Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

End group modulation of A-D-A type small donor molecules for DTP based organic photovoltaic solar cells: A DFT approach

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Table S1 : Coordinates of the designed compounds studied at HSEH1PBE/6-31G(d) level of theory in the angstrom unit.

1. **Compound C1**

Atoms	Coordinates (Angstroms) X	Y	Z
C	-7.081135	-0.069845	-0.171195
C	-6.638046	-1.381942	-0.334478
C	-5.250149	-1.495969	-0.396908
S	-5.702089	1.016449	-0.103071
C	-4.576725	-0.280915	-0.284743
C	-3.164039	-0.052217	-0.298390
C	-2.497368	1.158426	-0.210168
C	-1.105688	0.981104	-0.241670
C	-0.699602	-0.363795	-0.348609
C	0.699621	-0.363789	-0.348647
C	1.105701	0.981113	-0.241730
C	2.497382	1.158447	-0.210305
C	3.164058	-0.052190	-0.298565
C	4.576747	-0.280875	-0.284999
C	5.250176	-1.495920	-0.397238
C	6.638074	-1.381885	-0.334846
C	7.081156	-0.069799	-0.171458
N	0.000005	1.797976	-0.193420
S	-2.058912	-1.421213	-0.422906
S	2.058936	-1.421195	-0.423019

S	5.702110	1.016497	-0.103387
H	-7.338812	-2.203819	-0.400183
H	-4.733532	-2.441841	-0.522863
H	-3.011418	2.109237	-0.123016
H	3.011429	2.109263	-0.123185
H	4.733562	-2.441792	-0.523203
H	7.338844	-2.203758	-0.400583
C	0.000004	3.227997	-0.000993
H	0.000028	3.495376	1.061897
H	0.883820	3.658399	-0.477599
H	-0.883838	3.658393	-0.477557
C	-8.357502	0.538801	-0.055078
C	-9.634911	0.028591	-0.020072
C	-10.856660	0.826208	0.119818
C	-10.041111	-1.400892	-0.057820
C	-11.503824	-1.420413	0.115666
C	-11.989928	-0.114098	0.229544
C	-14.214825	-1.027485	0.477267
C	-13.705302	-2.342007	0.355225
C	-13.360084	0.076137	0.412599
C	-12.334823	-2.524542	0.172828
C	8.357520	0.538836	-0.055257
C	9.634921	0.028611	-0.020209
C	10.856669	0.826212	0.119757
C	10.041106	-1.400876	-0.057954
C	11.989915	-0.114108	0.229588
C	11.503805	-1.420416	0.115655
C	13.360057	0.076108	0.412776
C	14.214777	-1.027524	0.477512
C	13.705250	-2.342038	0.355406
C	12.334785	-2.524556	0.172882
O	-9.341301	-2.392143	-0.195297
O	9.341294	-2.392115	-0.195508
C	10.983538	2.201075	0.128833
C	12.235257	2.866553	0.272657
C	9.901335	3.116199	-0.015673
C	-10.983521	2.201073	0.128899
C	-9.901307	3.116198	-0.015513
C	-12.235251	2.866552	0.272615
N	13.234027	3.451659	0.388831
N	9.047374	3.898542	-0.130959
N	-9.047344	3.898555	-0.130699

N	-13.234028	3.451660	0.388714
H	13.788632	1.065886	0.511095
H	11.908511	-3.519845	0.076824
H	8.292574	1.619137	0.033080
H	-8.292550	1.619103	0.033229
H	-11.908551	-3.519837	0.076818
H	-13.788658	1.065920	0.510867
C	15.686271	-0.807398	0.678917
H	16.044873	-1.303435	1.589356
H	16.270811	-1.217621	-0.154009
H	15.919985	0.256954	0.760974
C	14.625455	-3.524686	0.423465
H	15.389322	-3.485261	-0.362973
H	15.161260	-3.562379	1.380102
H	14.073336	-4.461231	0.310037
C	-15.686335	-0.807338	0.678530
H	-16.270801	-1.217566	-0.154446
H	-16.045029	-1.303356	1.588942
H	-15.920043	0.257019	0.760548
C	-14.625527	-3.524642	0.423212
H	-15.161420	-3.562319	1.379800
H	-15.389322	-3.485217	-0.363296
H	-14.073409	-4.461195	0.309845

