Electronic Supplementary Information (ESI)

Grape bunches of novel conjugated chain bonded fullerene oligomers: Design of a potential electron trap carbonaceous molecular material

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Content of the Electronic Supplementary Information (ESI):

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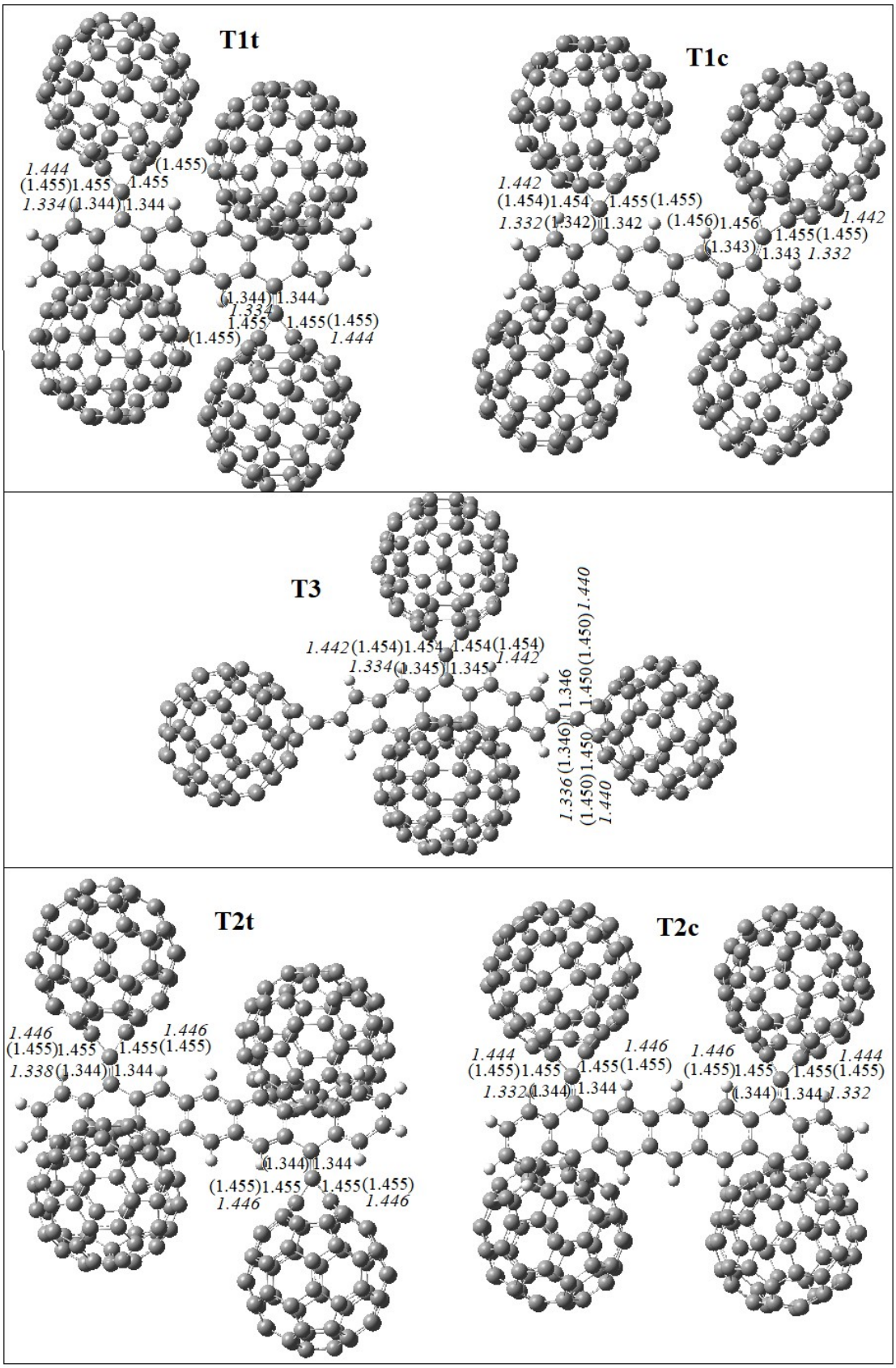

Fig. S1 Key bond length parameters (in Å) of the five **CBFOs** structures at B3LYP/6-31G(d), B3LYP/6-31+G(d) (in brackets) and B3LYP-GD3BJ/def2-tzvp (in italic)

