei Huang,* [*a] *and Hong Meng,* [*ab]

[a] Frontiers Science Center for Flexible Electronics Institute of Flexible Electronics, Northwestern Polytechnical University, Xian 710072, P. R. China.

[b] School of Advanced Materials Peking University Shenzhen Graduate School Shenzhen, 518055, P. R. China.

E-mail: jonyymm123@gmail.com (Minming Yan);
E-mail: iamwhuang@nwpu.edu.cn;
E-mail: menghong@pku.edu.cn (Hong Meng).

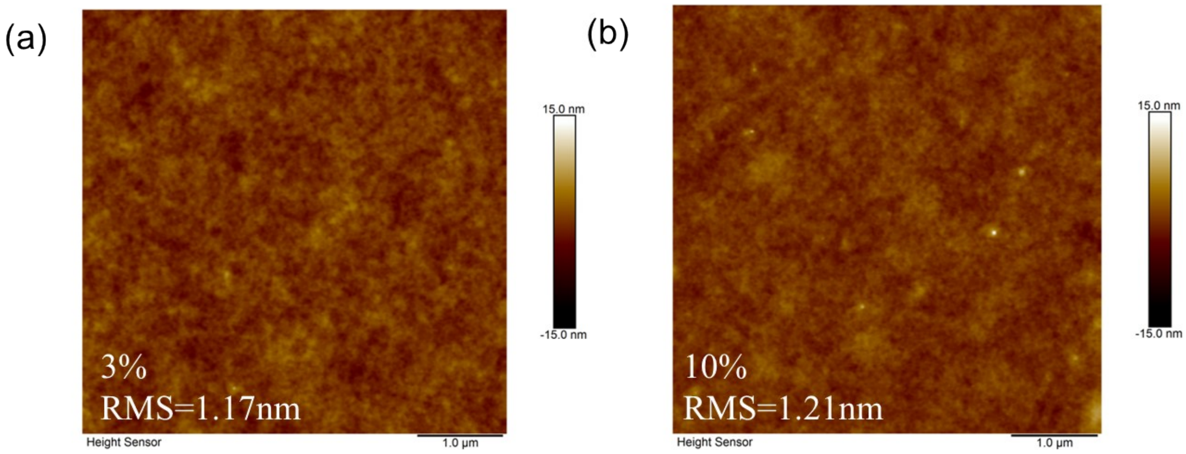


Figure S1 AFM of 3%DTE-Br and 10% DTE-Br in $PC_{61}BM$ and P3HT.