2. **Compound C2**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-7.080839	-0.093900	-0.023840
C	-6.635353	-1.416710	-0.041815
C	-5.247792	-1.535073	-0.053445
S	-5.701531	0.994978	-0.022901
C	-4.575125	-0.313111	-0.045123
C	-3.162765	-0.086858	-0.052256
C	-2.496539	1.127877	-0.046190
C	-1.105399	0.949136	-0.053959
C	-0.699337	-0.400762	-0.059322
C	0.699338	-0.400760	-0.059335
C	1.105397	0.949140	-0.053979
C	2.496536	1.127884	-0.046242
C	3.162765	-0.086850	-0.052323

C	4.575126	-0.313098	-0.045221
C	5.247797	-1.535057	-0.053712
C	6.635358	-1.416691	-0.042064
C	7.080838	-0.093881	-0.023893
N	-0.000003	1.767369	-0.064910
S	-2.057706	-1.461242	-0.066171
S	2.057710	-1.461237	-0.066212
S	5.701527	0.994992	-0.022837
H	-7.334353	-2.242594	-0.045484
H	-4.729588	-2.488255	-0.067843
H	-3.010918	2.082392	-0.033043
H	3.010913	2.082400	-0.033117
H	4.729596	-2.488238	-0.068252
H	7.334360	-2.242571	-0.045849
C	-0.000005	3.208330	0.018973
H	-0.000013	3.554537	1.058681
H	0.883776	3.601409	-0.488790
H	-0.883779	3.601408	-0.488803
C	-8.356098	0.522615	-0.006754
C	-9.638875	0.019725	0.002320
C	-10.859473	0.828202	0.021588
C	-10.048187	-1.405645	0.000134
C	-11.523130	-1.414547	0.023574
C	-12.008695	-0.101674	0.037236
C	-14.216640	-0.994701	0.070393
C	-13.712231	-2.301186	0.056031
C	-13.388876	0.115854	0.061218
C	-12.348517	-2.527395	0.032237
C	8.356096	0.522633	-0.006696
C	9.638872	0.019739	0.002336
C	10.859474	0.828207	0.021742
C	10.048176	-1.405632	-0.000044
C	12.008690	-0.101678	0.037263
C	11.523118	-1.414547	0.023401
C	13.388872	0.115838	0.061287
C	14.216630	-0.994722	0.070305
C	13.712214	-2.301203	0.055744
C	12.348499	-2.527400	0.031904
O	-9.352204	-2.408014	-0.016530
O	9.352187	-2.407995	-0.016876
C	10.980285	2.202870	0.023751
C	12.238196	2.871453	0.043679

C	9.884434	3.112919	0.005108
C	-10.980269	2.202867	0.023392
C	-9.884405	3.112898	0.004636
C	-12.238172	2.871469	0.043210
N	13.245883	3.452266	0.059764
N	9.018537	3.890204	-0.009634
N	-9.018494	3.890164	-0.010217
N	-13.245847	3.452305	0.059210
H	13.847986	1.096055	0.073419
H	11.943001	-3.533688	0.020568
H	8.289957	1.606294	0.002024
H	-8.289960	1.606277	0.001823
H	-11.943024	-3.533686	0.021053
H	-13.847985	1.096074	0.073201
F	15.536646	-0.837130	0.093400
F	14.575958	-3.311518	0.065614
F	-15.536655	-0.837099	0.093455
F	-14.575981	-3.311496	0.066044

3. **Compound C3**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-7.079087	0.081488	-0.120110
C	-6.632499	-1.237560	-0.224807
C	-5.245729	-1.352339	-0.265183
S	-5.700748	1.171141	-0.077118
C	-4.574012	-0.131396	-0.193682
C	-3.162197	0.096031	-0.203431
C	-2.496183	1.309695	-0.143576
C	-1.105305	1.132038	-0.166149
C	-0.699189	-0.216269	-0.237337
C	0.699262	-0.216231	-0.237334
C	1.105305	1.132096	-0.166147
C	2.496173	1.309830	-0.143573
C	3.162253	0.096201	-0.203425
C	4.574080	-0.131149	-0.193672
C	5.245861	-1.352059	-0.265165
C	6.632624	-1.237205	-0.224786
C	7.079134	0.081869	-0.120102

