Electronic Supplementary Material (ESI) for RSC Advances.

Effects of different functional groups on the optical and charge transport properties of copolymers for polymer solar cells

Supplementary Information

Content

Table S1a. Selected bond lengths and dihedral angles of QTT (n=1-3).

		TT-Q	Q-TT	TT-Q	Q-TT	TT-Q	Q-TT
Bond	n=1	1.46337	1.46358				
lengths(Å)	n=2	1.46205	1.46150	1.46144	1.46236		
	n=3	1.46199	1.46137	1.46086	1.46060	1.46096	1.46293
Dihedral	n=1	-23.63928	-26.15308				
angles(°)	n=2	-24.90429	-17.87959	-17.42984	-21.26147		
	n=3	-24.87192	-16.90961	-16.16270	-19.36750	-19.18454	-16.66149

Table S1b. Selected bond lengths and dihedral angles of BDT-DTBTBPz (Pz) (n=1-3).

		BDT-T	T-PZ	PZ-T	T-BDT	BDT-T	T-PZ	PZ-T	T-BDT	BDT-T	T-PZ	PZ-T
Bond lengths(Å)	n=1	1.44559	1.44987	1.45509								
	n=2	1.44514	1.44811	1.44724	1.44326	1.44540	1.44968	1.45493				
	n=3	1.44431	1.44742	1.44719	1.44261	1.44431	1.44862	1.44793	1.44448	1.44358	1.44901	1.45484
Dihedral angles(°)	n=1	-170.49803	5.61816	13.39008								
	n=2	170.71515	-5.03109	-5.48157	-173.56378	-158.08324	7.68750	11.70502				
	n=3	176.68680	3.44255	2.72084	-179.08794	158.05137	0.36958	8.30794	-160.10313	-175.84670	4.05776	12.77740

Table S1c. Selected bond lengths and dihedral angles of BDT-DTBTQx (Qx) (n=1-3).

		BDT-T	T-QX	QX-T	T-BDT	BDT-T	T-QX	QX-T	T-BDT	BDT-T	T-QX	QX-T
Bond lengths(Å)	n=1	1.44394	1.45271	1.45600								
	n=2	1.44380	1.45190	1.45019	1.44136	1.44090	1.45047	1.45596				
	n=3	1.44225	1.45033	1.45051	1.44179	1.44062	1.44914	1.44890	1.44057	1.44108	1.45052	1.45661
Dihedral angles(°)	n=1	-158.88276	4.50387	15.11273								
	n=2	-158.64403	5.64618	4.28348	-164.62392	170.31989	2.72739	9.13454				
	n=3	-174.88722	-4.84456	6.84659	-161.24158	178.96522	-3.00885	-3.68527	-179.89621	-173.25962	-2.86104	-11.93687

Table S1d. Selected bond lengths and dihedral angles of D1 (n=1-3).

		TT-QF	QF-TT	TT-QF	QF-TT	TT-QF	QF-TT
Bond	n=1	1.46414	1.46163				
lengths(Å)	n=2	1.46027	1.45967	1.46246	1.46310		
	n=3	1.46317	1.46244	1.45958	1.46229	1.46225	1.46340
Dihedral	n=1	17.47226	-31.20169				
angles(°)	n=2	25.65795	29.42143	-19.99886	-15.77639		
	n=3	-16.00495	-19.90711	31.36639	-15.42108	-15.11001	-19.76523

Table S1e. Selected bond lengths and dihedral angles of D2 (n=1-3).

		TT-QX	QX-TT	TT-QX	QX-TT	TT-QX	QX-TT
Bond	n=1	1.45686	1.45632				
lengths(Å)	n=2	1.45004	1.44666	1.45194	1.45520		
	n=3	1.44964	1.45078	1.44356	1.44464	1.45106	1.45513
Dihedral	n=1	16.93201	11.11547				
angles(°)	n=2	21.65745	23.27112	-14.39769	-11.02407		
	n=3	-24.94180	10.39440	18.35110	20.95335	-14.28154	-10.38900

Table S1f. Selected bond lengths and dihedral angles of D3 (n=1-3).

		TT-PX	PX-TT	TT-PX	PX-TT	TT-PX	PX-TT
Bond lengths(Å)	n=1	1.47221	1.47351				
	n=2	1.47214	1.47429	1.47374	1.47298		
	n=3	1.47223	1.47172	1.48291	1.48047	1.47269	1.47235
Dihedral	n=1	-50.19274	-52.90048				
angles(°)	n=2	-49.56691	-56.94529	-56.13512	-46.95250		
	n=3	-50.58099	-50.67054	111.19093	58.33356	49.10815	41.56013

Table S2. Absorption peaks and oscillator strength of the seven monomers under external electric field.

Field ($\times 10^{-3}$ a.u.)	BSeTT	QTT	Pz	Qx	D1	D2	D3
0	498.34(0.6012)	409.66(0.6229)	740.50(0.4990)	641.87(0.5056)	400.44(0.6706)	660.97(0.4478)	397.08(0.2421)
1	500.49(0.6031)	412.27(0.6246)	774.32(0.5147)	661.59(0.5253)	405.07(0.6613)	662.28(0.4472)	400.44(0.2481)
2	—	418.90(0.6267)	817.75(0.5436)	—	414.01(0.6575)	668.81(0.4514)	406.55(0.2530)
3	—	429.22(0.6319)	875.33(0.5836)	—	—	678.96(0.4554)	415.67(0.2580)

Table S3. HOMO, LUMO energy levels and band gaps of the seven monomers under external electric field (eV).

	BSeTT			QTT			Pz			Qx			D1			D2			D3		
Field ($\times 10^{-3}$ a.u.)	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}
0	-5.15	-2.79	2.36	-5.16	-2.30	2.86	-4.78	-3.28	1.50	-4.89	-3.08	1.81	-5.25	-2.33	2.92	-4.88	-3.13	1.75	-5.26	-2.25	3.01
1	-5.14	-2.79	2.35	-5.14	-2.30	2.84	-4.76	-3.37	1.39	-4.86	-3.16	1.70	-5.21	-2.33	2.88	-4.88	-3.13	1.75	-5.21	-2.26	2.95
2	—	—	—	-5.08	-2.31	2.77	-4.70	-3.44	1.26	—	—	—	-5.13	-2.34	2.79	-4.86	-3.13	1.73	-5.13	-2.27	2.86
3	—	—	—	-5.00	-2.32	2.68	-4.63	-3.49	1.14	—	—	—	—	—	—	-4.82	-3.11	1.71	-5.04	-2.29	2.75

Table S4. Calculated transition energies and oscillator strengths for $PC_{60}BM$/BSeTT.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	2.4227	511.77	(0.67058)H-1→L	0.0013
S2	2.4562	504.79	(0.61842)H-1→L+1	0.0000
S3	2.5071	494.54	(0.68093)H→L+3	0.5180
S4	2.5273	490.58	(0.65414)H-2→L	0.0001
S5	2.5499	486.24	(0.64220)H-3→L	0.0018
S6	2.6818	462.31	(0.49227)H-4→L+1	0.0002
S7	2.7249	455.00	(0.50300)H-2→L+1	0.0007
S8	2.7865	444.94	(0.49832)H-4→L	0.0001
S9	2.8377	436.91	(0.43935)H-3→L+1	0.0002
S10	2.8683	432.26	(0.54433)H-5→L+1	0.0009
S11	2.9556	419.49	(0.56464)H-4→L+2	0.0020
S12	2.9866	415.14	(0.53492)H-1→L+2	0.0023
S13	3.0021	412.99	(0.50347)H-2→L+2	0.0001
S14	3.0648	404.54	(0.59659)H→L	0.0052
S15	3.0869	401.65	(0.63059)H-5→L	0.0003
S16	3.1225	397.07	(0.59383)H→L+1	0.0070
S17	3.1457	394.14	(0.51284)H-3→L+2	0.0030
S18	3.1770	390.26	(0.62641)H-5→L+2	0.0110
S19	3.3012	375.57	(0.67971)H→L+2	0.0001
S20	3.4585	358.49	(0.38654)H-9→L	0.0024
S21	3.5132	352.91	(0.46798)H-9→L+1	0.0000

S22	3.5371	350.53	(0.29889)H-4→L+4	0.0005
S23	3.6941	335.62	(0.28040)H-6→L+3	0.0159
S24	3.6962	335.44	(0.52439)H-6→L+3	0.0473
S25	3.7108	334.11	(0.27965)H-3→L+5	0.0006
S26	3.7202	333.28	(0.39877)H-1→L+4	0.0082
S27	3.7771	328.25	(0.34068)H-3→L+4	0.0008
S28	3.7873	327.37	(0.39072)H-15→L	0.0001
S29	3.8485	322.16	(0.29794)H-18→L	0.0057
S30	3.8681	320.53	(0.62019)H-1→L+3	0.0027

Table S5. Calculated transition energies and oscillator strengths for $PC_{60}BM$/QTT.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	2.4276	510.72	(0.66917)H-1→L	0.0015
S2	2.4522	505.60	(0.61556)H-1→L+1	0.0000
S3	2.5278	490.48	(0.67082)H-2→L	0.0000
S4	2.5517	485.90	(0.65369)H-3→L	0.0000
S5	2.6697	464.42	(0.49995)H-3→L+1	0.0002
S6	2.7205	455.73	(0.53756)H-2→L+1	0.0004
S7	2.7854	445.13	(0.44604)H-5→L	0.0001
S8	2.8351	437.32	(0.43602)H-3→L+1	0.0002
S9	2.8679	432.32	(0.53764)H-6→L+1	0.0007
S10	2.9534	419.81	(0.52560)H-5→L+2	0.0013
S11	2.9800	416.05	(0.54803)H-1→L+2	0.0143
S12	2.9992	413.39	(0.50802)H-2→L+2	0.0171
S13	3.0220	410.28	(0.66053)H→L+3	0.4922
S14	3.0973	400.29	(0.63329)H-6→L	0.0046
S15	3.1389	394.99	(0.54866)H-3→L+2	0.0040
S16	3.1509	393.49	(0.60800)H→L	0.0027
S17	3.1788	390.04	(0.63202)H-6→L+2	0.0124
S18	3.2493	381.57	(0.61902)H→L+1	0.0000
S19	3.3945	365.26	(0.68315)H→L+2	0.0021
S20	3.4601	358.33	(0.34988)H-12→L	0.0010
S21	3.5128	352.95	(0.44232)H-12→L+1	0.0001
S22	3.5361	350.62	(0.29489)H-1→L+6	0.0012
S23	3.6053	343.89	(0.56140)H-4→L+3	0.2245
S24	3.6958	335.47	(0.40801)H-20→L	0.0012
S25	3.7108	334.12	(0.38112)H-21→L	0.0000
S26	3.7176	333.51	(0.45725)H-1→L+4	0.0118
S27	3.7234	332.99	(0.38586)H-17→L+3	0.0353
S28	3.7793	328.06	(0.34392)H-3→L+4	0.0020
S29	3.7875	327.35	(0.40878)H-19→L	0.0000
S30	3.8141	325.07	(0.54274)H-4→L+1	0.0005

Table S6. Calculated transition energies and oscillator strengths for $PC_{60}BM$/Pz.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	1.6909	733.24	(0.68362)H→L	0.4166
S2	2.4210	512.12	(0.66791)H→L	0.0023
S3	2.4502	506.01	(0.61328)H-2→L+2	0.0000
S4	2.5271	490.62	(0.62097)H-3→L+1	0.0000
S5	2.5459	487.00	(0.61741)H-4→L+1	0.0000
S6	2.6562	466.77	(0.67460)H→L+1	0.0000
S7	2.6713	464.13	(0.47402)H-5→L+2	0.0001
S8	2.6963	459.83	(0.60865)H→L+2	0.0035
S9	2.7146	456.72	(0.50903)H-1→L	0.0263
S10	2.7224	455.41	(0.43038)H-3→L+2	0.0003
S11	2.7829	445.52	(0.50026)H-5→L+1	0.0002
S12	2.8307	438.00	(0.42184)H-5→L+2	0.0000
S13	2.8601	433.50	(0.54228)H-7→L+2	0.0008
S14	2.9348	422.47	(0.66114)H→L+3	0.0016
S15	2.9470	420.72	(0.54355)H-5→L+3	0.0013
S16	2.9823	415.73	(0.46893)H-2→L+3	0.0002
S17	2.9865	415.15	(0.41221)H-17→L	0.0071
S18	3.0008	413.18	(0.45733)H-3→L+3	0.0002
S19	3.0827	402.19	(0.62888)H-7→L+1	0.0009
S20	3.1345	395.55	(0.37217)H-4→L+3	0.0674
S21	3.1495	393.67	(0.28425)H-8→L	0.1368
S22	3.1686	391.29	(0.62468)H-7→L+3	0.0127
S23	3.2336	383.43	(0.54468)H-8→L	0.0104
S24	3.2364	383.09	(0.67521)H-2→L	0.0049
S25	3.3505	370.05	(0.60470)H-3→L	0.0047
S26	3.3973	364.95	(0.50391)H→L+6	0.3122
S27	3.4160	362.95	(0.60492)H-5→L	0.0010
S28	3.4227	362.24	(0.44578)H→L+8	0.1253
S29	3.4349	360.95	(0.35148)H-10→L	0.1349
S30	3.4354	360.90	(0.63613)H-1→L+1	0.0438