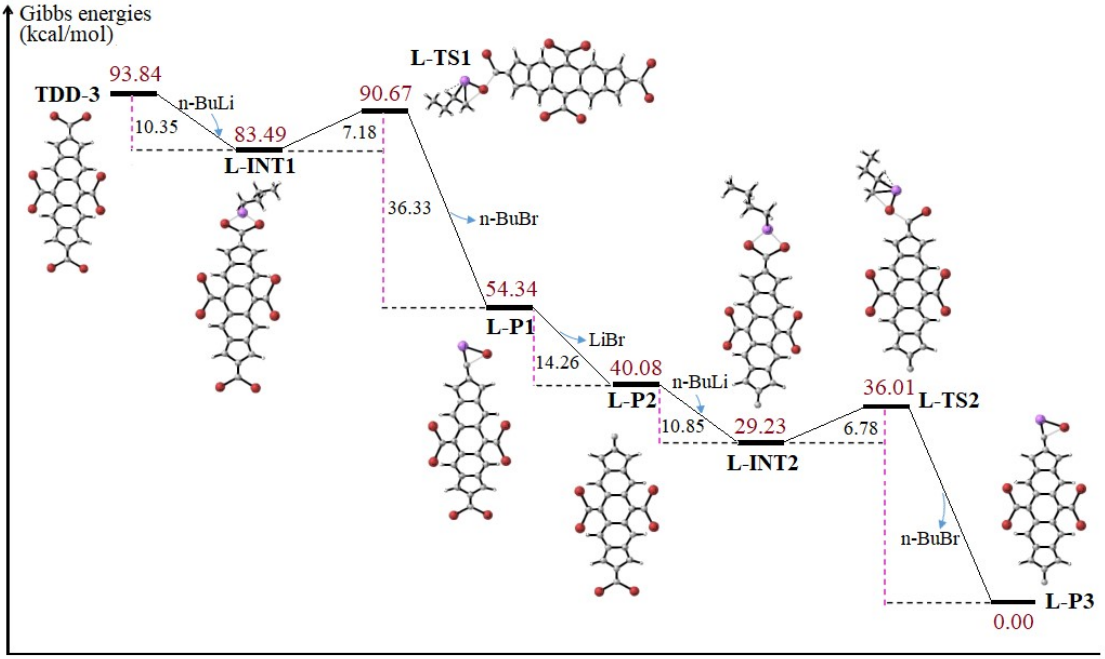

Fig. S2 Kinetic study of geometries in Path 2 and the change in the reaction Gibbs free energies for **TDD-3**-carbene (**L-P3**).

