Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Suppoting Information

Structural Modulation of Phenothiazine and Coumarin Based Derivatives for High Performance Dye Sensitized Solar Cells

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Table S1. Coordinates of the studied compounds studied at B3LYP/6-31G(d,p) level of theory in angstorm unit.

1. COU-BTZ

C	-9.34634300	2.68927300	-0.33734300
C	-7.41650900	1.13032900	0.03278900
C	-6.52462500	2.25534500	0.08793400
C	-7.09666700	3.65308600	0.09827100
C	-8.32264800	3.71335400	-0.81308900
C	-6.90277600	-0.20062300	0.11200100
C	-5.16567500	2.04781500	0.10356100
C	-4.61269800	0.75189200	0.07913600
C	-5.51000300	-0.33753100	0.07922200
C	-3.63885700	-1.92232900	0.00078000
C	-2.70297000	-0.79081200	0.01838500
C	-3.22161500	0.48415400	0.05528400
H	-9.83433900	3.04660400	0.58368900
H	-6.33323100	4.37233700	-0.21733700
H	-8.02570300	3.49375800	-1.84598200
H	-4.49406500	2.90317700	0.12504500
H	-2.51510200	1.31015300	0.06549300
N	-8.76782000	1.36468700	-0.09468100
O	-4.99706600	-1.60455500	0.02736700
C	-9.71563800	0.26342100	-0.19371100
C	-7.83679600	-1.42316400	0.20481800
C	-9.24165900	-0.93014300	0.61358400
C	-7.40522400	-2.42457500	1.30555500
C	-7.90043200	-2.15929700	-1.15409300
H	-8.21158600	-3.15199700	1.46204200
H	-6.50156800	-2.97287400	1.04271900
H	-7.23248600	-1.90858900	2.25722700
H	-8.57690700	-3.02091000	-1.08649500
H	-8.26059500	-1.50630500	-1.95688400
H	-6.91163900	-2.52762800	-1.44027100
O	-3.36718500	-3.10480300	-0.03691200
N	-1.32529000	-0.91858600	-0.00080600
C	-0.69986300	-2.05063700	-0.05108200
H	-1.20957900	-3.01476200	-0.08450200
C	0.74158500	-2.07935300	-0.06547300
C	1.54493700	-3.20883500	-0.12391700

S	1.69558600	-0.62123900	-0.00165000
C	2.91616200	-2.90856600	-0.12154000
H	1.14254100	-4.21546300	-0.16539100
C	3.19285200	-1.54414000	-0.06018700
H	3.68417900	-3.67225400	-0.15808500
C	4.51036800	-0.93915900	-0.04581400
C	4.72860800	0.48171500	0.07665700
C	5.67499700	-1.70265800	-0.14891500
C	6.06816700	1.04106500	0.09515800
C	6.97492800	-1.16342600	-0.13112500
H	5.59255400	-2.77855000	-0.25230700
C	7.23552900	0.20152100	-0.01032300
N	3.76978400	1.40416100	0.18337600
N	6.08493200	2.37052600	0.21579500
S	4.51902100	2.86072000	0.29732800
H	-10.68049400	0.61516500	0.19140500
H	-9.87541800	-0.00733700	-1.25042700
H	-9.22966300	-0.64763900	1.67436800
H	-9.95939200	-1.75193700	0.50673600
H	-8.78119100	4.70831100	-0.80635700
H	-7.39450800	3.93819200	1.11894900
H	-10.13778300	2.57405000	-1.08919600
H	7.80062400	-1.85890500	-0.21803500
C	8.53017800	0.83325200	0.01643400
H	8.50777100	1.91569000	0.11885800
C	9.79166600	0.31223800	-0.06446800
C	10.08899400	-1.07579400	-0.20341000
C	10.93044600	1.27191000	-0.00208900
N	10.31378000	-2.21340900	-0.31687600
O	10.81998000	2.47509800	0.11558200
O	12.12721800	0.64781000	-0.09221900
H	12.80206400	1.35000400	-0.04223500

2. PTZ-BTZ

C	10.70642800	-1.42325400	-0.95814600
C	8.73918400	-0.22171700	-0.19955300
C	8.20329600	-1.42814200	0.28417400
C	8.90897100	-2.61989000	0.11545600
C	10.16630500	-2.62144700	-0.49242400
C	5.86744700	-0.01850300	0.45966600
C	6.63597400	1.05251800	-0.03676000
C	4.58683200	2.27942600	-0.48960600
C	3.81322600	1.21243600	0.00407100
C	4.48015800	0.05214100	0.43998500
H	11.68134700	-1.40971200	-1.43690000
H	8.47400400	-3.54763200	0.47662100
H	10.71346200	-3.55289000	-0.60138600
H	3.88181200	-0.78123100	0.79429000