Table S7. Calculated transition energies and oscillator strengths for $PC_{60}BM$/Qx.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	1.8991	652.87	(0.68631)H→L	0.4554
S2	2.4223	511.85	(0.66372)H-3→L+1	0.0021
S3	2.4528	505.48	(0.61209)H-3→L+2	0.0000
S4	2.5260	490.83	(0.65731)H-4→L+1	0.0000
S5	2.5458	487.01	(0.64315)H-5→L+1	0.0000
S6	2.6748	463.54	(0.48495)H-6→L+2	0.0001
S7	2.7220	455.49	(0.51530)H-4→L+2	0.0030
S8	2.7312	453.95	(0.55413)H-1→L	0.2273
S9	2.7599	449.23	(0.52843)H→L+1	0.0006
S10	2.7751	446.77	(0.49210)H→L+2	0.0020
S11	2.8044	442.10	(0.39356)H→L+1	0.0012
S12	2.8429	436.11	(0.41046)H-6→L+2	0.0001
S13	2.8640	432.91	(0.52521)H-7→L+2	0.0007
S14	2.9370	422.15	(0.46096)H-6→L+3	0.0006
S15	2.9854	415.30	(0.46751)H-3→L+3	0.0008
S16	3.0016	413.06	(0.44920)H-4→L+3	0.0004
S17	3.0050	412.59	(0.50546)H→L+3	0.0012
S18	3.0848	401.92	(0.35993)H-2→L	0.0968
S19	3.0890	401.37	(0.57793)H-7→L+1	0.0139
S20	3.1390	394.98	(0.32658)H-5→L+3	0.0341
S21	3.1462	394.08	(0.41911)H-5→L+3	0.0360
S22	3.1761	390.36	(0.63300)H-7→L+3	0.0098
S23	3.3750	367.36	(0.67524)H-3→L	0.0047
S24	3.4467	359.72	(0.45254)H-1→L+1	0.0010
S25	3.4571	358.64	(0.36540)H-12→L+1	0.0021
S26	3.4730	357.00	(0.38830)H-5→L	0.0443
S27	3.4891	355.34	(0.45466)H-5→L	0.0575
S28	3.4999	354.25	(0.33247)H-1→L+2	0.0041
S29	3.5119	353.04	(0.50956)H→L+6	0.5663
S30	3.5137	352.86	(0.33891)H-12→L+2	0.0032

Table S8. Calculated transition energies and oscillator strengths for $PC_{60}BM$/D1.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	2.4278	510.69	(0.66893)H-1→L	0.0016
S2	2.4543	505.17	(0.61561)H-1→L+1	0.0000
S3	2.5280	490.45	(0.60178)H-3→L	0.0000
S4	2.5507	486.08	(0.63809)H-4→L	0.0000
S5	2.6728	463.88	(0.48294)H-4→L+1	0.0002
S6	2.7218	455.52	(0.47791)H-3→L+1	0.0005
S7	2.7835	445.42	(0.48951)H-5→L	0.0000
S8	2.8360	437.19	(0.44387)H-5→L+1	0.0001
S9	2.8674	432.39	(0.52308)H-6→L+1	0.0007
S10	2.9470	420.71	(0.55920)H-5→L+2	0.0010
S11	2.9822	415.74	(0.52944)H-1→L+2	0.0028
S12	2.9992	413.39	(0.45950)H-3→L+2	0.0000
S13	3.0822	402.26	(0.55899)H→L+3	0.3940
S14	3.1010	399.82	(0.52782)H-6→L	0.1592
S15	3.1402	394.83	(0.52044)H-4→L+2	0.0326
S16	3.1742	390.60	(0.62955)H-6→L+2	0.0069
S17	3.2938	376.41	(0.56767)H→L	0.0039
S18	3.3566	369.37	(0.56651)H→L+1	0.0011
S19	3.4600	358.33	(0.37601)H-12→L	0.0001
S20	3.5012	354.12	(0.51979)H-2→L+3	0.2251
S21	3.5127	352.96	(0.47741)H-12→L+1	0.0016
S22	3.5203	352.20	(0.63405)H→L+2	0.0308
S23	3.5360	350.64	(0.29359)H-1→L+6	0.0030
S24	3.6955	335.50	(0.38621)H-9→L	0.0014
S25	3.7050	334.64	(0.52496)H-2→L+1	0.0009
S26	3.7107	334.13	(0.38286)H-10→L	0.0001
S27	3.7190	333.38	(0.46486)H-1→L+4	0.0077
S28	3.7376	331.72	(0.53770)H-2→L	0.0012
S29	3.7786	328.13	(0.33746)H-4→L+4	0.0035
S30	3.7870	327.39	(0.40462)H-8→L	0.0001

Table S9. Calculated transition energies and oscillator strengths for $PC_{60}BM$/D2.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	1.8644	665.03	(0.69552)H→L	0.3754
S2	2.4257	511.13	(0.66534)H-1→L+1	0.0018
S3	2.4516	505.73	(0.61713)H-1→L+2	0.0000
S4	2.5244	491.13	(0.63272)H-3→L+1	0.0001
S5	2.5490	486.40	(0.61280)H-4→L+1	0.0000
S6	2.6173	473.70	(0.48609)H→L+1	0.0035
S7	2.6696	464.43	(0.44609)H-5→L+2	0.0001
S8	2.7012	458.99	(0.43590)H→L+2	0.0011
S9	2.7229	455.33	(0.44368)H-3→L+2	0.0002
S10	2.7816	445.73	(0.47111)H-5→L+1	0.0000
S11	2.8233	439.15	(0.52870)H→L+3	0.0048
S12	2.8303	438.06	(0.53809)H-2→L	0.1579
S13	2.8361	437.16	(0.33659)H-2→L	0.0567
S14	2.8637	432.95	(0.52260)H-6→L+2	0.0036
S15	2.9477	420.61	(0.56915)H-5→L+3	0.0014
S16	2.9778	416.35	(0.54472)H-1→L+3	0.0010
S17	2.9969	413.70	(0.48028)H-3→L+3	0.0001
S18	3.0722	403.57	(0.39918)H-17→L	0.0070
S19	3.0907	401.15	(0.61285)H-6→L+1	0.0000
S20	3.1362	395.33	(0.51248)H-4→L+3	0.0012
S21	3.1713	390.96	(0.61937)H-6→L+3	0.0081
S22	3.2649	379.75	(0.59860)H-7→L	0.0823
S23	3.3127	374.27	(0.49975)H-8→L	0.0162
S24	3.3487	370.24	(0.44606)H-1→L	0.0032
S25	3.3774	367.10	(0.46078)H-9→L	0.0022
S26	3.4538	358.98	(0.29858)H-12→L+1	0.0011
S27	3.4698	357.33	(0.34513)H-3→L	0.0014
S28	3.5104	353.19	(0.47164)H-12→L+2	0.0003
S29	3.5246	351.76	(0.50414)H-3→L	0.0037
S30	3.5378	350.46	(0.27957)H-1→L+6	0.0021

Table S10. Calculated transition energies and oscillator strengths for $PC_{60}BM$/D3.

State	*E* (eV)	Absorption peak λ (nm)	Contribution MO	Strength *f*
S1	2.4266	510.94	(0.67128)H-2→L	0.0015
S2	2.4547	505.10	(0.61468)H-2→L+1	0.0000
S3	2.5250	491.02	(0.61561)H-3→L	0.0000
S4	2.5474	486.70	(0.60835)H-4→L	0.0000
S5	2.6733	463.80	(0.48331)H-5→L+1	0.0002
S6	2.7219	455.51	(0.43218)H-3→L+1	0.0005
S7	2.7815	445.75	(0.48935)H-5→L	0.0001
S8	2.8316	437.87	(0.43023)H-5→L+1	0.0001
S9	2.8664	432.55	(0.49970)H-7→L+1	0.0007
S10	2.9463	420.82	(0.56201)H-5→L+2	0.0010
S11	2.9788	416.22	(0.55634)H-2→L+2	0.0028
S12	2.9961	413.82	(0.42700)H-3→L+2	0.0003
S13	3.0944	400.68	(0.61905)H-7→L	0.0062
S14	3.1214	397.21	(0.62427)H→L+3	0.1555
S15	3.1358	395.39	(0.43619)H-4→L+2	0.0164
S16	3.1716	390.92	(0.58793)H-7→L+2	0.0396
S17	3.2027	387.12	(0.57249)H-1→L+3	0.3206
S18	3.2705	379.10	(0.44927)H→L+1	0.0118
S19	3.3116	374.39	(0.38158)H→L	0.0049
S20	3.3784	366.99	(0.47808)H-1→L	0.0046
S21	3.3965	365.03	(0.47019)H-1→L+1	0.0029
S22	3.4576	358.59	(0.48857)H→L+2	0.0040
S23	3.4619	358.14	(0.39831)H→L+2	0.0007
S24	3.5138	352.84	(0.41949)H-2→L+5	0.0001
S25	3.5327	350.97	(0.29286)H-5→L+4	0.0021
S26	3.5727	347.03	(0.60880)H-1→L+2	0.0013
S27	3.6875	336.23	(0.43782)H-6→L+3	0.0181
S28	3.6955	335.50	(0.39163)H-23→L	0.0012
S29	3.7085	334.32	(0.37389)H-24→L	0.0004
S30	3.7143	333.80	(0.46911)H-2→L+4	0.0032

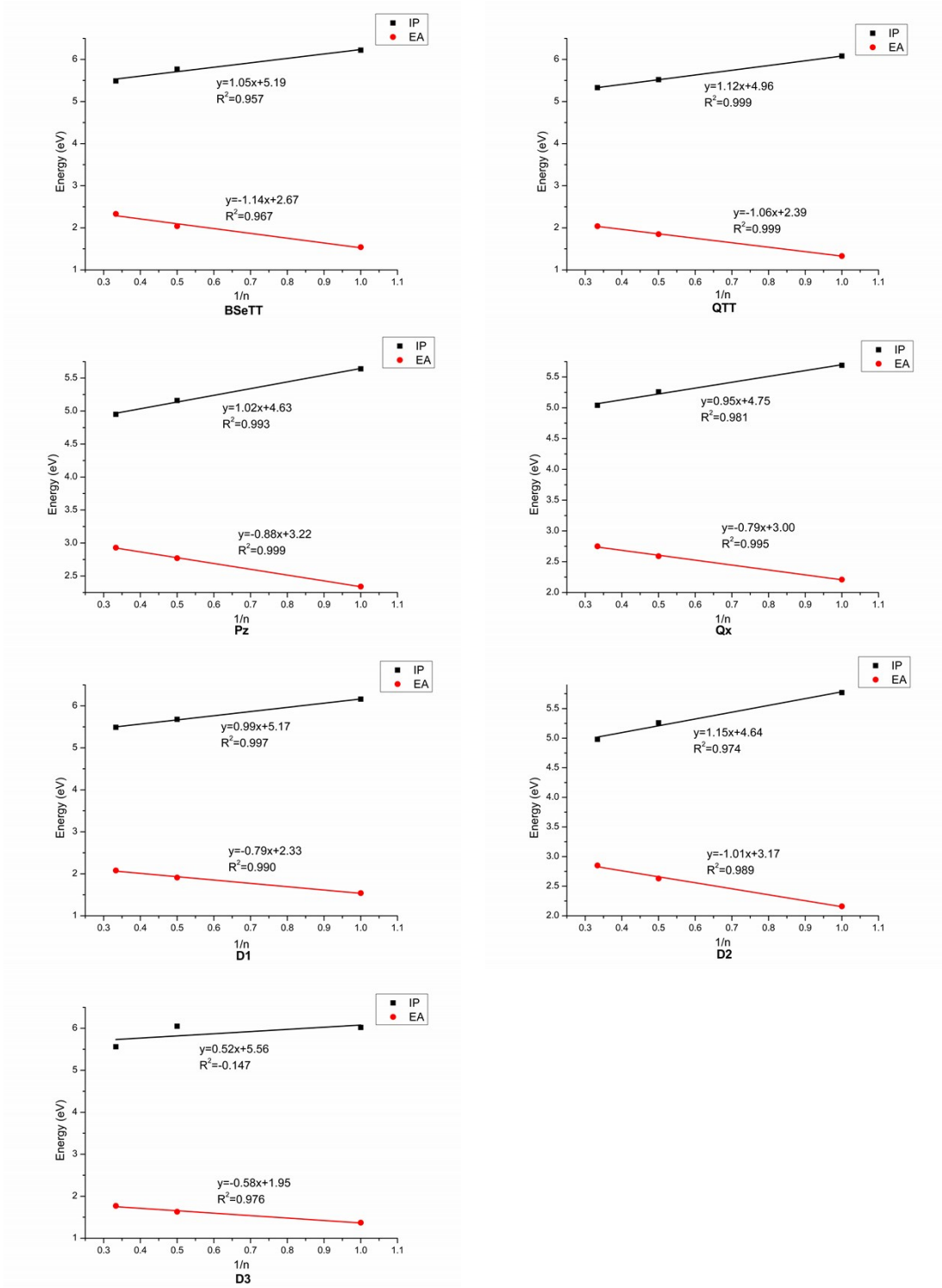
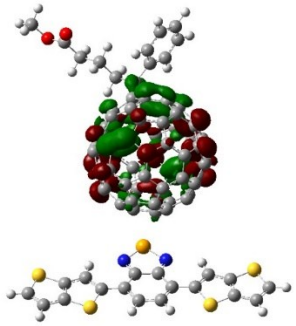


Figure S1. Relationship between the ionization potentials and electron affinities of all oligomers and the reciprocal of conjugated unit (1/n).