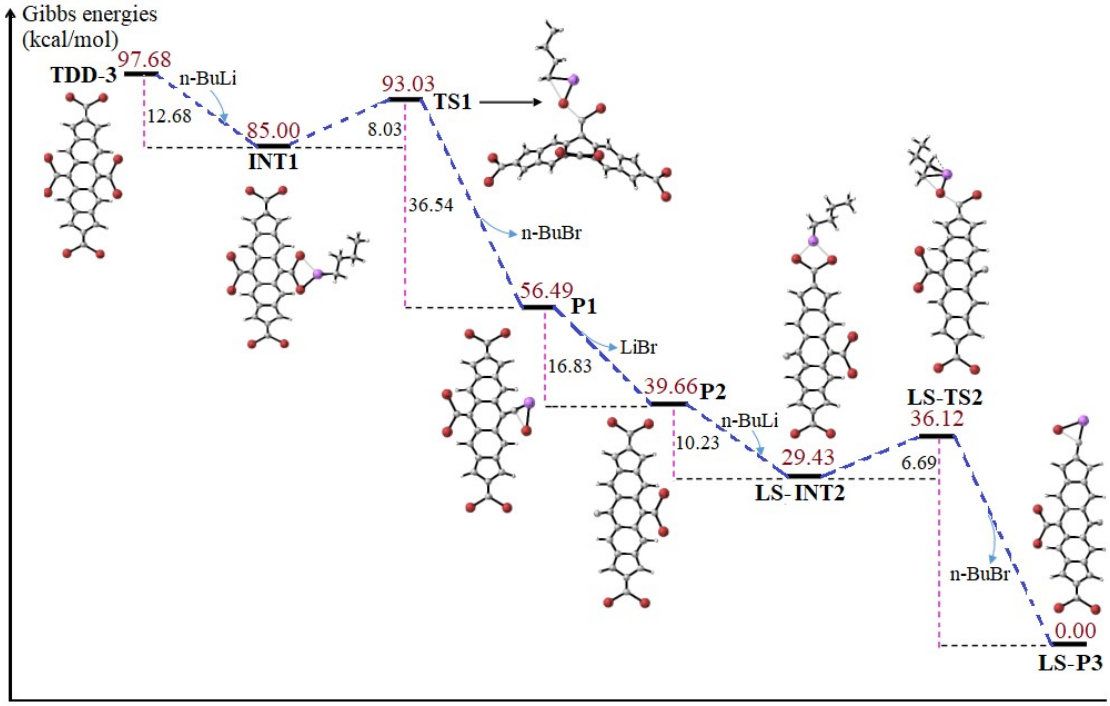

Fig. S3 Kinetic study of geometries in Path 3 and the change in the reaction Gibbs free energies for **TDD-3**-carbene (**LS-P3**).

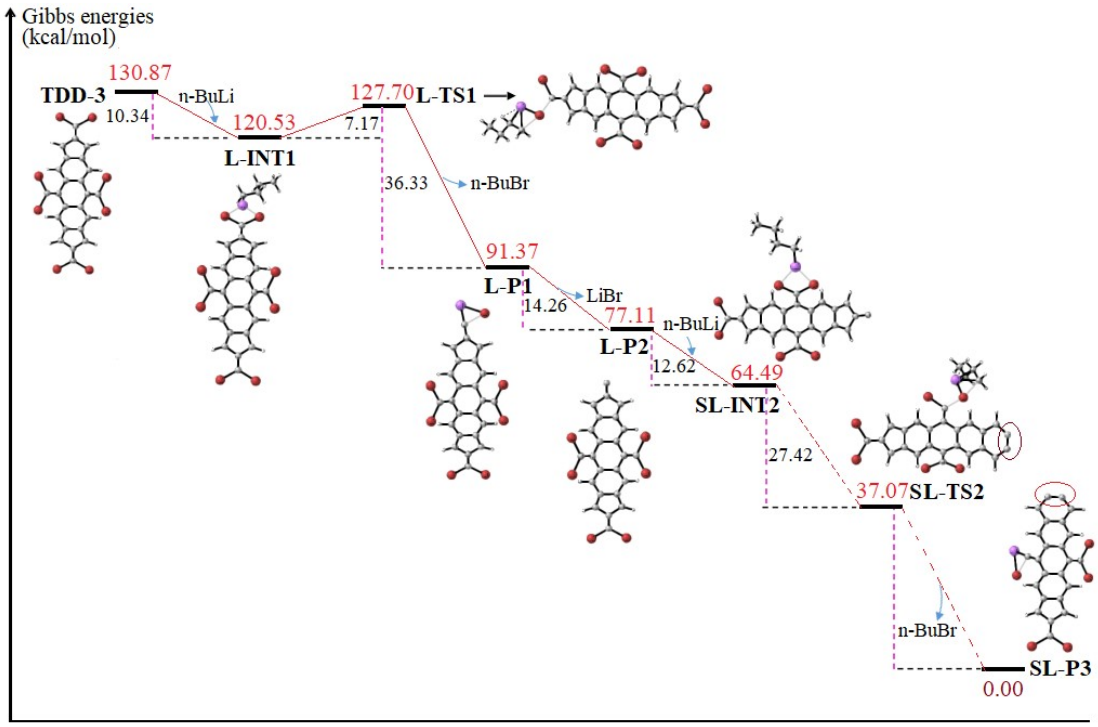

Fig. S4 Kinetic study of geometries in Path 4 and the change in the reaction Gibbs free energies for phenylalkyne intermediate (**SL-P3**).