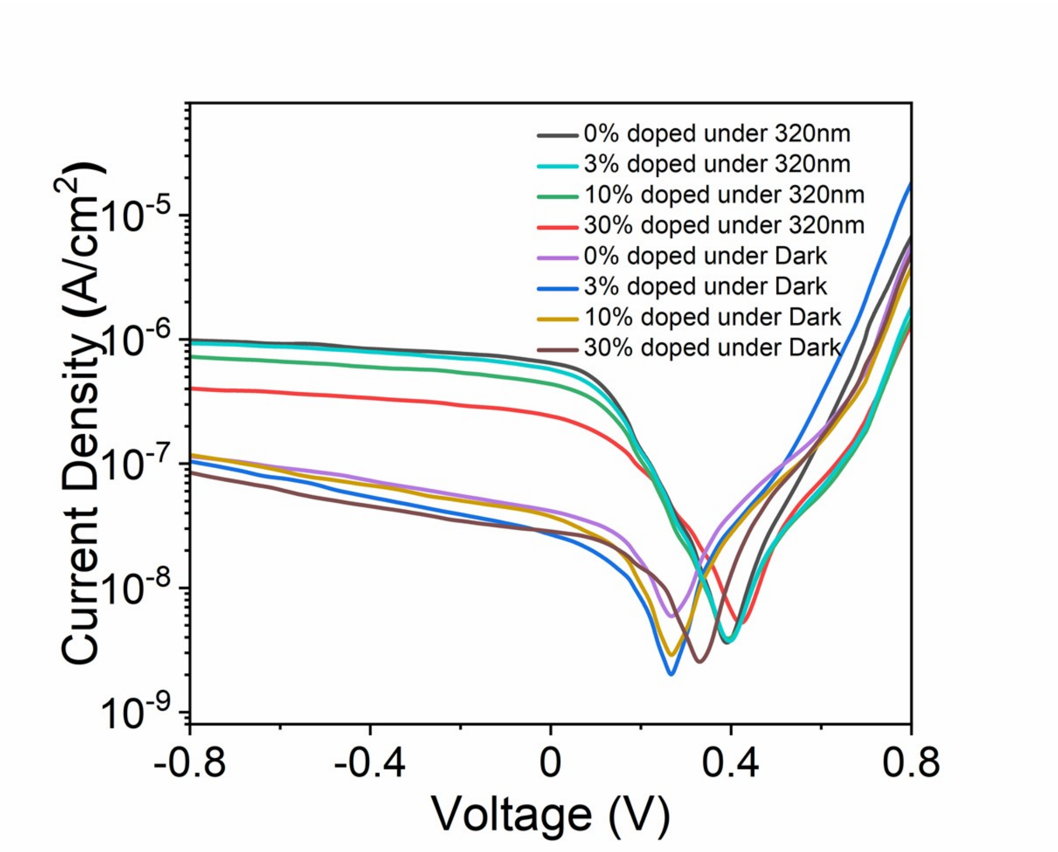


Figure S2. The dark current and photocurrent at 320 nm under 100 μW/cm^2 light intensity for different doping concentrations

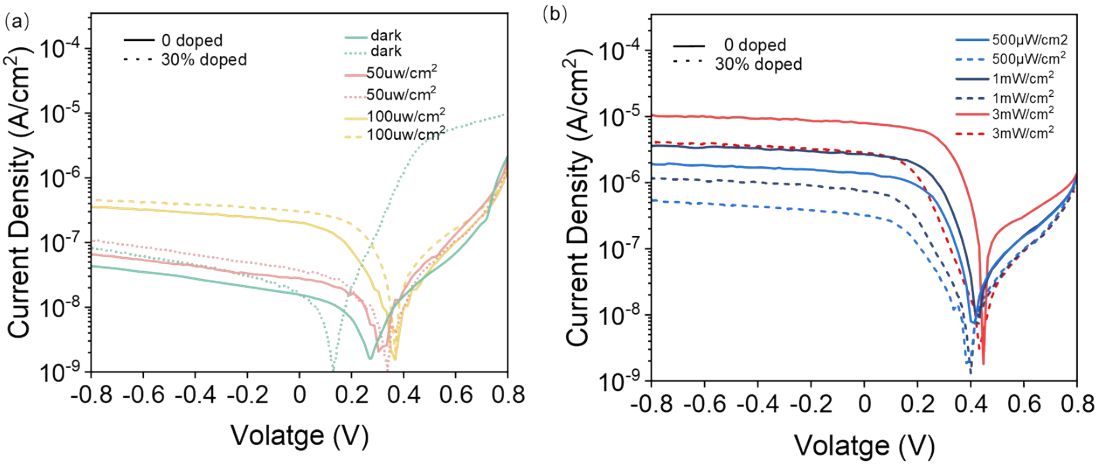


Figure S3. a) photocurrent and dark current under different doping conditions at a wavelength of 320nm and below a light intensity of 100μW. b) photoresponse at light intensities ranging from 500μW to 3mW.

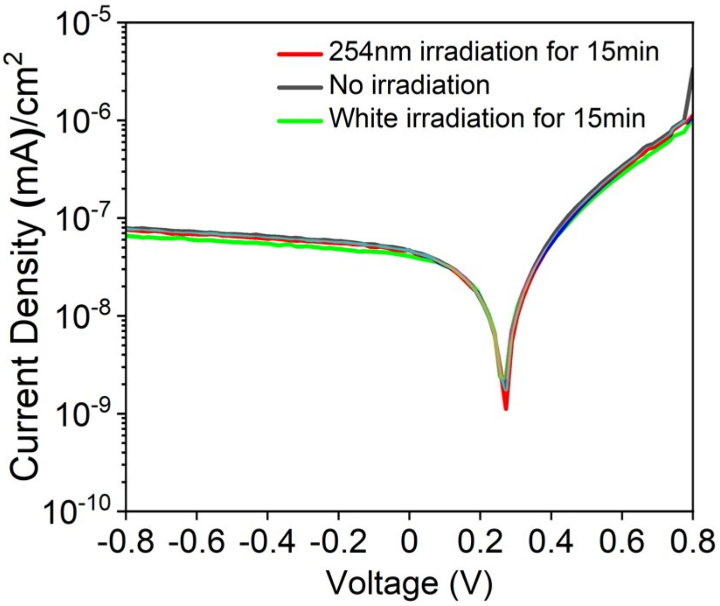


Figure S4. The photocurrent of the undoped device after exposure to 254 nm and white light treatment.