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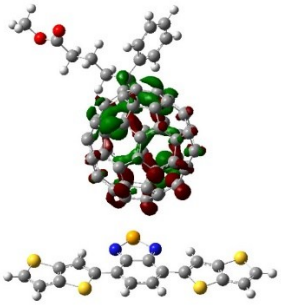

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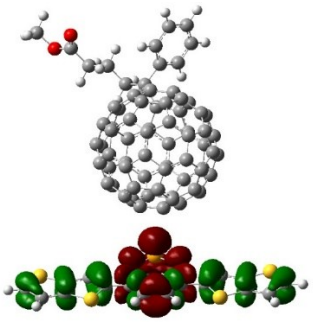

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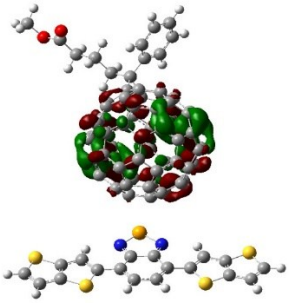

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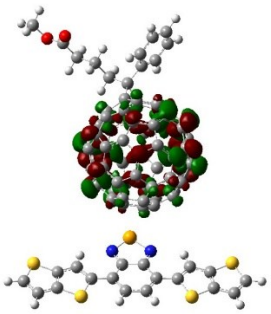

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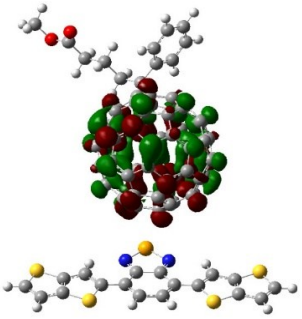

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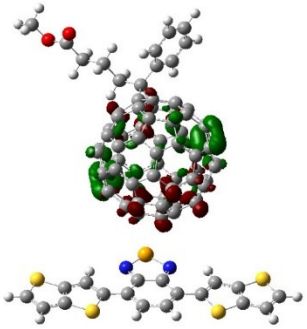

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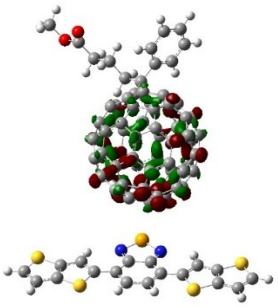

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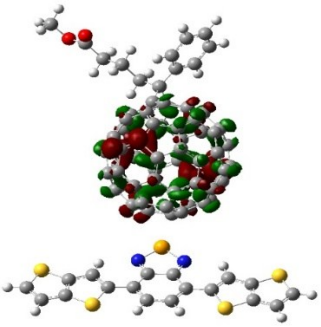

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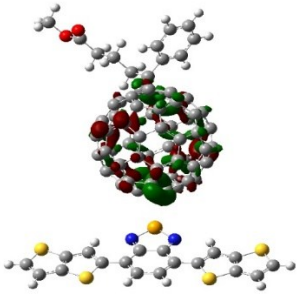

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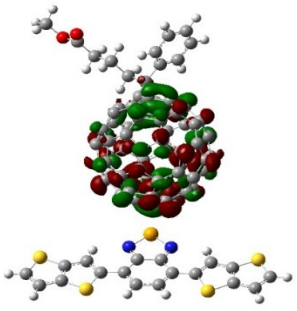

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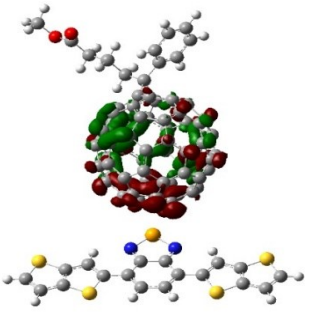

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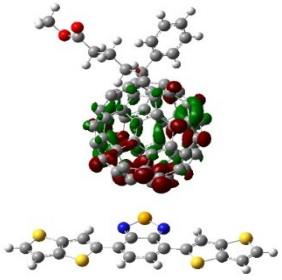

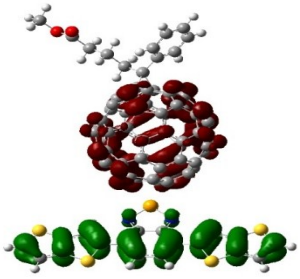

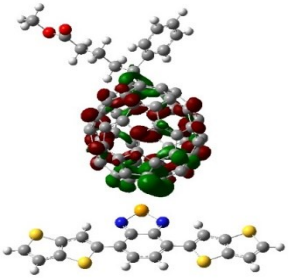

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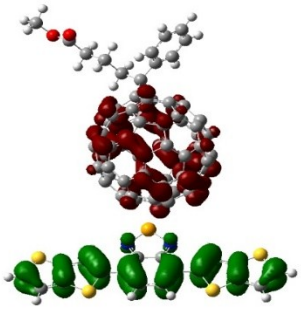

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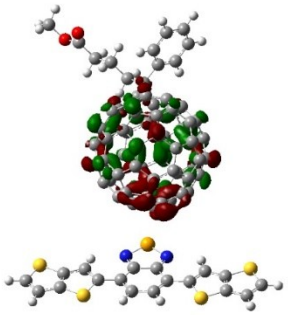

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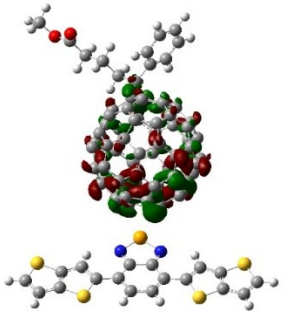

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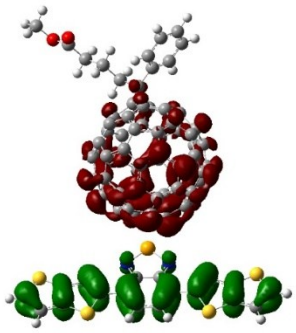

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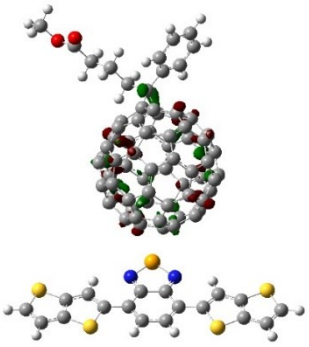

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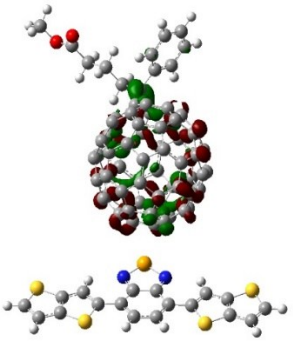

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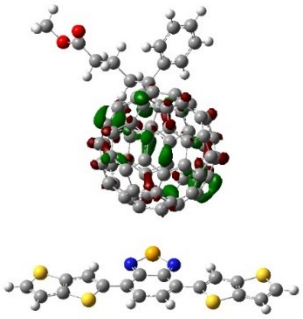

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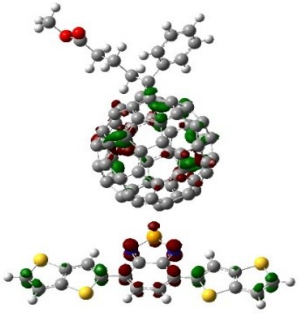

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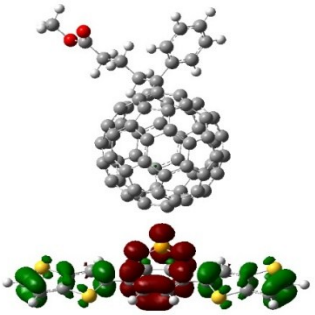

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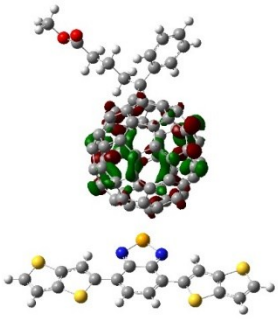

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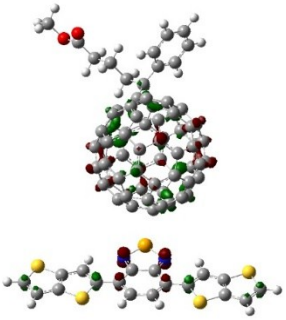

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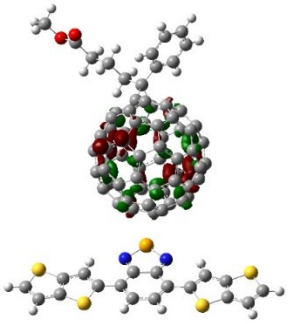

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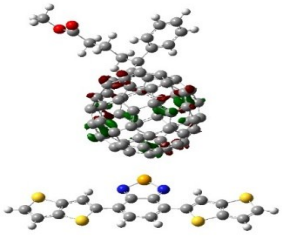

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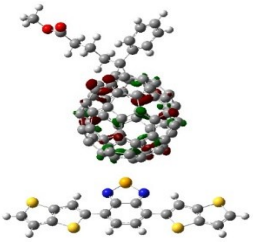

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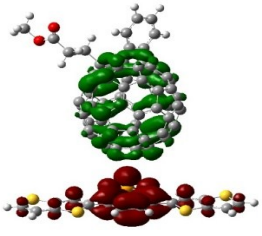
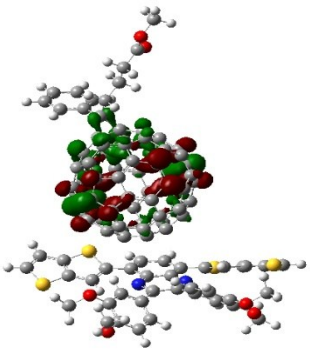


S28 S29 S30

Figure S2. Charge difference density (CDD) of $PC_{60}BM$/BSeTT, where the green and red stand for the hole and electron, respectively.