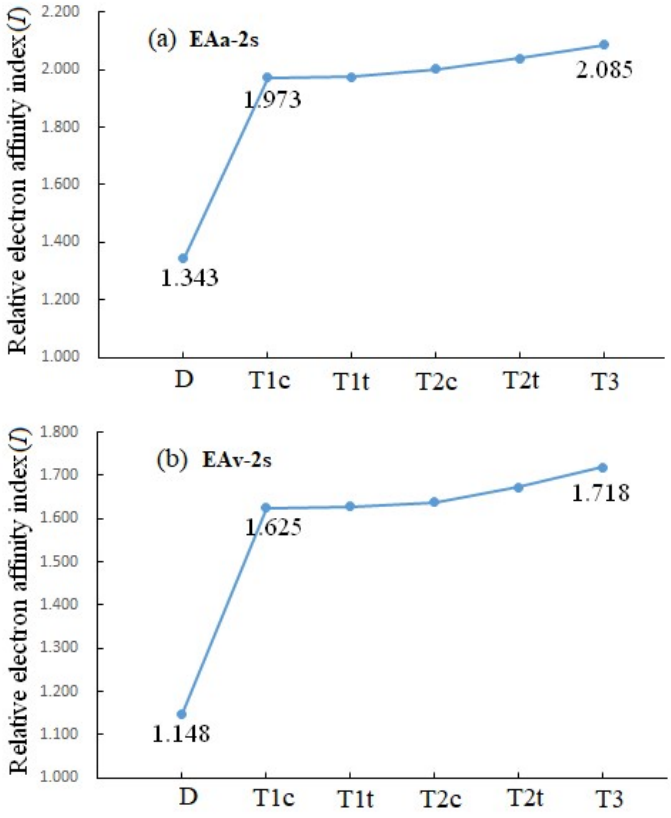

Fig. S5 Relative electrophilic index (*I*) of **D** and **CBFO**s for $EA_{a\text{-}2s}$ (singlet) and $EA_{v\text{-}2s}$(singlet).

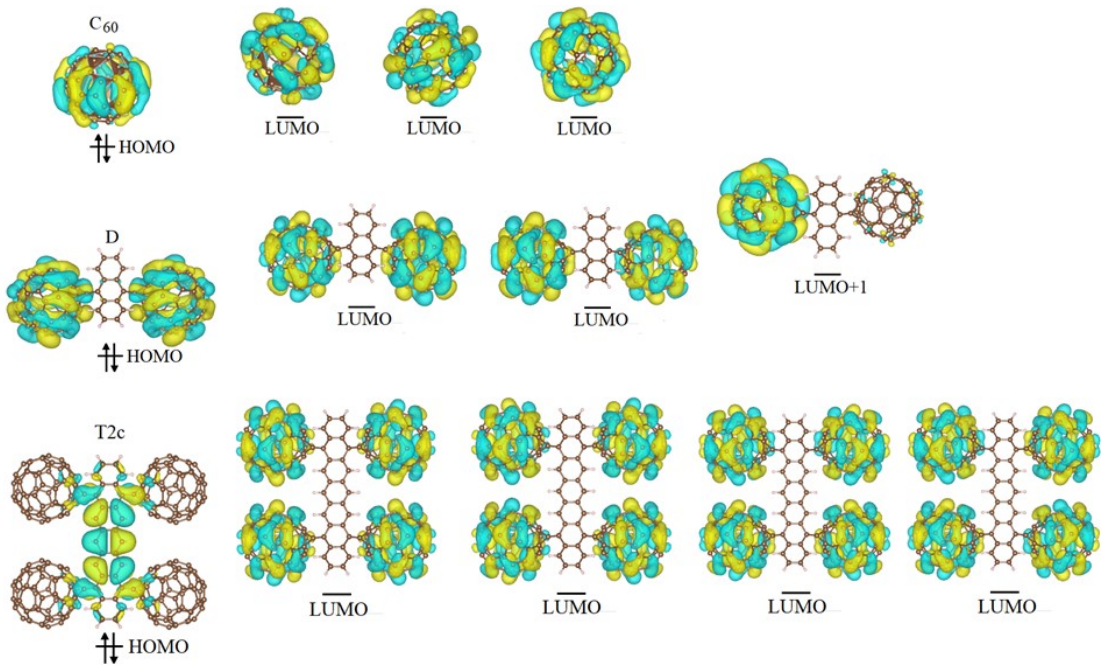

Fig. S6 Highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and LUMO+1 of C_{60}, **D** and **T2c**.