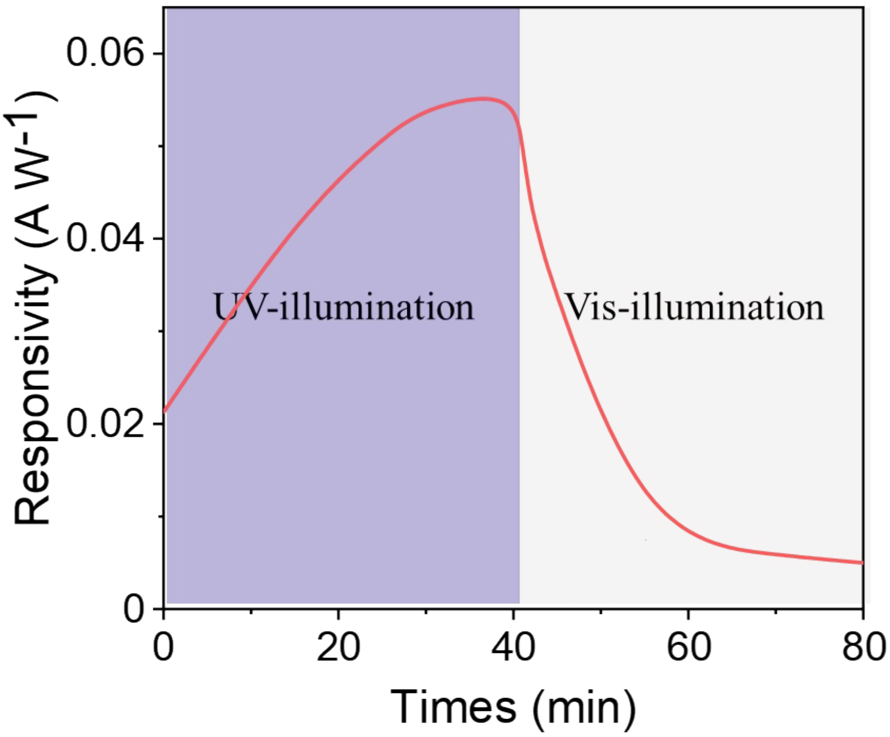
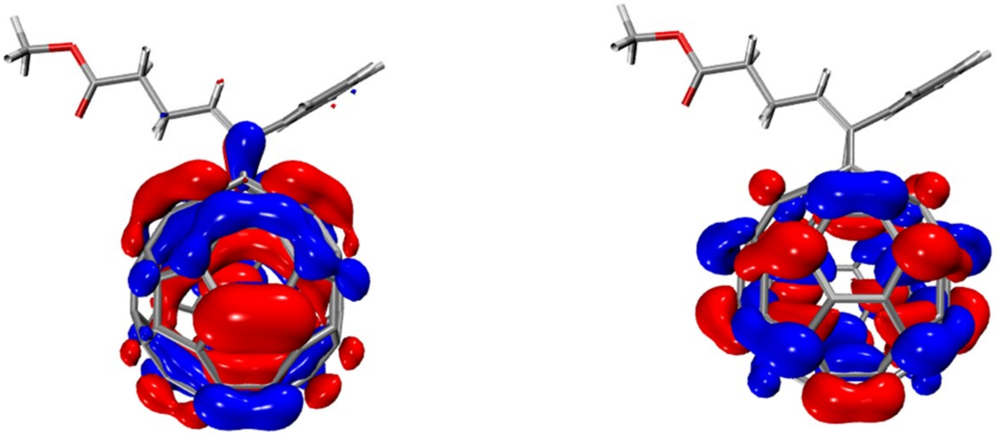


Figure S5. Responsivity changes over time with illumination.