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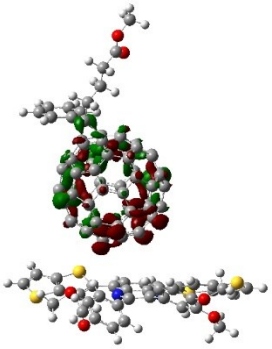

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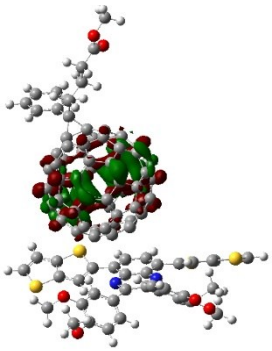

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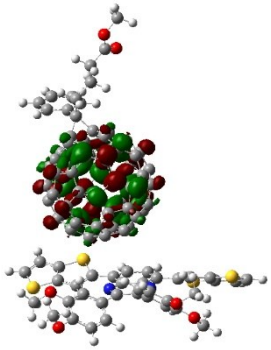

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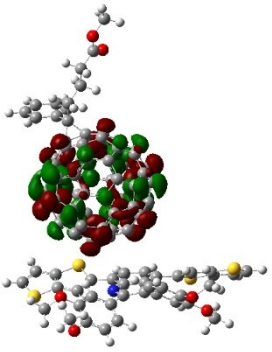

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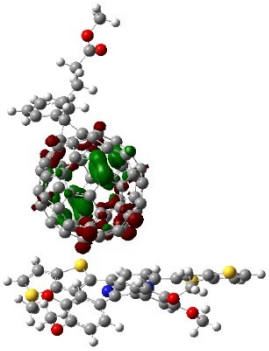

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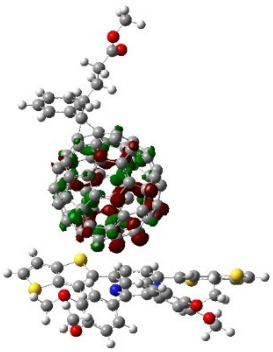

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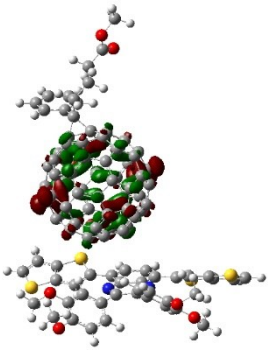

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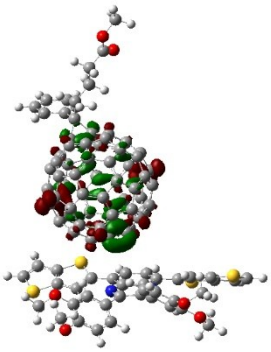

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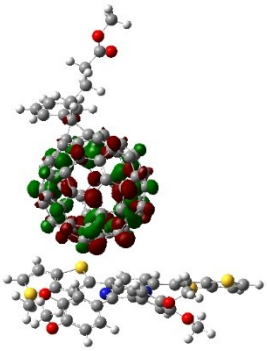

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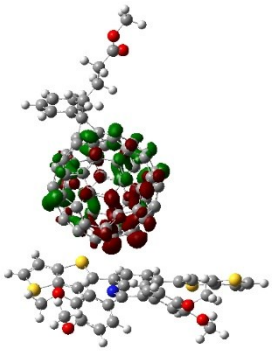

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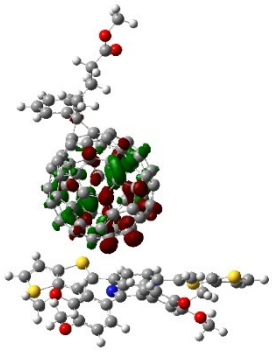

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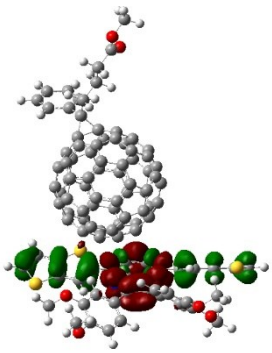

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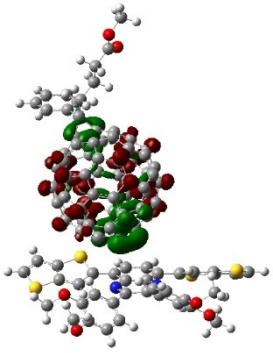

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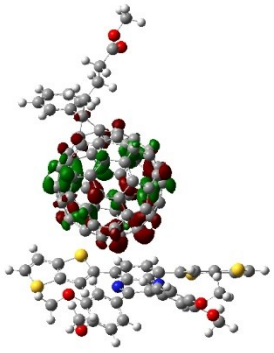

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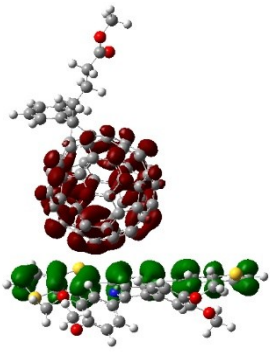

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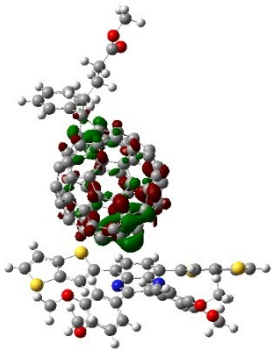

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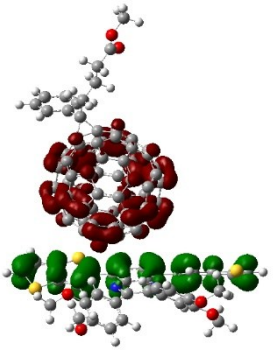

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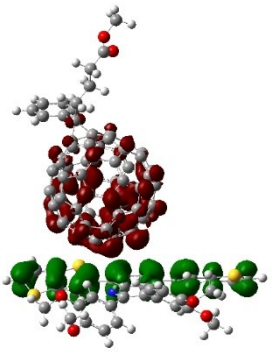

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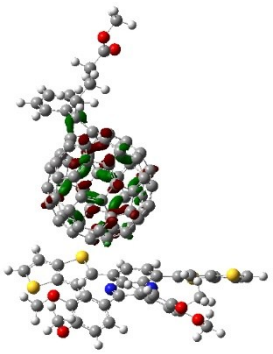

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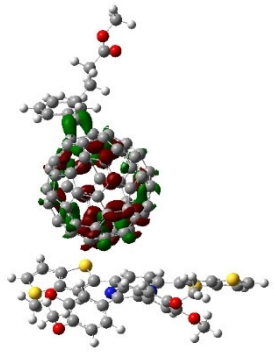

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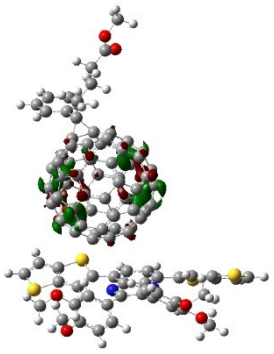

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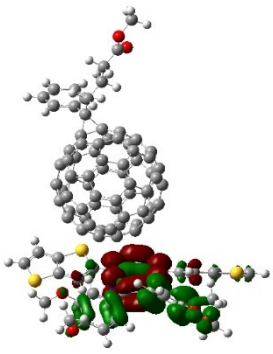

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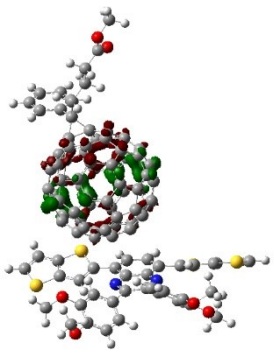

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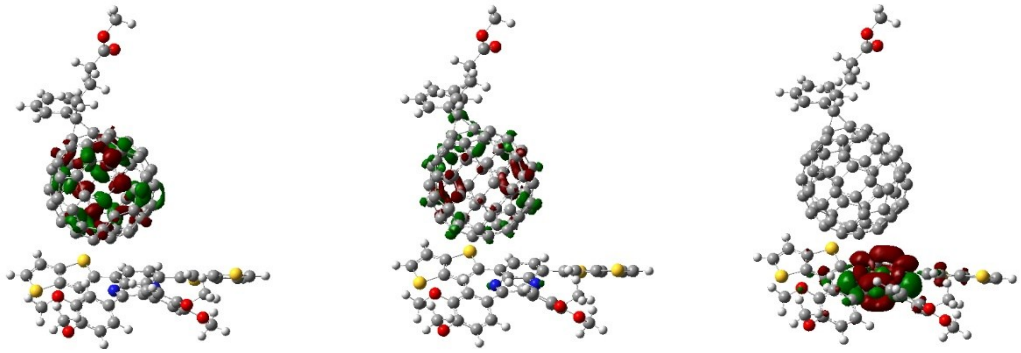

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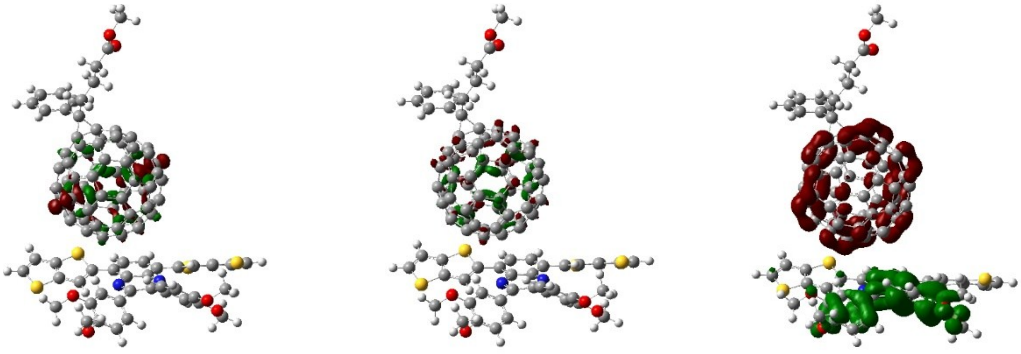
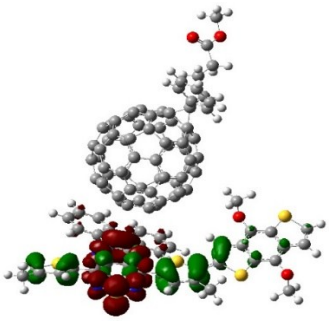


S28 S29 S30

Figure S3. Charge difference density (CDD) of $PC_{60}BM$/QTT, where the green and red stand for the hole and electron, respectively.



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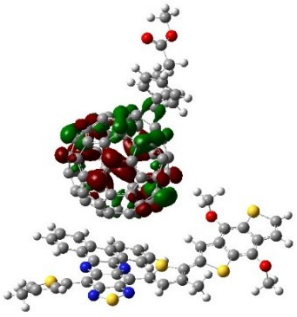

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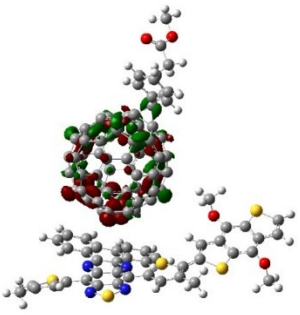

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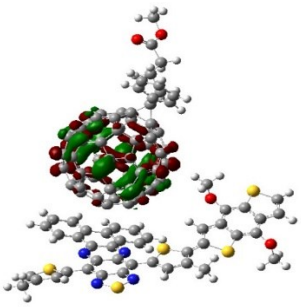

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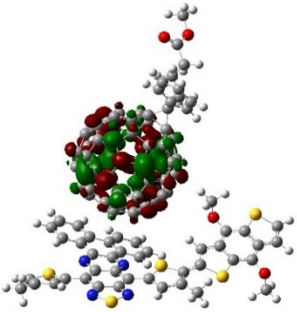

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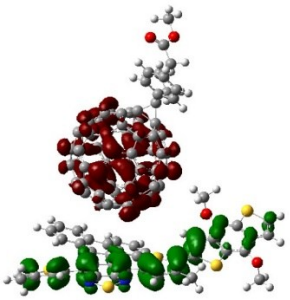

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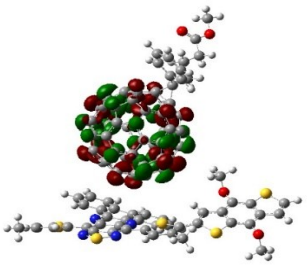

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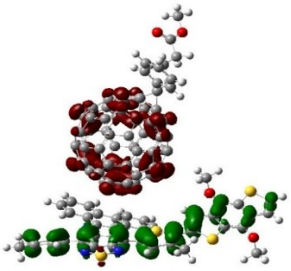

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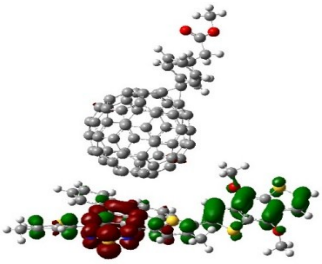

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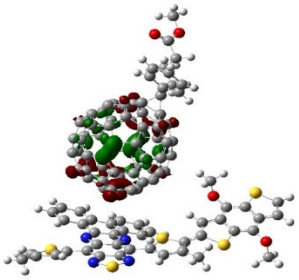

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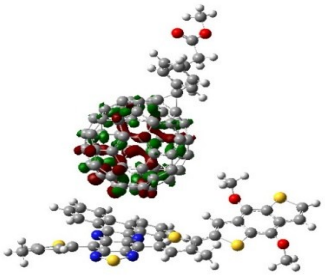

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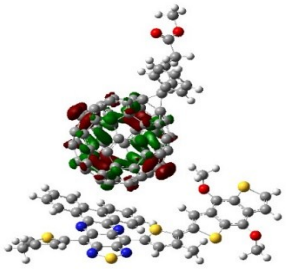

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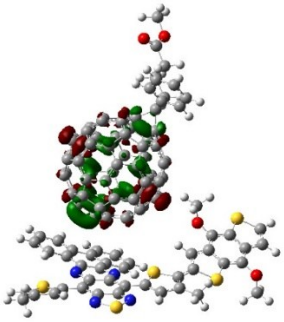