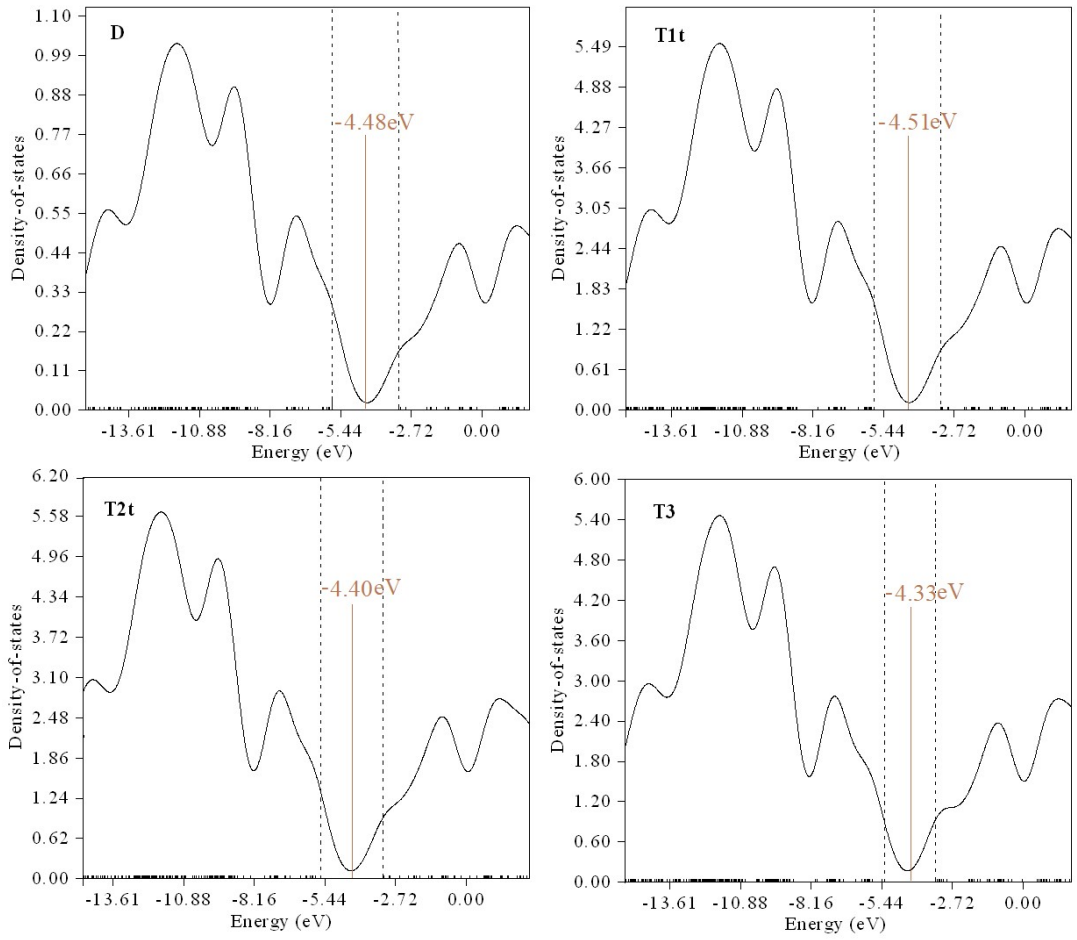

Fig. S7 Density of states (DOS) of **D**, **T1t**, **T2t** and **T3**. The brown lines represent the Fermi levels, defined as the midpoint between the highest occupied and lowest unoccupied states.