N	2.41641300	1.19087500	0.05724900
C	1.73051800	2.27724300	0.13151600
H	2.19031900	3.27231000	0.21524000
C	0.28767000	2.26600800	0.13293900
C	-0.54990100	3.36612000	0.22823400
S	-0.61665400	0.78124500	0.01737800
C	-1.91176400	3.02189400	0.20890400
H	-0.18273900	4.38377300	0.31194500
C	-2.14213600	1.65328600	0.09712200
H	-2.70430600	3.75728300	0.28091400
C	-3.43991800	1.00382300	0.04734600
C	-3.60515700	-0.42674600	-0.01932300
C	-4.63012900	1.73130200	0.06041500
C	-4.92295200	-1.03243800	-0.06316700
C	-5.91119700	1.14669100	0.01927800
H	-4.58729400	2.81372700	0.10162800
C	-6.12038100	-0.22996800	-0.04247600
N	-2.61249800	-1.31892300	-0.04703300
N	-4.89039900	-2.36596000	-0.12273000
S	-3.30779000	-2.80405900	-0.12300600
N	8.03186900	0.98271900	-0.05142400
C	9.99034900	-0.23388400	-0.82747500
C	5.97277000	2.18813700	-0.52475100
S	6.67479500	-1.42407300	1.20904900
H	8.48751200	1.78717800	-0.46284000
H	10.40309200	0.69776900	-1.20930300
H	6.55738100	3.00516500	-0.94271000
H	4.10461900	3.16327300	-0.89591800
H	-6.76188500	1.81672700	0.03596900
C	-7.39223700	-0.90869900	-0.08708900
C	-8.67128500	-0.42860700	-0.08101300
C	-9.77549900	-1.43021800	-0.13670200
C	-9.01904700	0.95371800	-0.02536300
O	-9.61907700	-2.63255400	-0.18755300
O	-10.99370600	-0.84392200	-0.12412700
N	-9.28424700	2.08725400	0.02042600
H	-7.32953000	-1.99339800	-0.13318700
H	-11.64426500	-1.56948500	-0.16261400

3. COU-IND

C	9.63922300	2.58504200	-0.49160000
C	7.68773600	1.00890200	-0.46262900
C	6.80171900	2.10843200	-0.72529100
C	7.38190600	3.46504200	-1.04840100
C	8.63811300	3.69860200	-0.20870600
C	7.16358600	-0.30054400	-0.23730800
C	5.44147900	1.92120800	-0.65114100
C	4.88177800	0.66765000	-0.33492200

C	5.77140900	-0.40862100	-0.13196100
C	3.89357900	-1.91647500	0.33540900
C	2.96536200	-0.80202400	0.10903200
C	3.48988300	0.42947800	-0.20991500
H	10.10105000	2.73707500	-1.48048400
H	6.63395800	4.24460200	-0.86756600
H	8.37409400	3.70243600	0.85600800
H	4.77511600	2.76201400	-0.83051200
H	2.78881100	1.24447900	-0.37059400
N	9.04498600	1.24664100	-0.43688900
O	5.25234000	-1.62844900	0.20505900
C	9.98959800	0.18036200	-0.13570400
C	8.08662100	-1.52561900	-0.08815300
C	9.47865900	-1.15411800	-0.64396700
C	7.61217300	-2.74254900	-0.92231400
C	8.19448300	-1.94101300	1.39784400
H	8.41040300	-3.49509600	-0.93931300
H	6.71649400	-3.20839300	-0.51358000
H	7.40727200	-2.44975600	-1.95870200
H	8.85428600	-2.81203400	1.50084400
H	8.59726600	-1.13414500	2.02039000
H	7.21255900	-2.21231400	1.79475000
O	3.61595000	-3.06159200	0.62766100
N	1.58682300	-0.90547700	0.19734300
C	0.95626600	-1.99470400	0.49242400
H	10.94044700	0.42569300	-0.62448100
H	10.19004800	0.14396800	0.94786900
H	9.42900400	-1.11203400	-1.73985200
H	10.19522900	-1.94217600	-0.38407700
H	9.10193600	4.66458000	-0.43692300
H	7.64765200	3.52545900	-2.11497400
H	10.45291200	2.61878200	0.24452200
H	1.45824200	-2.94119000	0.69961100
C	-0.48672400	-2.00066500	0.55610500
C	-1.29707200	-3.07974500	0.86962400
S	-1.42622700	-0.56423200	0.26140000
C	-2.66706800	-2.76289900	0.83368500
H	-0.90353100	-4.05919600	1.11973000
C	-2.92729600	-1.43469600	0.51112400
H	-3.44846100	-3.47813000	1.06461900
C	-4.26985500	-0.89160800	0.30235100
C	-4.70654800	0.43771100	0.48099000
C	-5.27978900	-1.79134000	-0.13601900
C	-6.03753400	0.81380900	0.25504200
C	-6.59242300	-1.41871200	-0.35726500
H	-5.00074400	-2.81856300	-0.34081600
C	-7.03208800	-0.08453100	-0.16849600
H	-7.28683800	-2.17456000	-0.70050200
C	-3.97153300	1.65128600	0.96395300