N	-0.000021	1.949934	-0.138362
S	-2.057136	-1.275761	-0.288636
S	2.057265	-1.275651	-0.288630
S	5.700742	1.171453	-0.077105
H	-7.330670	-2.063062	-0.266718
H	-4.726914	-2.301887	-0.345565
H	-3.010643	2.262295	-0.082417
H	3.010580	2.262458	-0.082413
H	4.727098	-2.301635	-0.345543
H	7.330848	-2.062667	-0.266690
C	-0.000055	3.385388	0.013654
H	0.000031	3.681904	1.068607
H	0.883598	3.802037	-0.475144
H	-0.883826	3.801972	-0.474981
C	-8.353898	0.692433	-0.045623
C	-9.635940	0.184923	-0.026660
C	-10.856542	0.988313	0.060537
C	-10.039175	-1.241278	-0.059408
C	-11.512159	-1.256914	0.038158
C	-12.000758	0.051895	0.113482
C	-14.219622	-0.856800	0.242376
C	-13.708695	-2.165020	0.163274
C	-13.375140	0.254377	0.217145
C	-12.334958	-2.365286	0.059506
C	8.353929	0.692835	-0.045625
C	9.635928	0.185240	-0.026676
C	10.856644	0.988469	0.060514
C	10.038956	-1.241013	-0.059435
C	12.000719	0.051881	0.113475
C	11.511936	-1.256861	0.038151
C	13.375127	0.254170	0.217150
C	14.219453	-0.857126	0.242394
C	13.708342	-2.165274	0.163294
C	12.334578	-2.365349	0.059512
O	-9.342132	-2.239259	-0.144433
O	9.341743	-2.238876	-0.144446
C	10.982713	2.362410	0.080324
C	12.239922	3.026633	0.168783
C	9.892011	3.276075	0.008929
C	-10.982360	2.362274	0.080354
C	-9.891464	3.275707	0.008963
C	-12.239435	3.026754	0.168807

N	13.245789	3.606300	0.240805
N	9.029497	4.055192	-0.047398
N	-9.028729	4.054588	-0.047243
N	-13.245168	3.606653	0.240826
H	13.821917	1.237727	0.280827
H	11.916842	-3.364872	-0.002055
H	8.290141	1.775083	0.013342
H	-8.290088	1.774682	0.013338
H	-11.917362	-3.364868	-0.002061
H	-13.821794	1.237995	0.280823
Cl	15.916567	-0.585507	0.373592
Cl	14.753876	-3.533889	0.193497
Cl	-15.916698	-0.584943	0.373559
Cl	-14.754421	-3.533488	0.193460

4. **Compound C4**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-7.077267	-0.147174	-0.158151
C	-6.628401	-1.464490	-0.283386
C	-5.242407	-1.575726	-0.333878
S	-5.700671	0.944890	-0.110052
C	-4.572611	-0.353785	-0.250352
C	-3.161432	-0.125089	-0.264162
C	-2.495843	1.089022	-0.201847
C	-1.105196	0.911923	-0.226998
C	-0.699048	-0.436499	-0.302857
C	0.699055	-0.436492	-0.302857
C	1.105189	0.911935	-0.226998
C	2.495834	1.089049	-0.201847
C	3.161436	-0.125056	-0.264161
C	4.572618	-0.353736	-0.250351
C	5.242427	-1.575670	-0.333878
C	6.628419	-1.464419	-0.283385
C	7.077270	-0.147099	-0.158149
N	-0.000008	1.729746	-0.196967
S	-2.056266	-1.496352	-0.355419
S	2.056285	-1.496330	-0.355418
S	5.700663	0.944952	-0.110048

H	-7.324942	-2.290946	-0.331914
H	-4.722085	-2.522867	-0.430842
H	-3.010578	2.041254	-0.137398
H	3.010560	2.041286	-0.137398
H	4.722115	-2.522817	-0.430844
H	7.324971	-2.290868	-0.331912
C	-0.000015	3.164993	-0.040744
H	-0.000015	3.458161	1.015081
H	0.883628	3.582959	-0.528353
H	-0.883666	3.582949	-0.528350
C	-8.352142	0.458523	-0.066916
C	-9.632989	-0.054949	-0.036899
C	-10.855985	0.741916	0.069625
C	-10.028403	-1.480739	-0.061744
C	-11.501363	-1.509140	0.074388
C	-11.995262	-0.200999	0.159734
C	-14.170609	-1.134965	0.353884
C	-13.684326	-2.437466	0.264798
C	-13.367355	0.000071	0.304341
C	-12.315599	-2.628465	0.121316
C	8.352141	0.458603	-0.066916
C	9.632980	-0.054887	-0.036904
C	10.855998	0.741947	0.069621
C	10.028353	-1.480687	-0.061754
C	11.995247	-0.201002	0.159729
C	11.501312	-1.509130	0.074381
C	13.367346	0.000029	0.304337
C	14.170568	-1.135029	0.353878
C	13.684248	-2.437517	0.264792
C	12.315517	-2.628478	0.121309
O	-9.330900	-2.476902	-0.164834
O	9.330816	-2.476825	-0.164843
C	10.991181	2.113781	0.070384
C	12.248407	2.775802	0.179239
C	9.906368	3.030412	-0.047228
C	-10.991119	2.113755	0.070387
C	-9.906267	3.030340	-0.047225
C	-12.248318	2.775827	0.179239
N	13.248994	3.362061	0.266218
N	9.047463	3.809654	-0.141395
N	-9.047318	3.809534	-0.141385
N	-13.248878	3.362131	0.266211

