Supporting Information

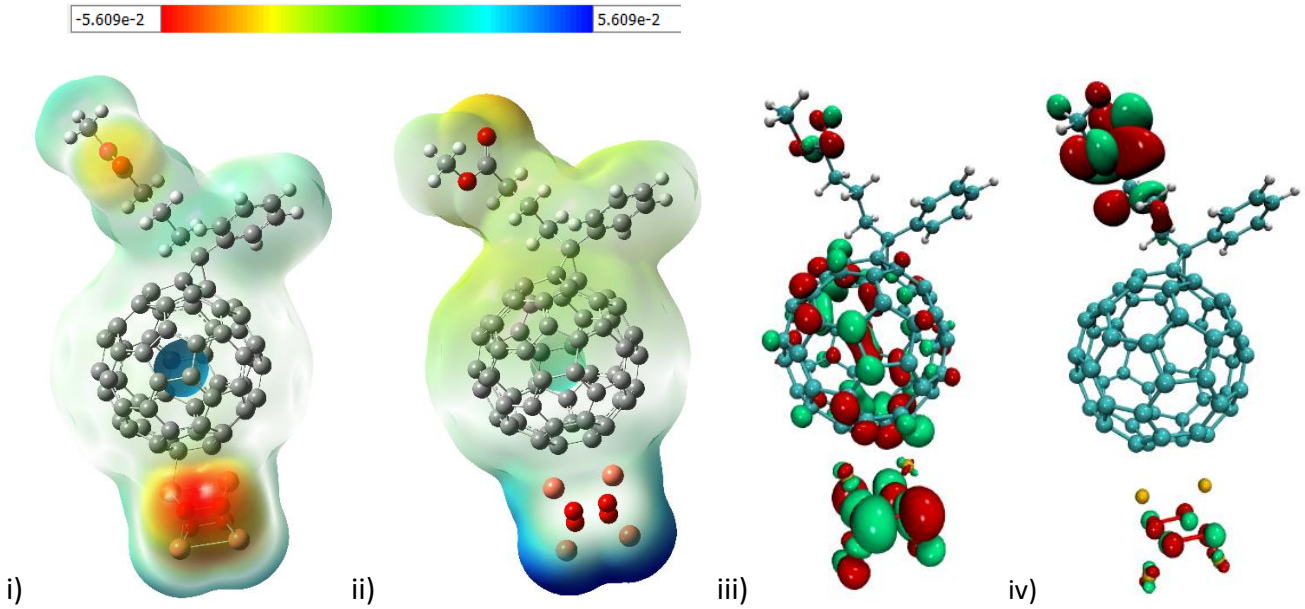

Figure 1: Electrostatic potential surface of i) PCBM-$(CuO)_4$ complex, ii) PCBM-$(CuO)_4$ + $\vec{E}_x$ and the HOMO isosurfaces of iii) PCBM-$(CuO)_4$ complex, iv) PCBM-$(CuO)_4$ + $\vec{E}_x$

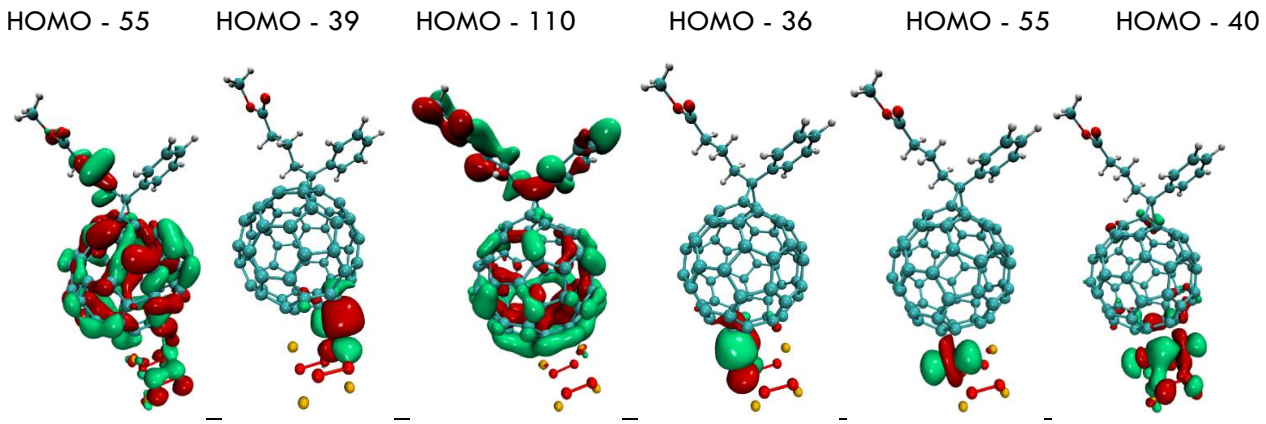

Figure 2: Isosurfaces of the orbitals involved in the chemical bond between PCBM and $(CuO)_4$ cluster**.**