C	-6.16989200	2.27597100	0.57204300
N	-4.91012100	2.69229500	0.98611400
O	-7.14580900	3.00090600	0.50409300
O	-2.80783800	1.78091200	1.28735600
C	-4.60586000	4.05367000	1.38993800
H	-3.54324300	4.09285300	1.63229300
H	-4.83206400	4.74849400	0.57630700
H	-5.19917900	4.33279200	2.26547600
C	-8.38979100	0.38895600	-0.38601400
C	-9.51513300	-0.28280300	-0.76086700
C	-10.77171900	0.51843400	-0.89901300
C	-9.59572000	-1.68360500	-1.02836800
N	-9.65925800	-2.82606500	-1.24548900
O	-10.85629300	1.71237800	-0.70917300
O	-11.82178300	-0.24952000	-1.26598200
H	-8.54002300	1.45274500	-0.22034600
H	-12.58777300	0.35078700	-1.33083500

4. PTZ-IND

C	11.18684000	-0.67458600	-0.49233600
C	9.03163300	0.05121400	0.35475100
C	8.54120900	-1.25670900	0.19367600
C	9.36683200	-2.24905800	-0.33595400
C	10.69384400	-1.96717200	-0.66755000
C	6.08833900	-0.10169000	0.53322400
C	6.82190400	1.09387600	0.66316500
C	4.75806500	2.35562100	0.42224200
C	4.02563200	1.16698600	0.25376100
C	4.71526800	-0.05762900	0.32576000
H	12.21562800	-0.43967500	-0.74989500
H	11.33178500	-2.75257500	-1.06133000
H	4.14524000	-0.97480900	0.21701000
N	2.64183800	1.09900100	0.05819300
C	1.99379800	2.06310600	-0.49220900
H	2.48112700	2.96611900	-0.88723400
C	0.55775900	2.02164500	-0.64900500
C	-0.24118700	2.98002400	-1.24894600
S	-0.37908500	0.66168300	-0.10077200
C	-1.60669700	2.63806800	-1.23532900
H	0.15367600	3.89086400	-1.68674900
C	-1.86795000	1.40858400	-0.64161200
H	-2.38067900	3.25835800	-1.67289300
H	8.96837500	-3.25036500	-0.47368000
C	-3.21405000	0.87885800	-0.40891600
C	-3.61090900	-0.47149200	-0.34563900
C	-4.26519300	1.81611100	-0.22443700
C	-4.94631600	-0.83897500	-0.13453100
C	-5.58332200	1.45215100	-0.01629700

H	-4.01931100	2.87200400	-0.21437000
C	-5.98368600	0.09417300	0.03754000
H	-6.31409300	2.23808200	0.12322000
C	-2.82185000	-1.73301800	-0.53065500
C	-5.02944300	-2.33897000	-0.16342900
N	-3.73310800	-2.78617400	-0.40697000
O	-5.99830300	-3.06048600	-0.01467500
O	-1.63701200	-1.89107500	-0.74706900
C	-3.35608900	-4.18499100	-0.51594300
H	-2.93155900	-4.38709100	-1.50326000
H	-2.61198700	-4.43659600	0.24488900
H	-4.25817900	-4.77990200	-0.36845100
C	-7.34566900	-0.36869400	0.25847100
N	8.20492400	1.06302900	0.86965900
S	6.90208400	-1.67456700	0.76693600
C	10.35648700	0.33181900	-0.00039400
C	6.13485600	2.31467400	0.60987300
H	6.69043400	3.24201800	0.73435600
H	4.25060200	3.31536700	0.43028000
H	10.73543600	1.34514800	0.11671000
C	-8.50423100	0.32950200	0.42186400
C	-8.62635800	1.75264700	0.40272600
C	-9.75436800	-0.46692900	0.63568500
O	-9.80464200	-1.67675800	0.67777700
O	-10.83851900	0.32657200	0.77922100
N	-8.72293000	2.91309900	0.38596400
H	-11.59795300	-0.27083000	0.91266000
H	-7.46648600	-1.44824900	0.29727300
H	8.64180400	1.97470500	0.91556000