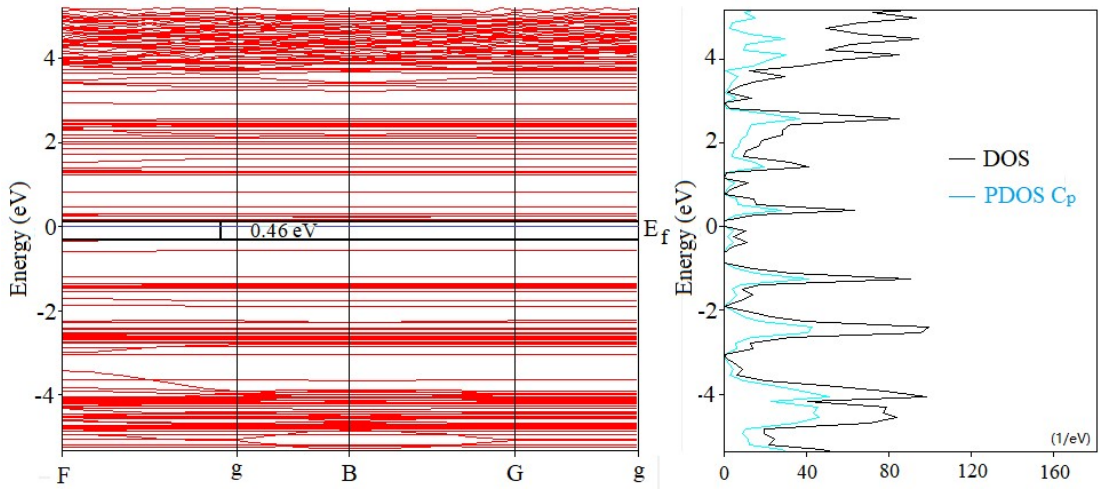

Fig. S8 Energetical band structure of **2D-T3** along high symmetry points, and the density of states, the partial density states of *p* orbitals of carbon atoms.

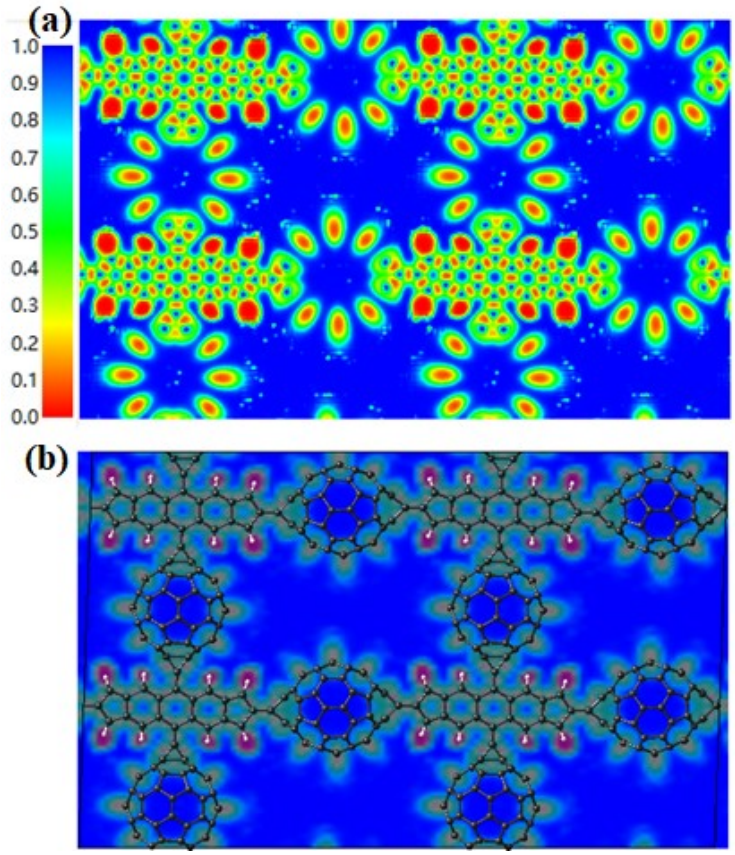

Fig. S9 Electron localization function (ELF) of (a) three-dimension and (b) two-dimension plot for **2D-T3**.

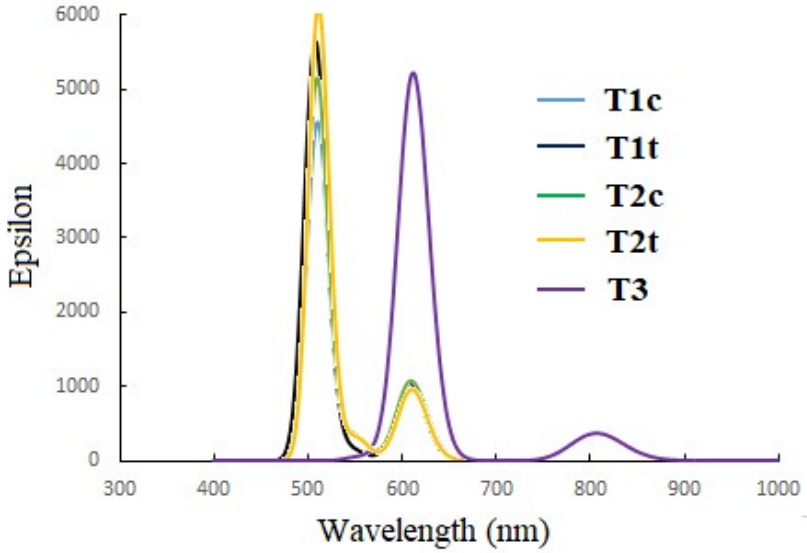

Fig. S10 UV-vis spectrum of the five **CBFO**s under PBE0/6-31G(d) theorectical level.