Density functional theory calculations

For the Monomers of DET-Brc, DET-Bro, P3HT and $PC_{61}BM$ the DFT calculations based on the Gaussian 16, Revision C.01.[1] B3LYP[2]-D3[3]/6-31G(d,p) [4] [5]was used for structure optimization. Geometry optimizations were carried out in a vacuum and frequency analysis was performed to ensure that no imaginary frequency occurs. The Molecular Orbital Levels (HOMO and LUMO) and Torsion Angle were studied at the B3LYP-D3/6-31G(d,p) level of theory after running the geometric optimization by the Multiwfn[6] and VMD[7] programs.

For the Dimer and Trimer, using Molclus[8] program, we generate 20 different conformations. MOPAC was called with Molclus program, and the dimers and trimers were preliminarily optimized at PM6[9] -DH[+10] level. The low energy conformations were selected. For low energy conformations, the DFT calculations based on the Gaussian 16, Revision C.01. B3LYP-D3/6-31G(d,p) was used for structure optimization, geometry optimizations were carried out in a vacuum and frequency analysis was performed to ensure that no imaginary frequency occurs. The Intermolecule Distance were studied at the B3LYP-D3/6-31G(d,p) level of theory after running the geometric optimization by the Multiwfn and VMD programs. The Intermolecular Interactions were evaluated at the B3LYP-D3/6-31G(d,p) level of theory after running the geometric optimization by Multiwfn based on the IGMH[11] proposed in Ref.[11] and the EDA-FF[12] proposed in Ref.[12]



HOMO = -5.59 eV

LUMO = -3.04 eV

Figure S6. DFT-calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) for the simplified structures of $PC_{61}BM$ under the B3LYP-D3/6-31G(d,p)level.

Supplementary Tables

Supplementary Table 1. EDA-FF for DET-Br - P3HT and C_{60} cage

	Electrostatic (kJ/mol)	Repulsion (kJ/mol)	Dispersion (kJ/mol)	Total (kJ/mol)
DET-Br_C - P3HT to C_{60} cage	-85.97	85.23	-166.18	-166.92
DET-Br_O - P3HT to C_{60} cage	-31.38	83.45	-171.38	-119.31
P3HT and C_{60} cage	-60.46	44.74	-103.91	-119.62

Supplementary Table 2. Intermolecule Distance of DET-Br - P3HT to $PC_{61}BM$

	Geometry center (DET-Br - P3HT) (Angstrom)	Geometrycenter ($PC_{61}BM$) (Angstrom)	Intermolecule Distance (Angstrom)
DET-Br_C - P3HT to $PC_{61}BM$	(-1.18, -2.14, 0.88)	(1.84, 1.46, -0.06)	4.79
DET-Br_O - P3HT to $PC_{61}BM$	(1.22, -2.12, 1.19)	(-2.38, 1.72, -0.80)	**5.63**
P3HT to $PC_{61}BM$	(-2.13, 3.08, -0.34)	(0.130, -1.47, 0.24)	5.11

References

[1]*Gaussian 16 Rev. B.01*; Wallingford, CT, 2016. (accessed.

[2]Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* 1994, **98**, 11623-11627.

[3]Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *The Journal of chemical physics* 2010, **132**,

[4]Hariharan, P.; Pople, J. A. *Molecular Physics* 1974, **27**, 209-214.

[5]Petersson, a.; Bennett, A.; Tensfeldt, T. G.; Al‐Laham, M. A.; Shirley, W. A.; Mantzaris, J. *The Journal of chemical physics* 1988, **89**, 2193-2218.

[6]Lu, T.; Chen, F. *Journal of computational chemistry* 2012, **33**, 580-592.

[7]Humphrey, W.; Dalke, A.; Schulten, K. *Journal of molecular graphics* 1996, **14**, 33-38.

[8]Lu, T. *Beijing Kein Research Center for Natural Science: Beijing, China*,

[9]Stewart, J. J. *Journal of Molecular modeling* 2007, **13**, 1173-1213.

[10]Korth, M. *Journal of Chemical Theory and Computation* 2010, **6**, 3808-3816.

[11]Lu, T.; Chen, Q. *Journal of computational chemistry* 2022, **43**, 539-555.

[12]Lu, T.; Liu, Z.; Chen, Q. *Materials Science and Engineering: B* 2021, **273**, 115425.