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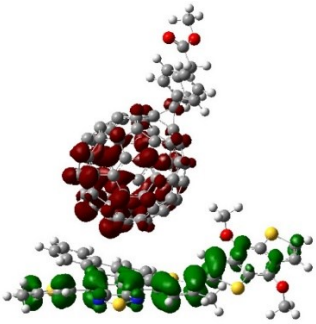

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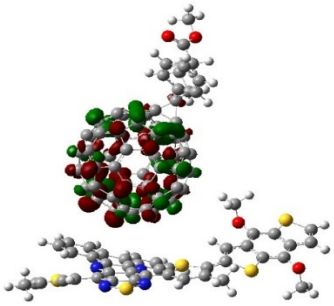

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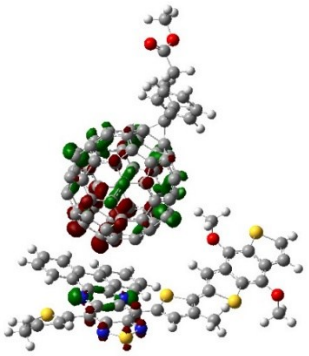

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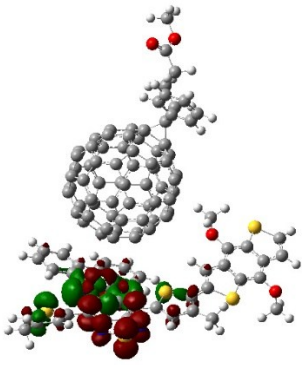

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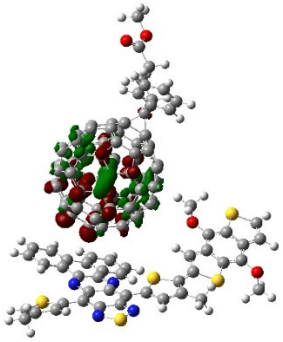

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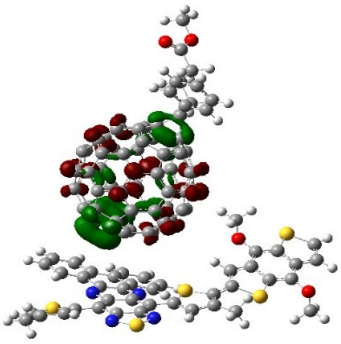

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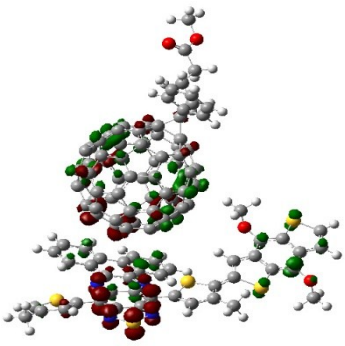

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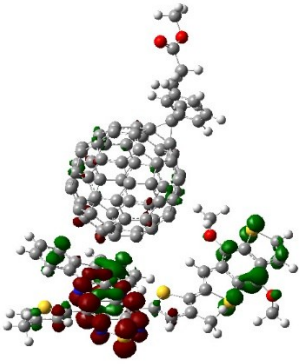

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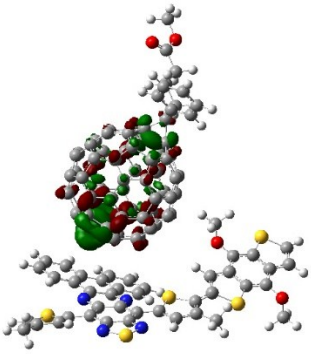

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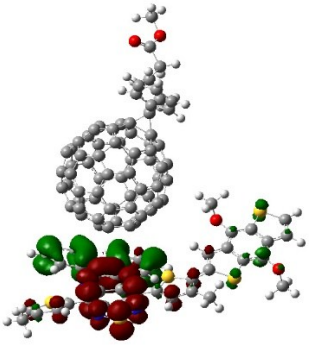

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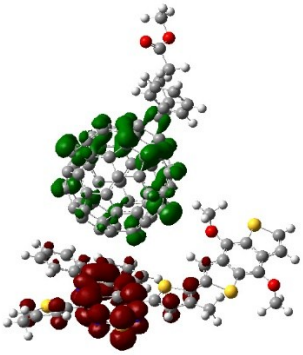

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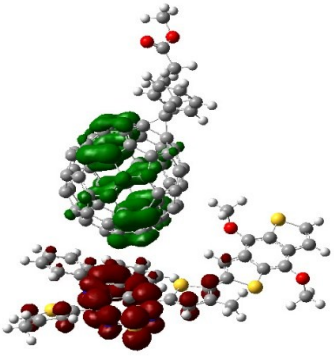

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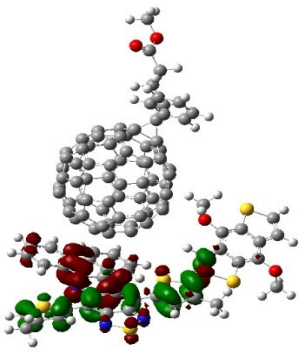

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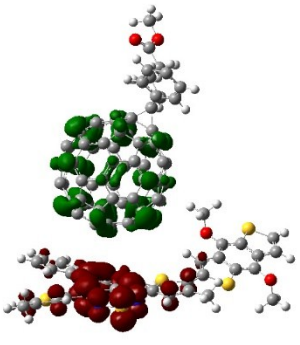

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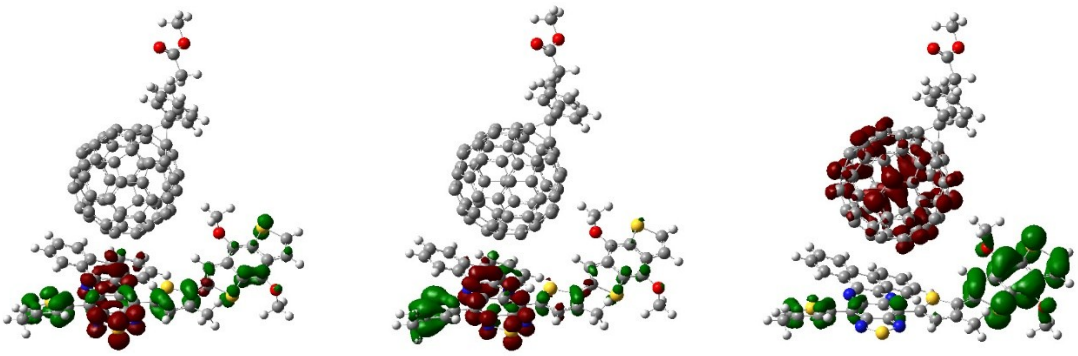
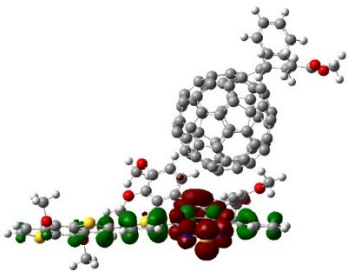


S28 S29 S30

Figure S4. Charge difference density (CDD) of $PC_{60}BM$/Pz, where the green and red stand for the hole and electron, respectively.



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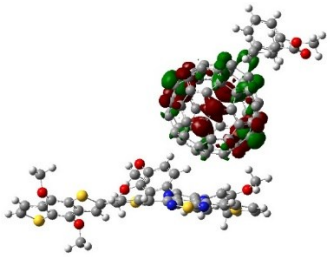

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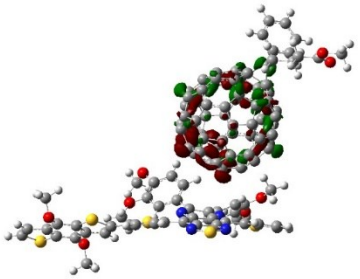

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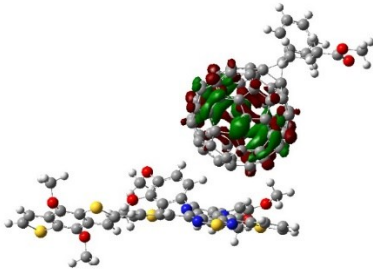

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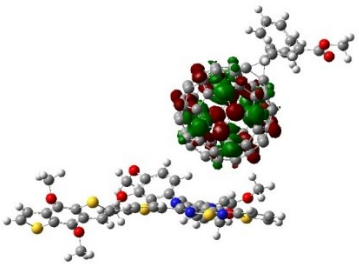

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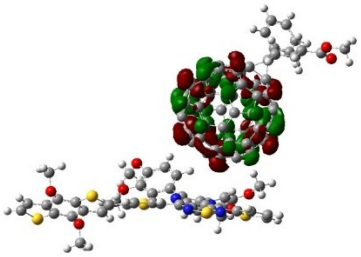

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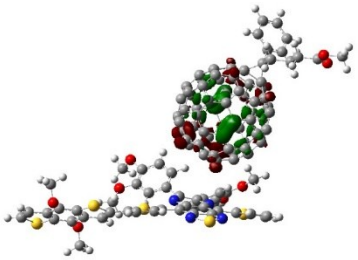

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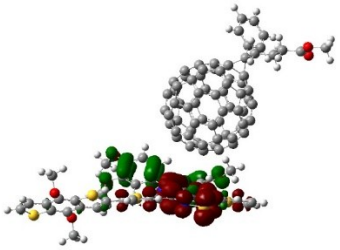

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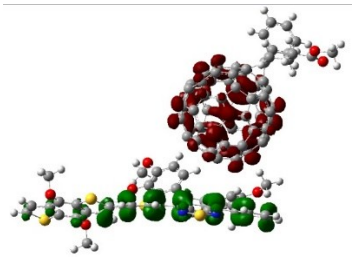

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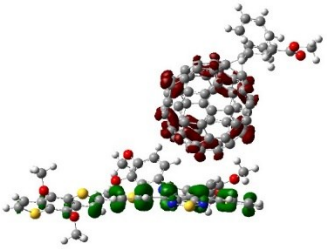

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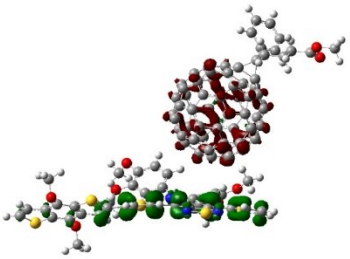

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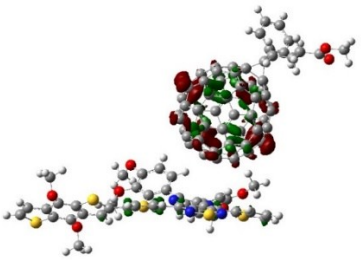

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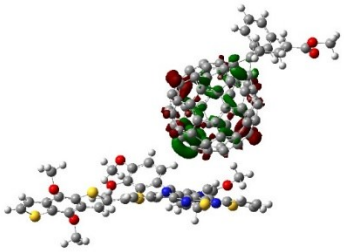

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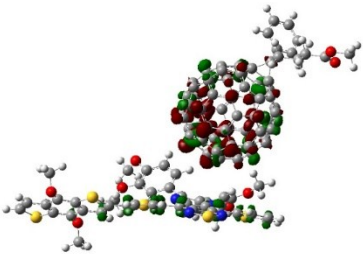

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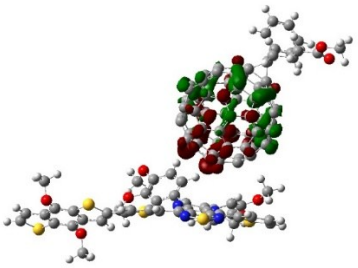