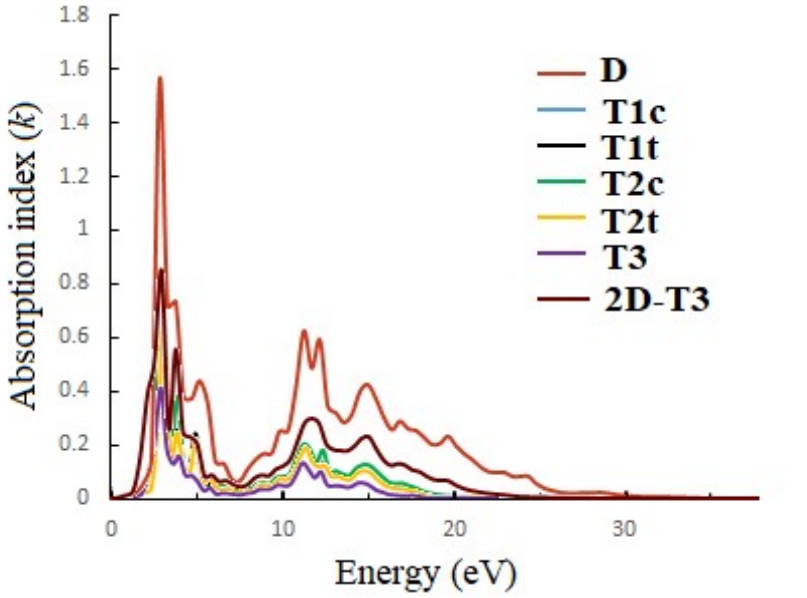

Fig S11 Relationship between absorption index and radiation energy for **D**, **CBFO**s and **2D-T3**.

Table S1 The energies of *cis* and *trans* configurations of **TDD-1** and **TDD-2**

B3LYP/6-31G(d)					
Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}	Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}
cis-**TDD-1**	-21743.76962	0.07	*cis*-**TDD-2**	-21897.44201	0.01
trans-**TDD-1**	-21743.76974	0	*trans*-**TDD-2**	-21897.44199	0
B3LYP-GD3BJ/def2-tzvp					
Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}	Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}
cis-**TDD-1**	-21744.38516	0	*cis*-**TDD-2**	-21898.09332	0.031
trans-**TDD-1**	-21744.38512	0.025	*trans*-**TDD-2**	-21898.09337	0

Table S2 The energies of *cis* and *trans* configurations of **T1c, T1t, T2c** and **T2t**

B3LYP/6-31G(d)					
Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}	Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}
T1c	-10295.012129	1.87	**T2c**	-10448.652896	0
T1t	-10295.015137	0	**T2t**	-10448.652851	0.03
B3LYP/6-31+G(d)					
Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}	Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}
T1c	-10295.231754	2.06	**T2c**	-10448.876825	0
T1t	-10295.235037	0	**T2t**	-10448.876049	0.48
B3LYP-D3BJ/def2-tzvp					
Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}	Configurations	Energy/a.u.	Relative energy kcal·mol^{-1}
T1c	-10299.690314	0.13	**T2c**	-10453.395411	0
T1t	-10299.690520	0	**T2t**	-10453.391247	2.61

Table S3 The first vertical electron affinity (EA_{v1}, eV) of C_{60}, dimer (**D**) and five **CBFO**s at B3LYP/6-31G(d) and B3LYP/6-31+G(d) levels of theory

	C_{60}	**D**	**T1c**	**T1t**	**T2c**	**T2t**	**T3**
EA_{v1}(6-31+g(d))	-2.52	-2.86	-3.07	-3.08	-3.07	-3.1	-3.16
EA_{v1}(6-31g(d))	-1.99	-2.38	-2.61	-2.61	-2.61	-2.63	-2.71
ΔEA_{v1}	0.53	0.48	0.46	0.47	0.46	0.47	0.45

ΔEA_{v1} is the difference between two levels of theory for the corresponding structure