H	13.835435	0.972905	0.381261
H	14.382706	-3.264466	0.310936
H	11.879438	-3.619729	0.048611
H	8.292103	1.540571	0.000552
H	-8.292099	1.540492	0.000547
H	-11.879548	-3.619729	0.048620
H	-14.382807	-3.264396	0.310943
H	-13.835417	0.972959	0.381264
N	-15.620865	-0.948449	0.510664
N	15.620829	-0.948554	0.510658
O	16.034619	0.194034	0.593468
O	16.311986	-1.953578	0.547730
O	-16.034626	0.194152	0.593444
O	-16.312052	-1.953453	0.547710

5. **Compound C5**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-7.084151	-0.079598	-0.150608
C	-6.641671	-1.392815	-0.293703
C	-5.252427	-1.508655	-0.350461
S	-5.705070	1.006552	-0.093299
C	-4.578689	-0.293734	-0.254010
C	-3.165450	-0.064687	-0.268339
C	-2.498371	1.146511	-0.200539
C	-1.106047	0.968312	-0.227233
C	-0.699813	-0.377546	-0.309993
C	0.699817	-0.377548	-0.310004
C	1.106055	0.968309	-0.227249
C	2.498380	1.146505	-0.200570
C	3.165455	-0.064694	-0.268372
C	4.578693	-0.293745	-0.254051
C	5.252426	-1.508676	-0.350416
C	6.641672	-1.392836	-0.293689
C	7.084158	-0.079609	-0.150702
N	0.000006	1.785839	-0.193600
S	-2.059888	-1.435765	-0.366886
S	2.059890	-1.435769	-0.366918
S	5.705082	1.006550	-0.093468
H	-7.343070	-2.214925	-0.349579

H	-4.736144	-2.456625	-0.461722
H	-3.012394	2.098826	-0.131405
H	3.012405	2.098819	-0.131433
H	4.736139	-2.456654	-0.461590
H	7.343068	-2.214953	-0.349506
C	0.000010	3.218590	-0.025628
H	0.000050	3.504560	1.032517
H	0.883916	3.640893	-0.509383
H	-0.883935	3.640888	-0.509315
C	-8.362589	0.532290	-0.047145
C	-9.638315	0.023221	-0.013214
C	-10.862413	0.823709	0.108051
C	-10.048170	-1.406374	-0.037505
C	-11.508110	-1.419900	0.121335
C	-11.993498	-0.108635	0.211504
C	-14.214205	-1.009776	0.452289
C	-13.707889	-2.333289	0.305651
C	-13.364517	0.091933	0.387716
C	-12.336705	-2.526793	0.160293
C	8.362601	0.532281	-0.047319
C	9.638323	0.023204	-0.013341
C	10.862423	0.823700	0.107817
C	10.048165	-1.406400	-0.037381
C	11.993492	-0.108636	0.211517
C	11.508095	-1.419912	0.121548
C	13.364500	0.091955	0.387773
C	14.214178	-1.009750	0.452589
C	13.707858	-2.333283	0.306146
C	12.336683	-2.526803	0.160740
O	-9.349079	-2.402038	-0.156501
O	9.349070	-2.402077	-0.156248
C	10.983205	2.201742	0.106944
C	12.236117	2.866112	0.237308
C	9.899778	3.114980	-0.031609
C	-10.983182	2.201754	0.107471
C	-9.899742	3.115018	-0.030802
C	-12.236100	2.866106	0.237870
N	13.242668	3.440076	0.346060
N	9.046775	3.899441	-0.142480
N	-9.046737	3.899513	-0.141416
N	-13.242648	3.440068	0.346663
H	13.792116	1.081643	0.495695

