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亚甲基富勒烯衍生物[6,6]-苯基-C_{61}丁酸甲酯的密度泛函研究

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DFT Study on Methanofullerene Derivative [6,6]-Phenyl-C_{61} Butyric Acid Methyl Ester

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Table s1 Computed excitation energies (eV), electronic transition configurations and oscillator strengths (*f*) for the optical transitions with *f*>0.001 of the absorption band in the visible region and near-UV region for PCBM in $CHCl_3$

State	|CI Coeff.| > 0.2 (corresponding transition orbitals)[a]	excitation energy ($eV \cdot nm^{-1}$)	*f*
1	0.69(231 → 232)	2.07/599	0.0030
2	0.67(231 → 233)	2.15/577	0.0000
3	0.68(230 → 232)	2.23/555	0.0000
4	0.66(229 → 232)	2.26/548	0.0000
5	0.55(228 → 233); −0.41(230 → 233)	2.33/532	0.0000
6	0.50(229 → 233); −0.40(231 → 234); 0.26(227 → 232)	2.34/529	0.0012
7	0.63(228 → 232); 0.28(229 → 234)	2.38/520	0.0000
8	0.52(230 → 233); 0.42(228 → 233)	2.43/509	0.0004
9	0.54(231 → 234); 0.40(229 → 233)	2.49/499	0.0034
10	0.65(227 → 233)	2.52/492	0.0001
11	0.63(229 → 234); −0.21(228 → 232)	2.56/483	0.0000
12	0.55(228 → 234); 0.39(230 → 234)	2.57/482	0.0027
13	0.64(227 → 232)	2.60/477	0.0004
14	0.49(230 → 234); −0.37(228 → 234); −0.25(227 → 233)	2.67/464	0.0021
15	0.68(227 → 234)	2.78/446	0.0084
16	0.67(226 → 232); 0.22(226 → 233)	3.07/403	0.0114
17	0.66(226 → 233); −0.22(226 → 232)	3.12/397	0.0052
18	0.48(225 → 232); −0.29(224 → 232); 0.23(225 → 233)	3.14/394	0.0062
19	0.38(225 → 233); −0.36(224 → 233); 0.26(231 → 236); 0.25(224 → 232); −0.24(225 → 232)	3.17/392	0.0019
20	0.48(224 → 232); 0.42(225 → 232)	3.27/380	0.0014
21	0.65(231 → 235)	3.29/376	0.0188
22	0.53(231 → 236); −0.43(225 → 233)	3.30/376	0.0002
23	0.50(224 → 233); 0.30(225 → 233); 0.24(226 → 234); 0.24(231 → 236)	3.34/371	0.0002
24	0.45(228 → 235); −0.27(220 → 233); 0.24(224 → 234); −0.22(230 → 235); −0.22(225 → 234)	3.35/370	0.0053
25	0.63(226 → 234)	3.36/368	0.0007
26	0.33(228 → 235); −0.32(229 → 236);	3.40/364	0.0010

	0.32(231 → 237); −0.27(217 → 232)		
27	0.46(230 → 236); −0.30(228 → 236); −0.29(218 → 232)	3.41/363	0.0015
28	0.51(230 → 235); 0.35(229 → 236)	3.44/361	0.0035
29	0.50(229 → 235); −0.25(224 → 232); −0.24(228 → 236)	3.48/356	0.0134
30	0.54(225 → 234); 0.23(222 → 232)	3.49/356	0.0110
31	0.56(221 → 232); −0.28(229 → 237)	3.52/352	0.0006
32	0.46(224 → 234); −0.21(217 → 232); 0.20(225 → 234)	3.56/348	0.0029
33	0.28(224 → 234); 0.28(219 → 232); −0.27(222 → 232); 0.24(225 → 234); −0.20(222 → 233)	3.58/346	0.0007
34	0.50(227 → 235)	3.60/345	0.0042
35	0.35(228 → 236); 0.31(227 → 235); 0.29(230 → 236); 0.25(218 → 232)	3.61/344	0.0109
36	0.41(231 → 237); 0.30(229 → 236); 0.25(222 → 232)	3.64/341	0.0162
37	0.44(220 → 232); 0.26(227 → 236); 0.22(217 → 233)	3.65/340	0.0047
38	0.45(216 → 232); 0.39(218 → 233)	3.66/339	0.0023
39	0.41(217 → 232); −0.23(229 → 236); −0.22(219 → 232); 0.21(231 → 237)	3.66/338	0.0002
40	0.38(218 → 232); −0.36(228 → 236)	3.67/338	0.0180

a HOMO is No. 231 orbital.