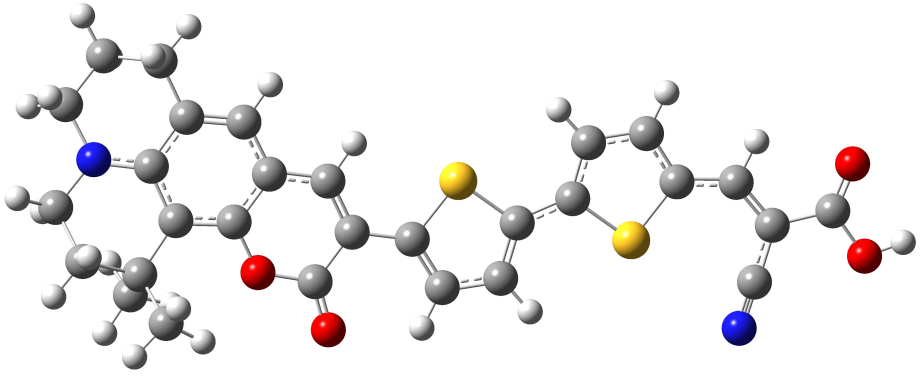

Fig. S1: Optimized structure of the test compound

Table S2: Calculated energies of HOMO, LUMO, Δ_{H-L} , λ_{max} values of the reference compound studied at different functionals.

Functionals	**E_{HOMO} (eV)**	**E_{LUMO} (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-5.26	-2.71	2.55	464
B3LYP	-5.08	-2.68	2.40	558
B3LYP-D3	-5.08	-2.68	2.40	558
CAM-B3LYP	-6.23	-1.59	4.64	454
MO6-2X-D3	-6.18	-1.92	4.26	439
PBEPBE	-4.94	-2.93	2.01	563
wB97XD	-6.80	-1.04	5.40	444