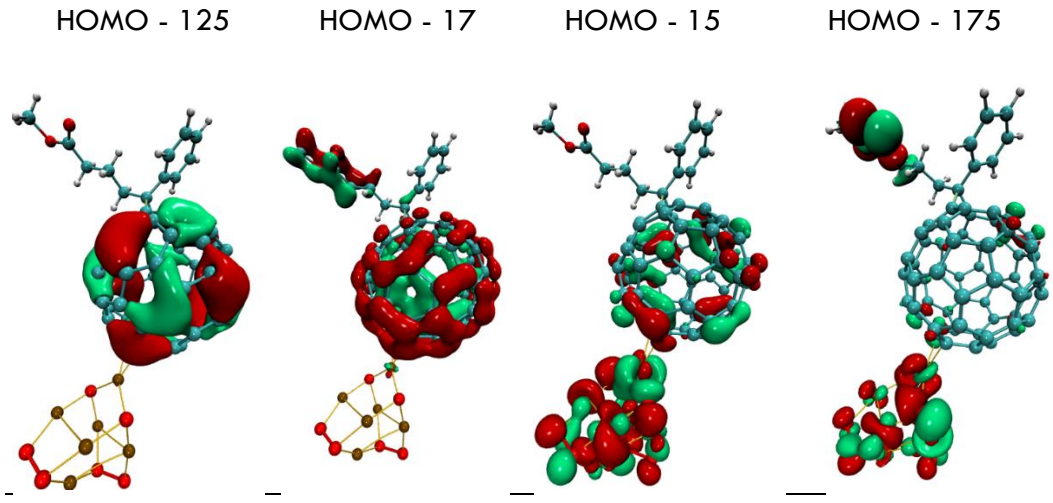

Figure 3: Isosurfaces of the orbitals involved in the chemical bond between PCBM and $(CuO)_6$ cluster**.**

Table 1: Electronic contribution from Cu atoms to the orbitals involved in BCP and RCP of PCBM-$(CuO)_4$ + $\vec{E}_x$

PCBM-$(CuO)_4$ + $\vec{E}_x$				
Critical Point	**Orbital**	**Energy Level (eV)**	**Contribution from Occupied Orbitals (%)**	**CuO contribution to each orbital (%)**
BCP1	HOMO - 27	-7.74	69	21.0
	HOMO - 35	-8.62	10	85.5
BCP-2	HOMO - 100	-13.21	66	16.7
	HOMO - 20	-7.47	13	88.6
RCP	HOMO - 27	-7.74	20	21.0
	HOMO - 30	-8.14	16	98.3
	HOMO - 31	-8.28	15	98.3
	HOMO - 100	-13.21	14	16.7

Table 2: Frequency, Raman activity, theoretical and experimental reports, and vibration types of a) PCBM, b) PCBM-$(CuO)_4$, c) PCBM-$(CuO)_4$+$\vec{E}_x$, d) PCBM-$(CuO)_6$

i) **PCBM**				
Frequency (Cm^{-1})	**Raman Activity (A4/Uma)**	**Theoretical (cm^{-1})** Vincenzo Schettino et al.	**Experimental (cm^{-1})** Kusmany et al.	**Vibration Type**
255.17	19.3864	261	273	Hg(1)
476.15	91.2743	487	498	Ag(1)
525.43	42.2190	577	----------	T1u(2)
862.66	25.9641	----------	----------	C-C-O Symmetrical stretching mode of the butyric acid group
1018.56	69.4882	----------	----------	C-C ring Symmetrical bending (phenyl group)
1105.77	15.4876	1100	1101	Hg(5)
1272.91	28.3103	1307	1310	Gu(5)
1331.55	51.4342	1308	1356	Gg(5)
1417.19	130.6115	----------	----------	C-C (bond C60-PBM) Symmetrical stretching mode
1523.31	724.7829	1467	1470	Ag(2)
1609.95	116.7676	1585	1574	Hg(8)
1654.12	68.6890	----------	----------	C-C ring symmetrical stretching (phenyl group)
ii) **PCBM-$(CuO)_4$**				
Frequency (Cm^{-1})	**Raman Activity (A4/Uma)**	**Theoretical (cm^{-1})** Vincenzo Schettino	**Experimental (cm^{-1})** Kusmany et al (41)	**Vibration Type**
447.99	86.1809	429	433	Hg(2)
724.48	485.6496	751	924	Gu(3)
754.28	950.9702	789	----------	T2g(3)
1094.42	147.0639	1100	1101	Hg(5)
1277.02	204.3552	1246	1251	Hg(6)
1403.56	2115.1874	1344	----------	T2g(4)
1467.52	630.8999	1434	1446	Gu(6)
1514.20	2941.4702	1462	1470	Ag(2)
1600.24	1533.0451	1585	1574	Hg(8)
iii) **PCBM-$(CuO)_4$ (Field)**				
Frequency (Cm^{-1})	**Raman Activity (A4/Uma)**	**Theoretical (cm^{-1})**	**Experimental (cm^{-1})**	**Vibration Type**

		Vincenzo Schettino (49)	Kusmany et al (48)	
144.95	178.0735	----------	----------	Butyric acid group torsional vibration mode
420.11	203.4326	429	433	Hg(2)
688.34	502.8613	705	711	Hg(3)
810.35	549.6100	962	924	Gu(4)
1083.29	836.9041	1099	1101	Hg(5)
1237.06	380.7367	1246	1251	Hg(6)
1366.53	979.4355	1343	1385	Hu(6)
1386.79	1089.3472	1344	----------	T2g(4)
1412.29	1584.4950	1426	1427	Hg(7)
1505.63	287.2294	1462	1470	Ag(2)
1572.12	523.2173	1576	1559	Hu(7)
iv) **PCBM-$(CuO)_6$**				
318.58	316.6434	----------	----------	O-Cu-O Symmetrical stretching mode
400.58	2069.9573	----------	----------	O-Cu-O Symmetrical stretching mode
469.14	1716.9873	----------	----------	O-Cu-O Symmetrical stretching mode
546.03	646.4512	527	----------	T1u(1)
596.71	7028.5128			Cu-O-Cu Symmetrical stretching mode
721.01	750.1502	705	711	Hg(3)
809.58	2706.7227	----------	----------	O-Cu-O Bending mode
1420.62	4152.4486	1344	----------	T2g(4)
1466.33	1598.4275	1434	1446	Gg(6)
1515.91	5305.6382	1462	1470	Ag(2)
1591.32	2519.2458	1576	1559	Hu(7)
1610.08	1586.2477	1585	1574	Hg(8)