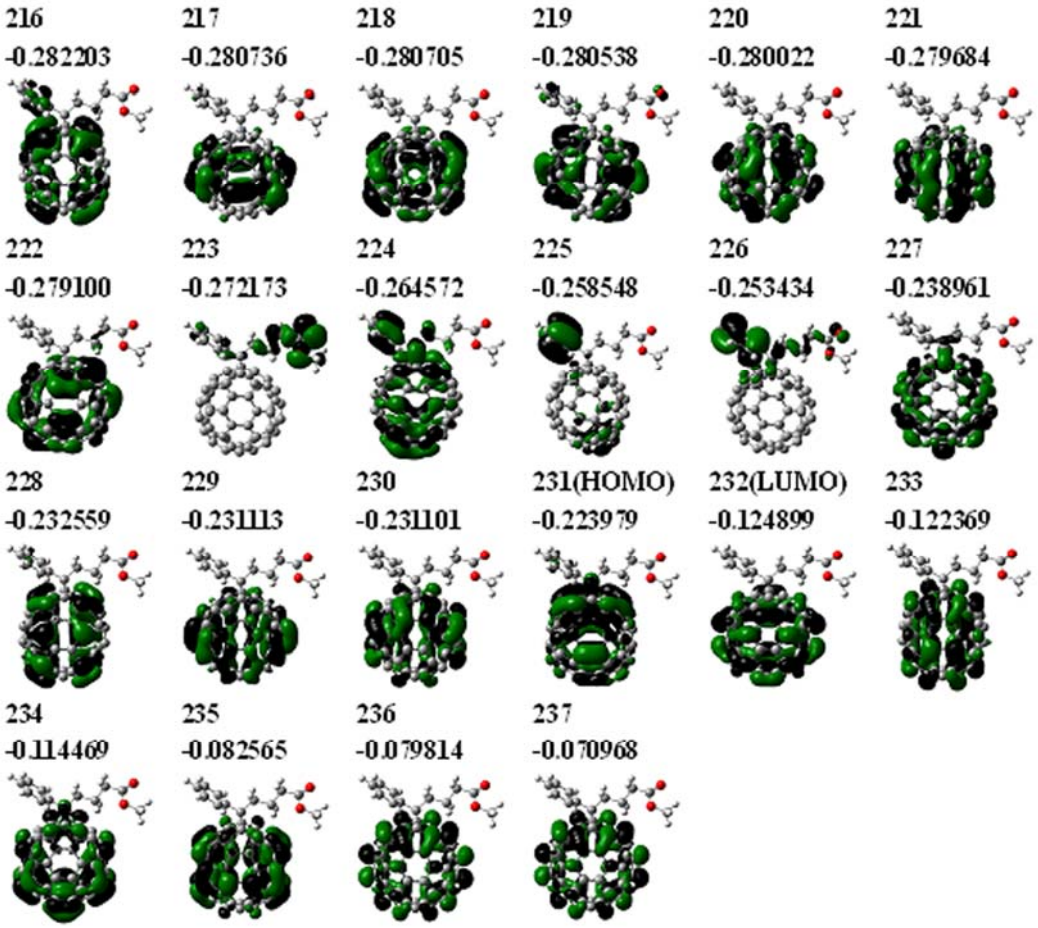

Fig. s1 Isodensity plots (isodensity contour=0.02) of the partial frontier orbital and energies (in Hartree) of PCBM in $CHCl_3$