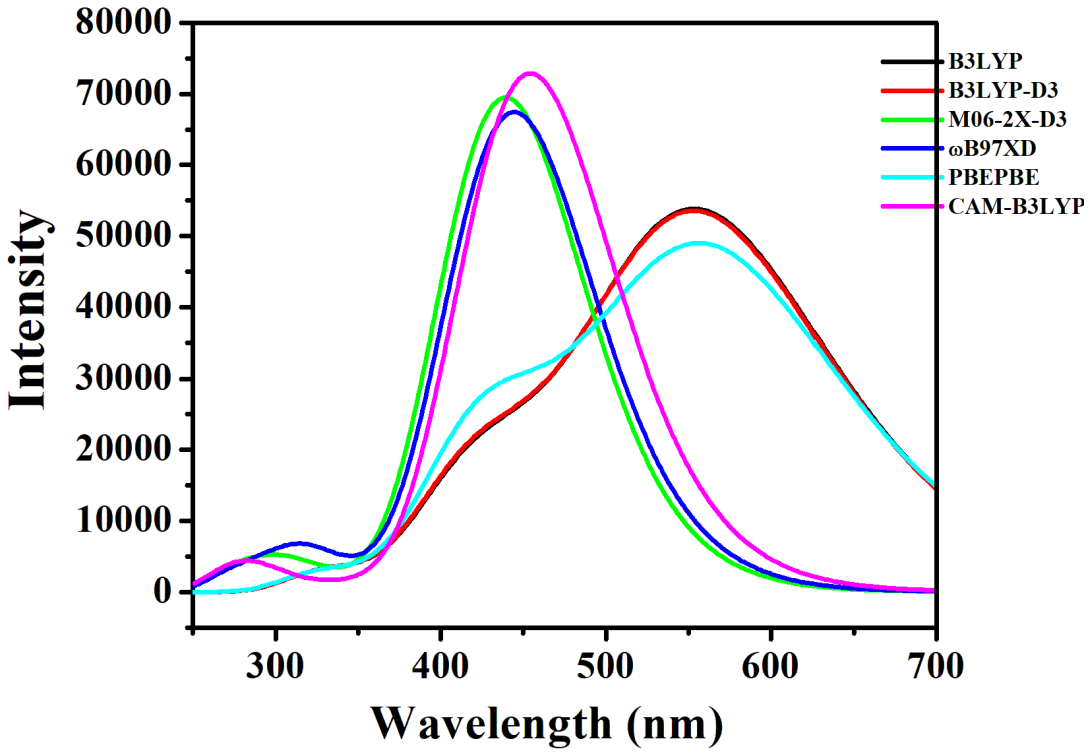

Fig. S2: Plot of uv-visible spectra of the test compound

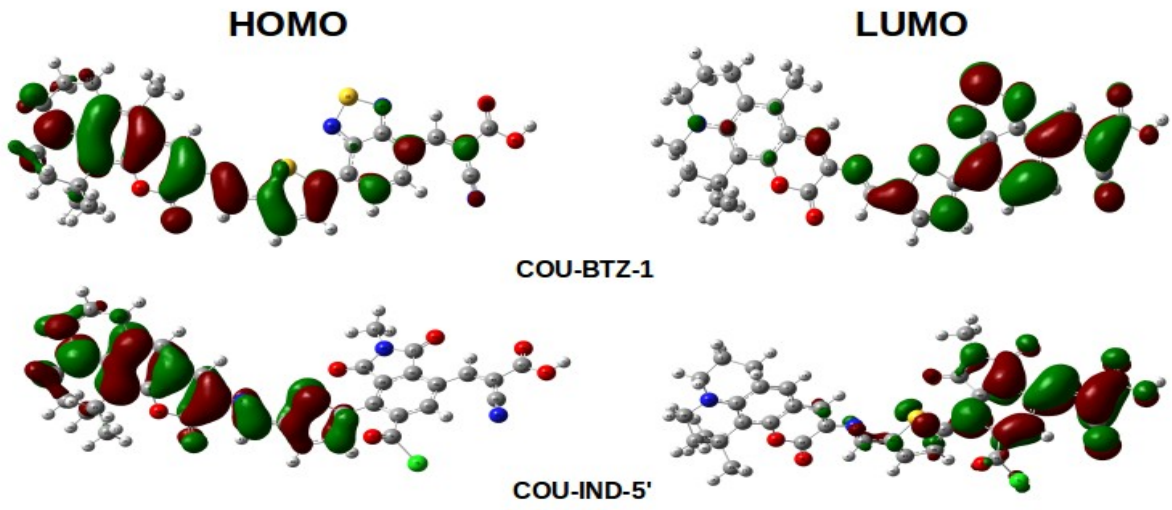

Fig. S3: Plot of frontier molecular orbitals of compounds COU-BTZ-1 and COU-IND-5'.