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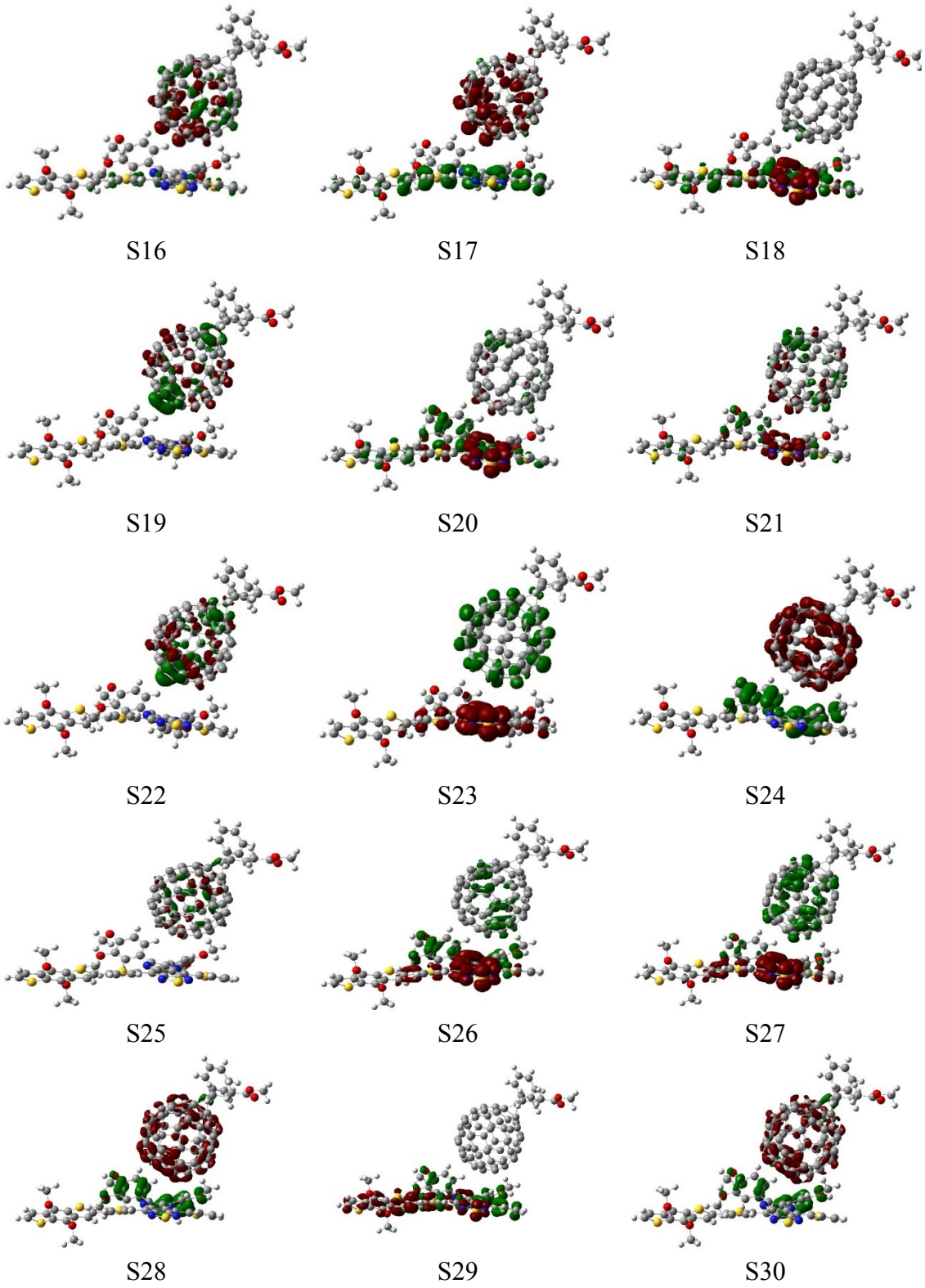
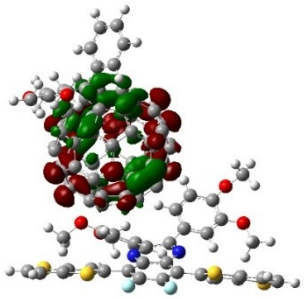


Figure S5. Charge difference density (CDD) of $PC_{60}BM$/Qx, where the green and red stand for the hole and electron, respectively.



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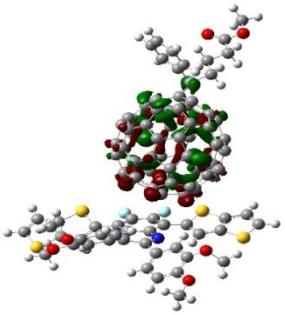

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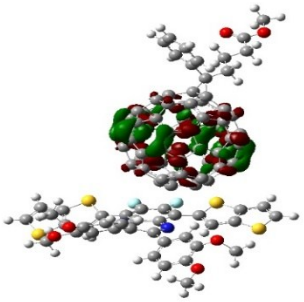

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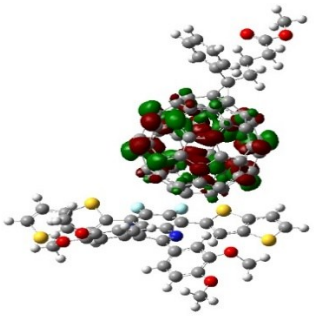

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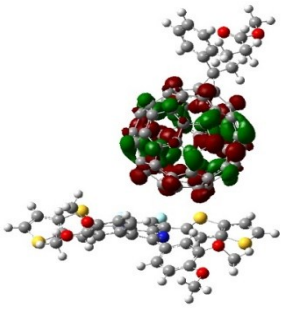

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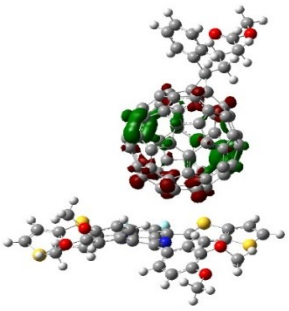

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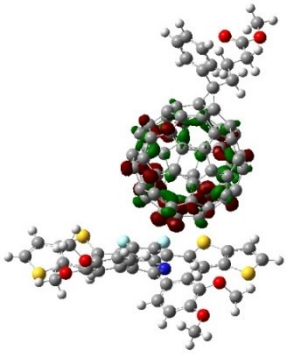

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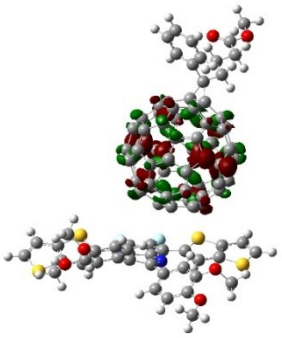

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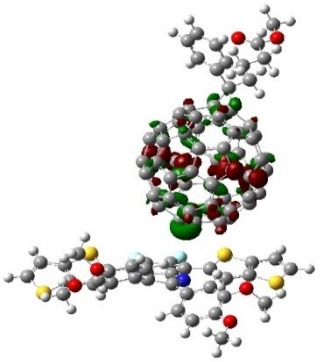

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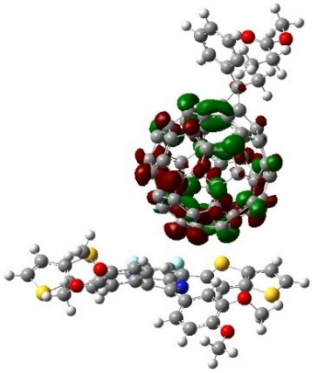

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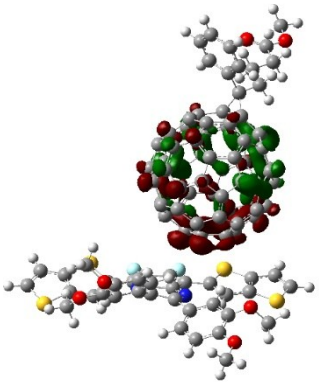

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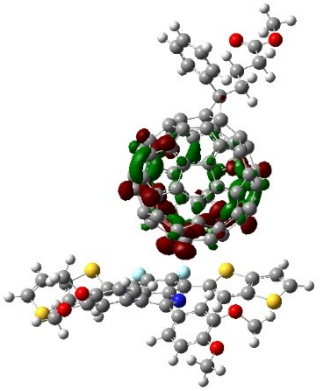

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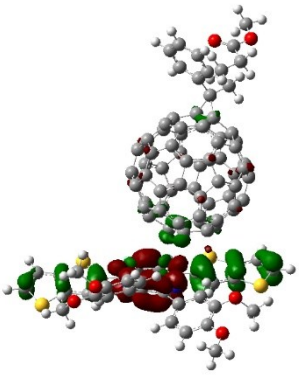

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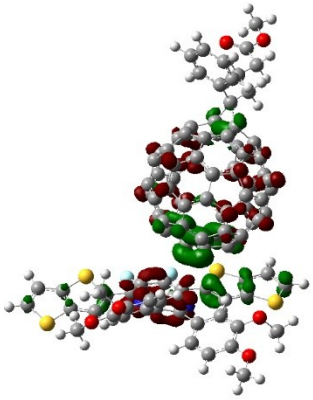

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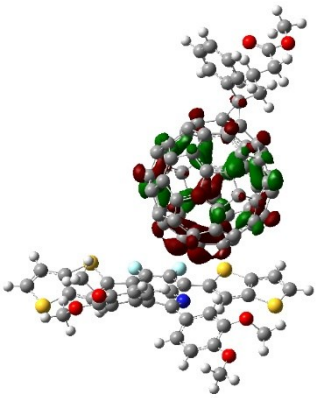

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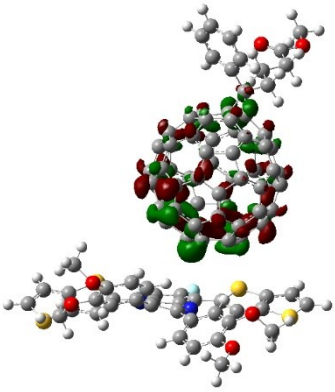

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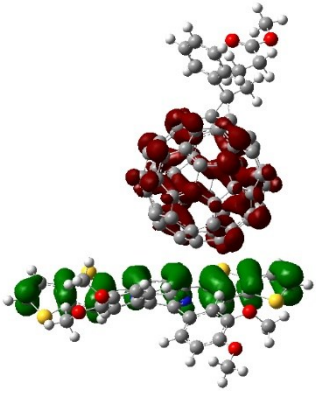

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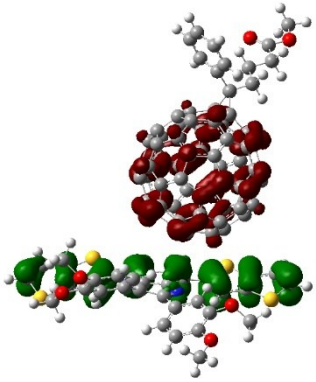

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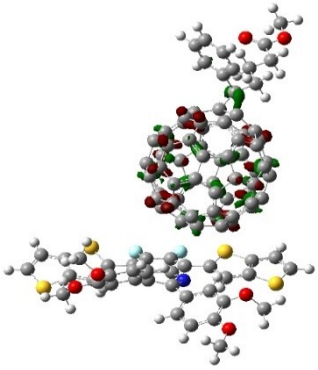

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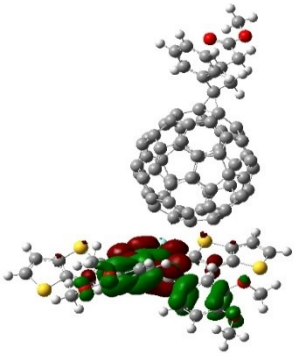

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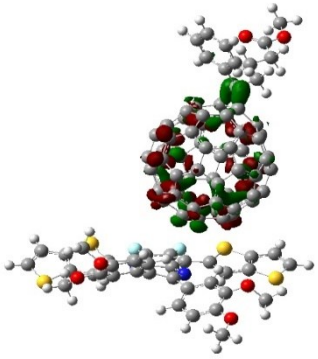

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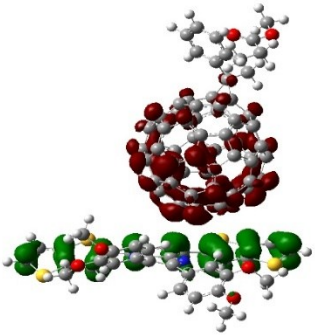

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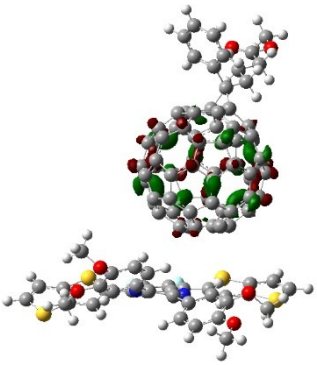

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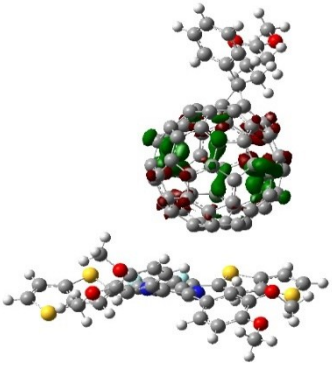

