



Correction to: Body centered non-fullerene acceptors substitution on triangular shaped Sub-phthalocyanines (SubPcs) based A-D-A organic solar cells: A step toward new strategies for better performances

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In the original publication of the article, the authors noticed errors in abstract, figure caption, reference, layout of tables and figures. These errors have been corrected with this Correction.

In Abstract, the first sentence should begin with the word “Four”. The corrected sentence should read, “For Acceptor–Donor–Acceptor (A-D-A) type of triangular shaped sub-phthalocyanines (SubPcs) donor molecules namely SubPcs-EDM (sub-phthalocyanines-ethylidene di-malononitrile as M1), SubPcs-ETFM (sub-phthalocyanines-ethylidene tetrafluoro-malononitrile as M2), SubPcs-ETFOM (sub-phthalocyanines-ethylidene tetrafluoro-oxo

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malononitrile as M3) and SubPcs-EOM (sub-phthalocyanines-ethylidene oxo malononitrile as M4) have been designed for computing its optoelectronic properties with state-of-the-art density functional theory B3LYP/LanL2DZ (d, p) model.”

In the caption of Fig. 7, the symbol “= >” was incorrectly published. The corrected caption is given below:

“Fig. 7 Charge transfer mechanism between $S_0 = > S_1$ state with exciton binding energy”

The reference, “Cui, Y., Yao, H., Hong, L., Zhang, T., Tang, Y., Lin, B., Bi, P. (2019). 17% efficiency organic photovoltaic cell with superior processability. *Natl. Sci. Rev* (<http://creativecommons.org/licenses/by/4.0/>)” has been removed.

The layout for Tables 1 and 3 and Figs. 5, 6 and 7 have been corrected. The corrected tables and figures are presented below:

The original article has been corrected.

Table 1 HOMO, LUMO, energy gap (HOMO–LUMO), first singlet (S_1) state excitation energy (E_{opt}) and binding energy of exciton at S_1 excited state with B3LYP and LanL2DZ basis set are given in the unit of electron volt (eV)

Molecules	E_{HOMO}	E_{LUMO}	E_{H-L}	E_{opt}	E_b
R	−5.93	−3.22	2.71	2.385	3.323
M1	−6.15	−3.59	2.56	2.071	2.183
M2	−6.13	−3.64	2.49	1.982	2.444
M3	−6.25	−3.77	2.48	1.921	2.308
M4	−6.11	−3.42	2.69	2.220	2.572

Table 3 Reorganization energy of hole and electron in the unit of electron volt (eV), ground state, excited state and the difference of dipole moment between excited and ground states in the unit of Debye are shown below

Molecules	λ_h	λ_e	μ_g	μ_e	$\mu_e - \mu_g$
R	0.063	0.282	2.073	2.324	0.251
M1	0.061	0.315	7.286	8.113	0.827
M2	0.054	0.102	8.056	8.844	0.788
M3	0.056	0.382	7.136	7.534	0.398
M4	0.053	0.611	5.715	6.292	0.577

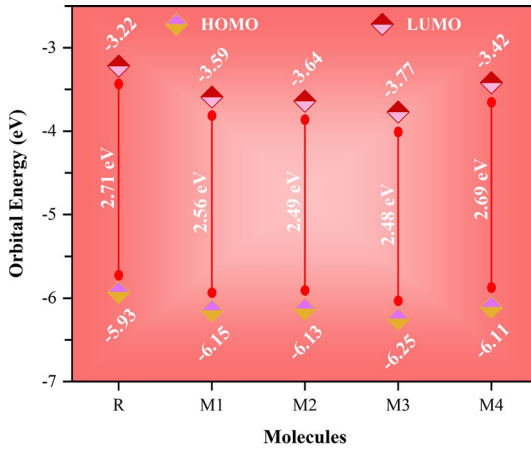


Fig. 5 Energy gap difference between HOMO to LUMO energy orbitals ($S_0 \Rightarrow S_1$)

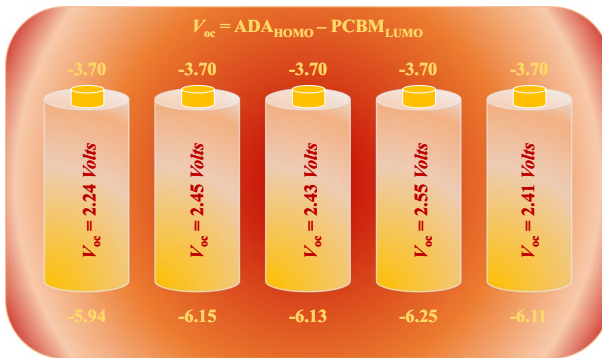


Fig. 6 Open circuit voltages of designed molecules with reference to PCBM LUMO

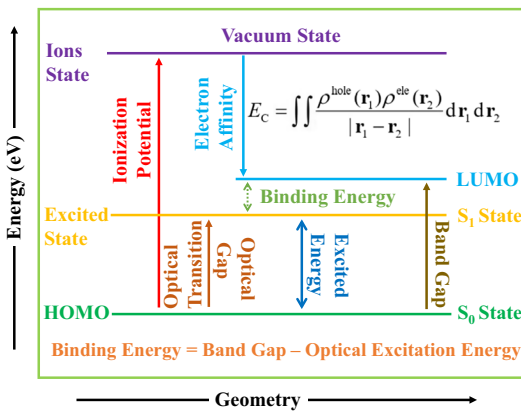


Fig. 7 Charge transfer mechanism between $S_0 \Rightarrow S_1$ state with exciton binding energy