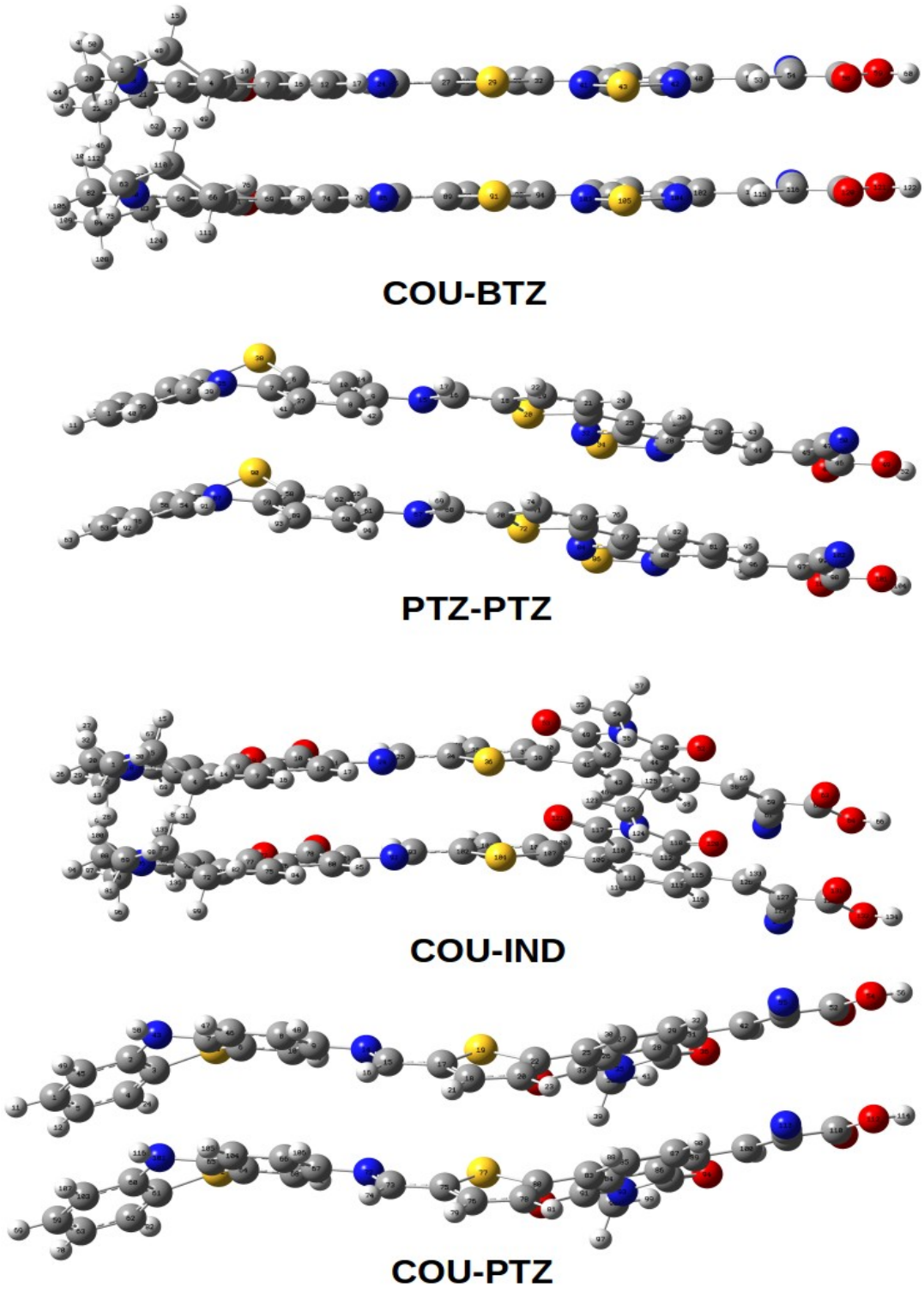

Fig. S4: Optimized structure of the stacked unsubstituted compound .

Table S3: Spectral data obtained from PDOS spectra.

Compound	**Groups**	**Contribution to HOMO(%)**	**Contribution to LUMO(%)**
COU-BTZ	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	76 24 0	53 44 3
COU-BTZ-1	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	77 23 0	53 44 3
COU-BTZ-2	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	69 31 0	54 44 2
COU-BTZ-3	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	76 24 0	54 44 2
COU-BTZ-4'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	56 41 2
COU-BTZ-5'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	58 40 2
COU-BTZ-6'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	76 24 0	52 46 2
COU-BTZ-7'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	58 41 2
PTZ-BTZ	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	90 10 0	53 45 2
PTZ-BTZ-1	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	90 10 0	53 45 2
PTZ-BTZ-2	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	92 8 0	53 45 2
PTZ-BTZ-3	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	53 45 2
PTZ-BTZ-4'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	57 41 2
PTZ-BTZ-5'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	58 40 2

PTZ-BTZ-6'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	90 10 0	52 46 2
PTZ-BTZ-7'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	58 40 2
COU-IND	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	36 57 7
COU-IND-1	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	36 57 7
COU-IND-2	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	78 22 0	36 57 7
COU-IND-3	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	36 57 7
COU-IND-4'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	80 20 0	39 55 6
COU-IND-5'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	80 20 0	41 54 5
COU-IND-6'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	79 21 0	35 59 6
COU-IND-7'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	80 20 0	40 55 5
PTZ-IND	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	36 59 5
PTZ-IND-1	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	36 59 5
PTZ-IND-2	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	93 7 0	36 58 6
PTZ-IND-3	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	36 59 5
PTZ-IND-4'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	40 55 5
PTZ-IND-5'	Acceptor and Donor unit	90	36

	Bridging unit and Anchoring group Ti_5O_{10} cluster	10 0	59 5
PTZ-IND-6'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	35 60 5
PTZ-IND-7'	Acceptor and Donor unit Bridging unit and Anchoring group Ti_5O_{10} cluster	91 9 0	41 55 4