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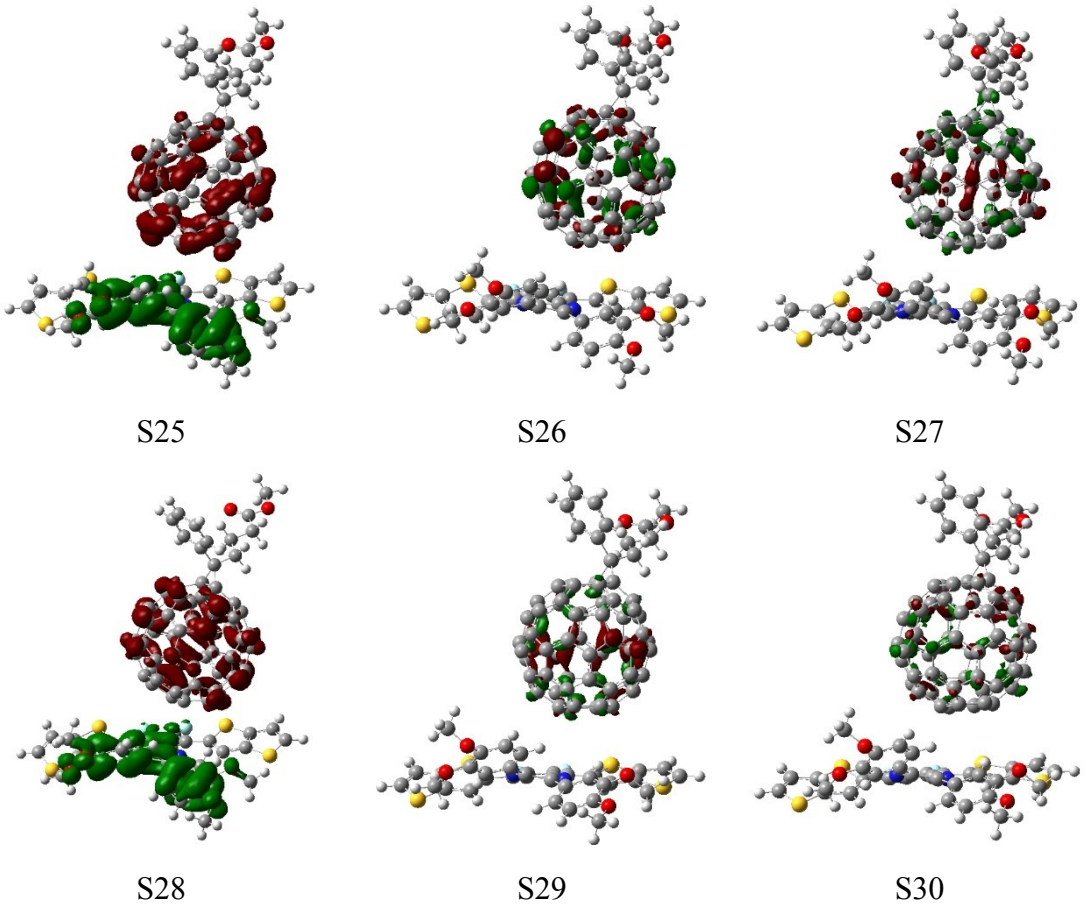
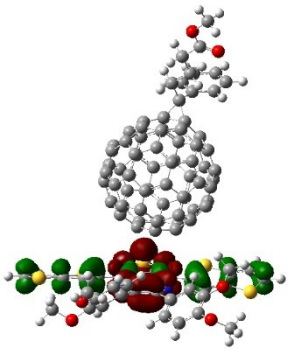


Figure S6. Charge difference density (CDD) of $PC_{60}BM$/D1, where the green and red stand for the hole and electron, respectively.



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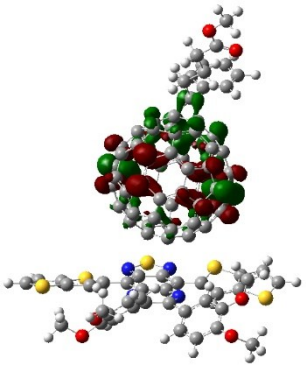

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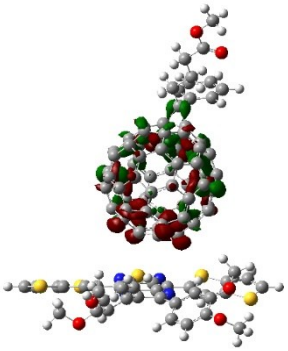

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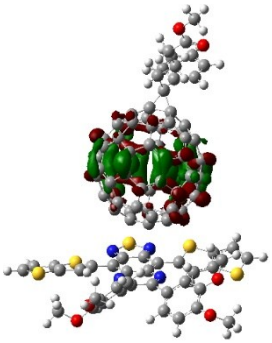

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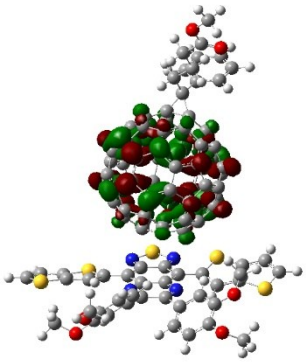

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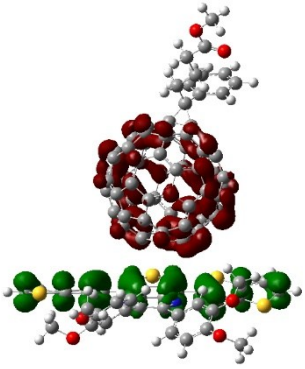

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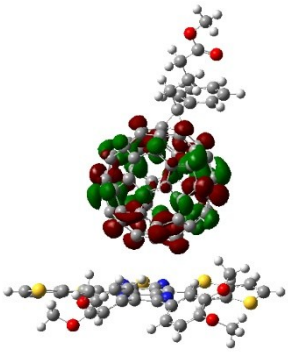

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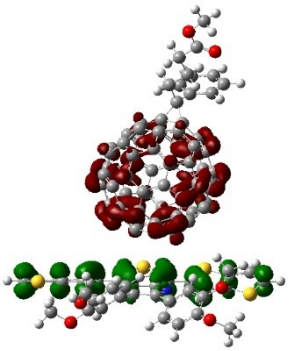

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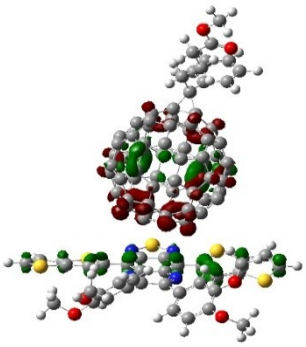

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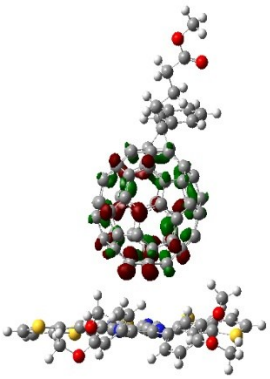

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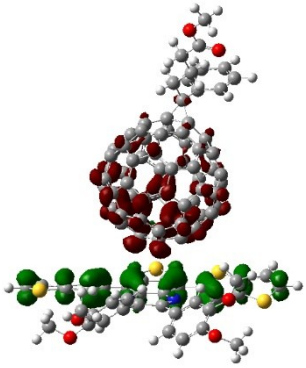

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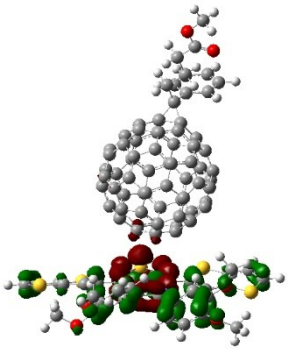

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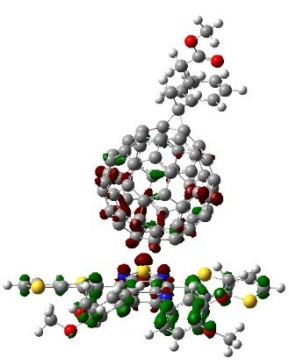

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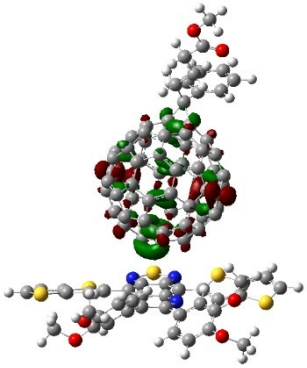

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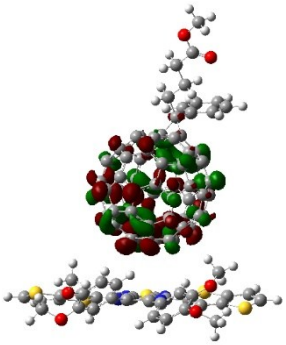

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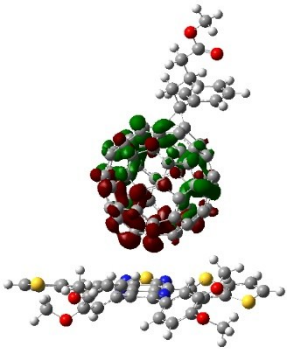

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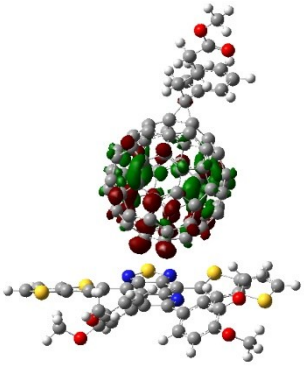

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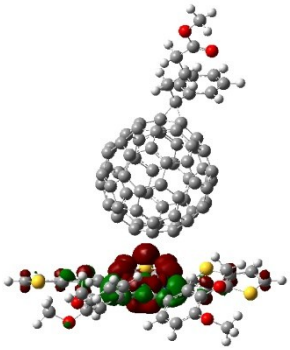

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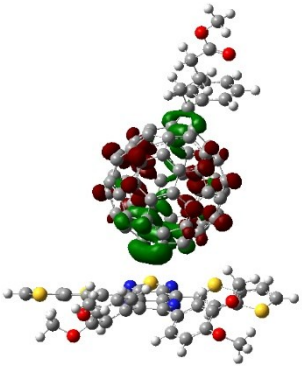

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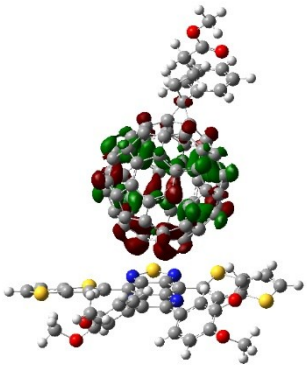

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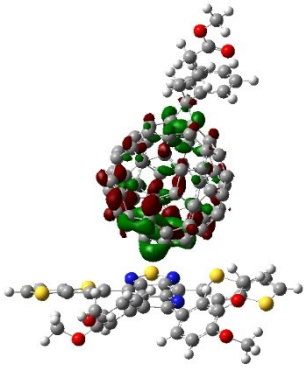

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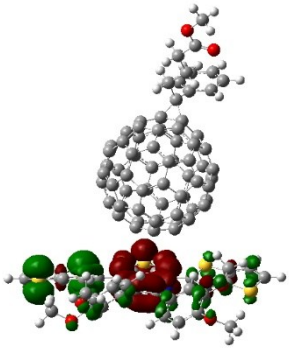

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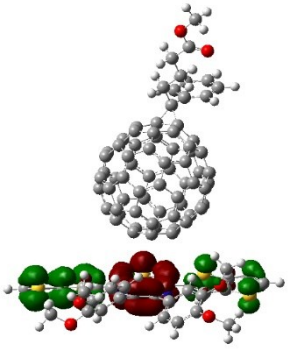

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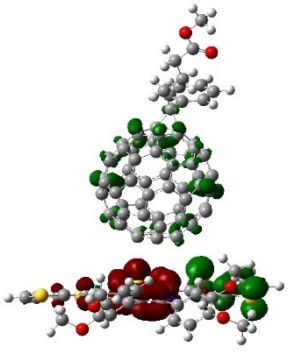