H	11.913082	-3.522704	0.057859
H	8.297222	1.613494	0.027810
H	-8.297200	1.613494	0.028098
H	-11.913103	-3.522678	0.057268
H	-13.792135	1.081604	0.495779
N	15.589690	-0.877307	0.602646
H	15.988207	-1.532976	1.266883
H	15.894660	0.067936	0.796647
N	14.619369	-3.373506	0.366855
H	14.246753	-4.277004	0.107303
H	15.494038	-3.175875	-0.107660
N	-15.589733	-0.877352	0.602270
H	-15.894704	0.067867	0.796391
H	-15.988286	-1.533101	1.266409
N	-14.619407	-3.373512	0.366133
H	-15.494079	-3.175773	-0.108332
H	-14.246804	-4.276968	0.106418

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

Functional	**HOMO (eV)**	**LUMO (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-5.13	-3.57	1.56	648
B3LYP	-4.65	-2.74	1.91	710
B3LYP-D3	-4.65	-2.72	1.93	703
CAM-B3LYP	-5.85	-1.67	4.18	520
B3PW91	-4.76	-2.82	1.94	698
HSEH1PBE	-4.52	-2.99	1.53	732
WB97XD	-6.46	-1.11	5.35	492

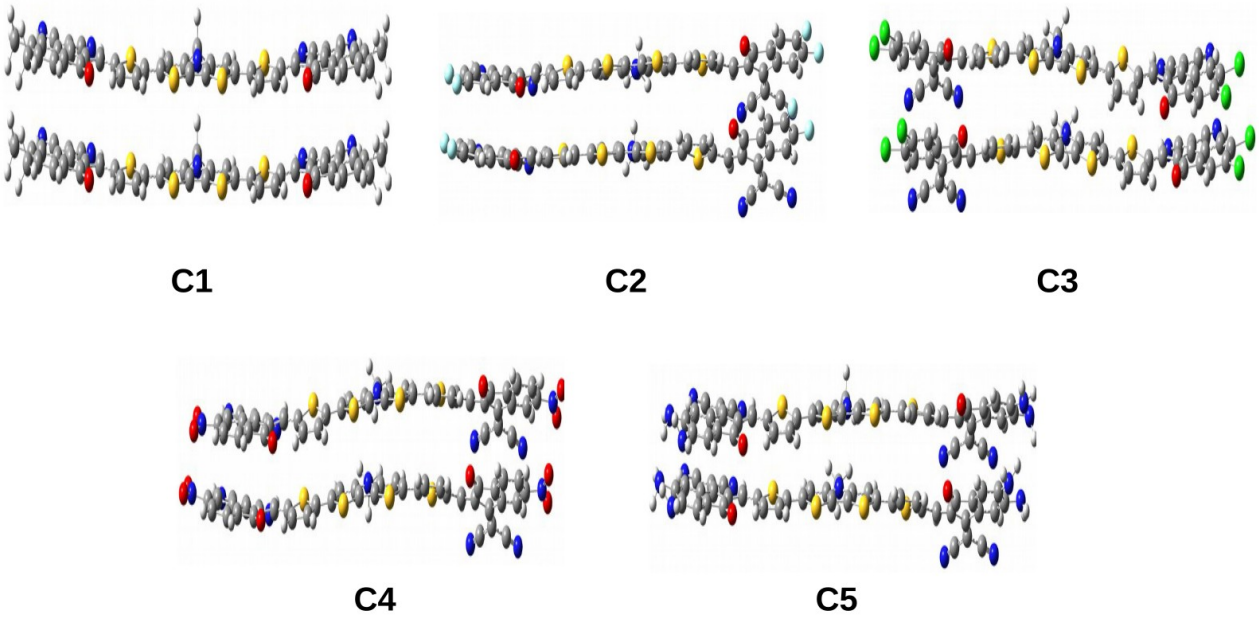

Fig. S1 : Optimized structures of the studied compounds in the π-stacked orientation.

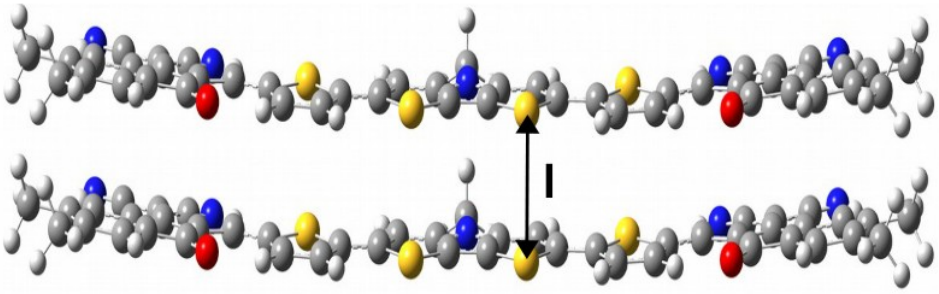

Fig. S2 : Representative structure of two stacked molecules along with distance l.