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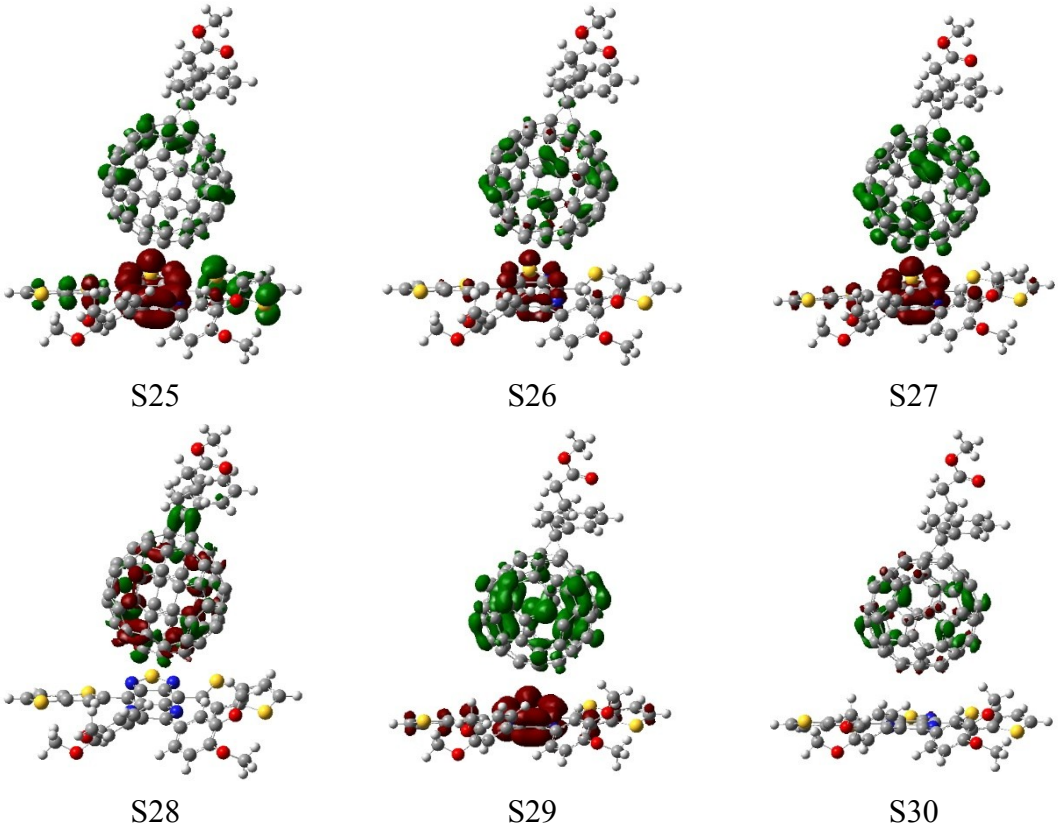
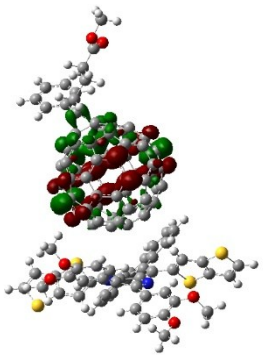


Figure S7. Charge difference density (CDD) of $PC_{60}BM$/D2, where the green and red stand for the hole and electron, respectively.



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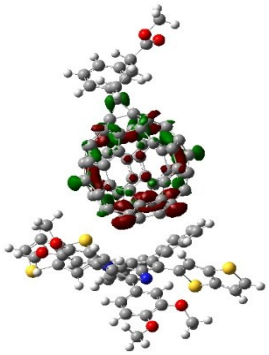

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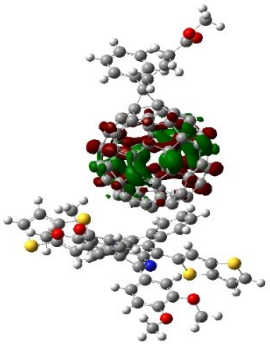

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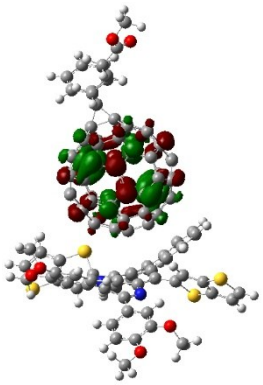

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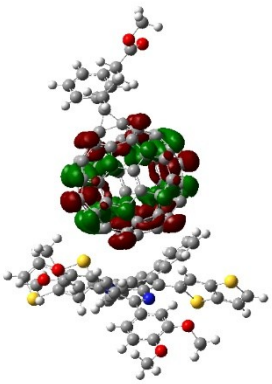

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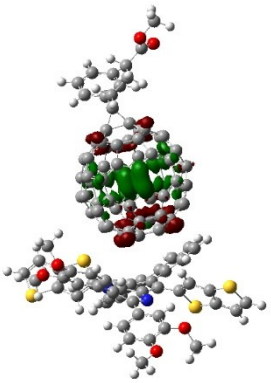

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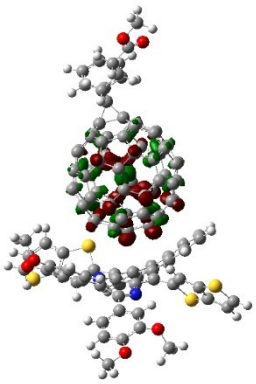

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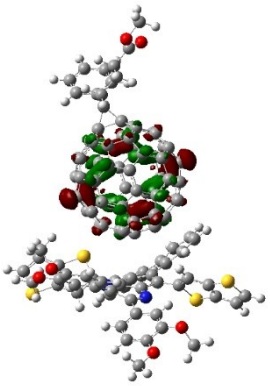

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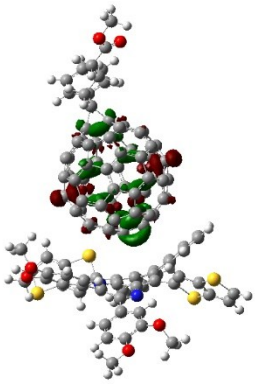

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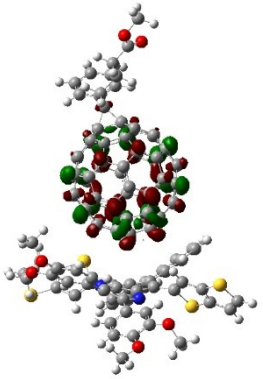

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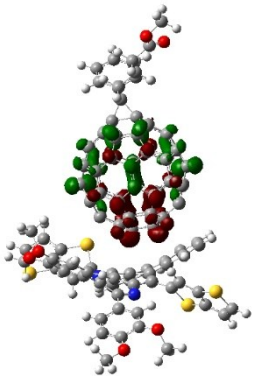

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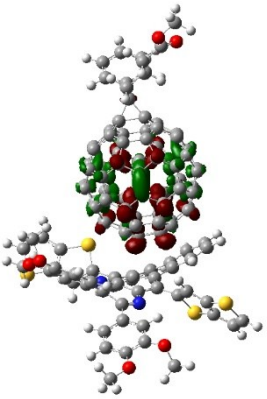

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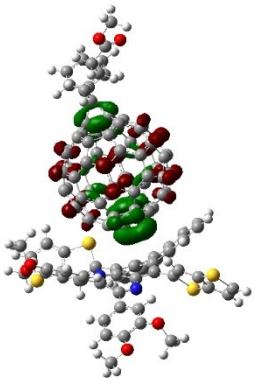

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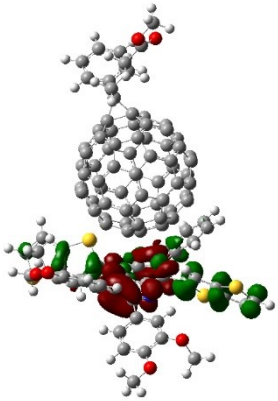

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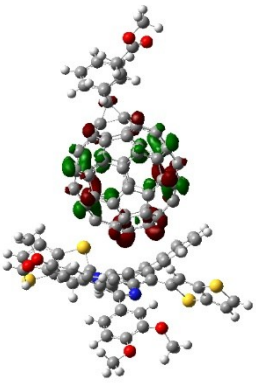

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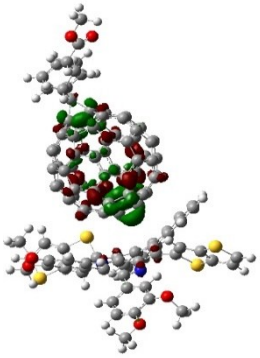
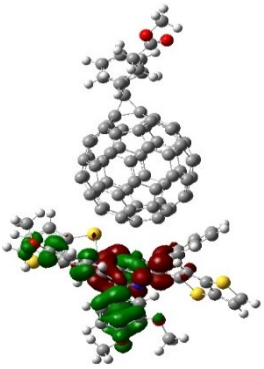


S16



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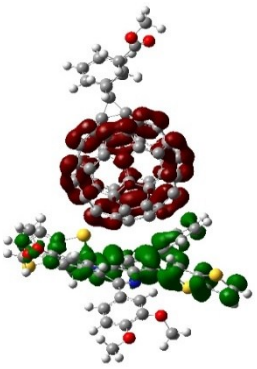

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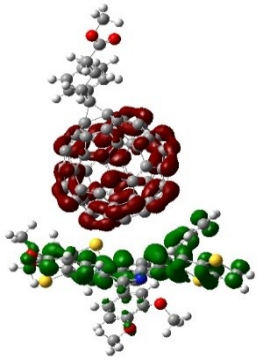

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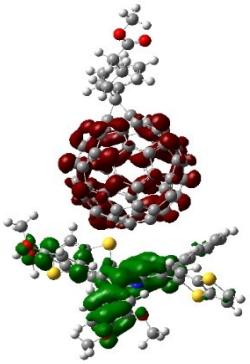

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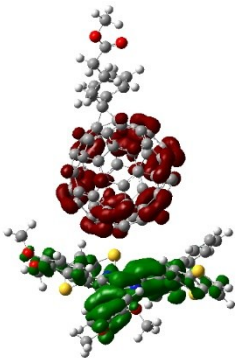

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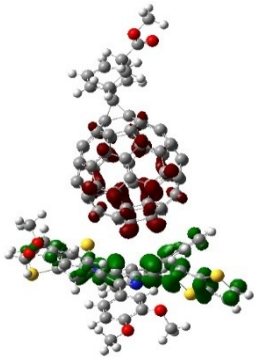

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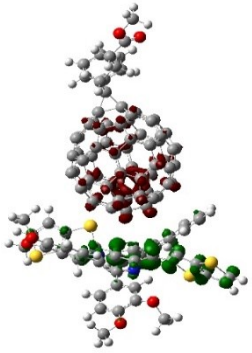

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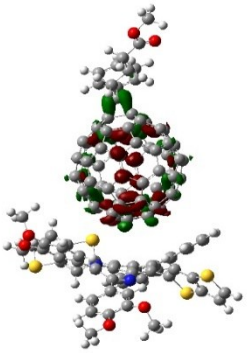

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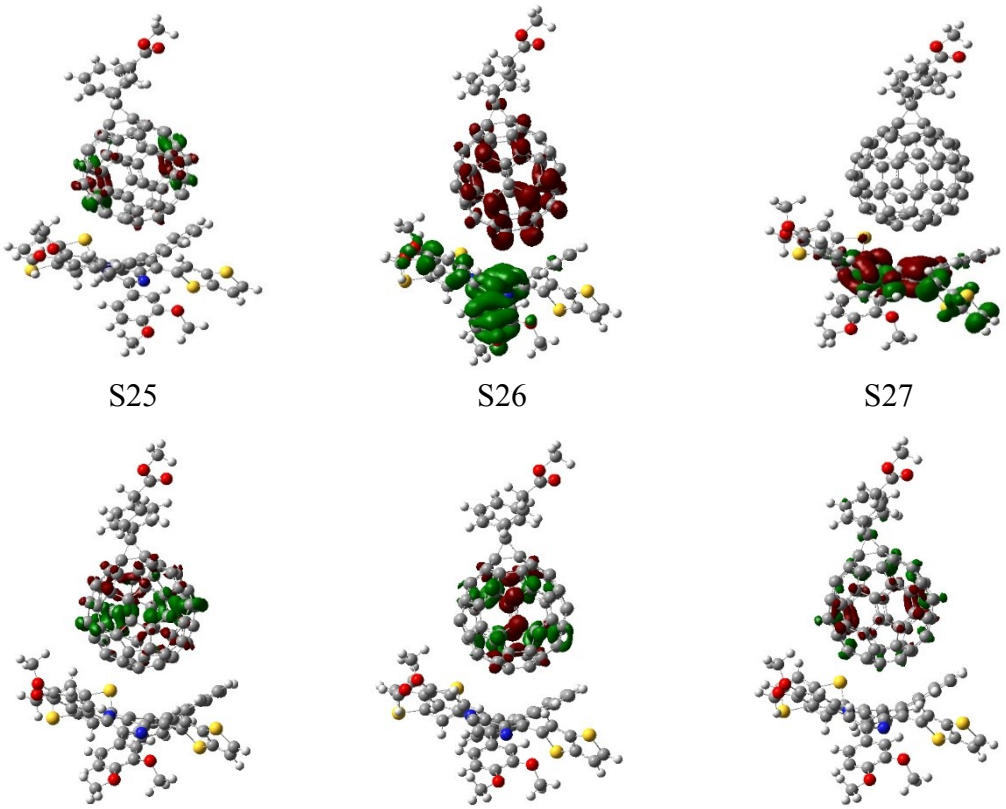

Figure S8. Charge difference density (CDD) of $PC_{60}BM$/D3, where the green and red stand for the hole and electron, respectively.