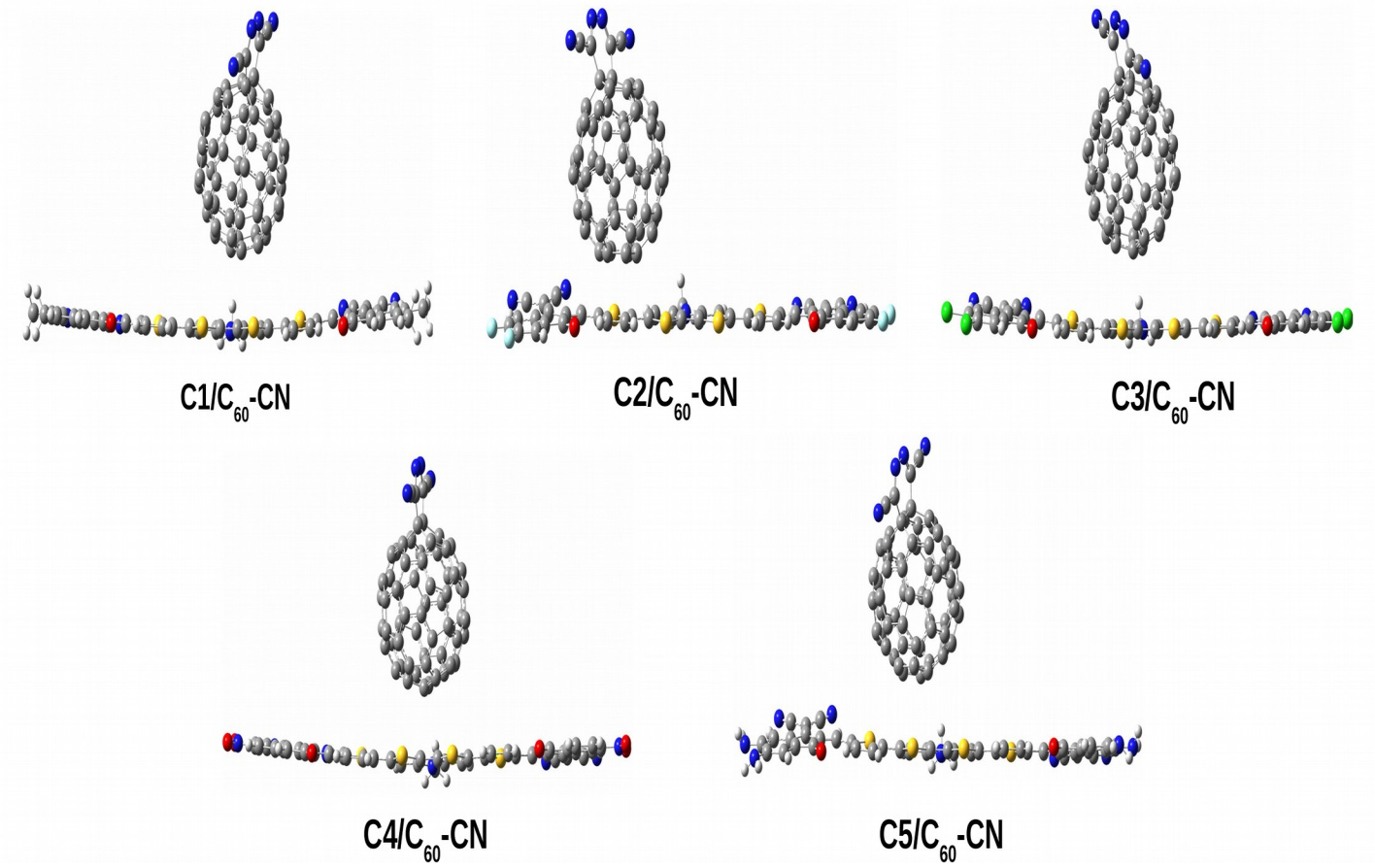

Fig. S3 : Optimized structures of the C1- C5/ C_{60}-CN complexes.