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Addition/Correction

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Correction to "Inapplicability of Electron-Hopping Models for the Organic Semiconductor Phenyl-C61-butyric Acid Methyl Ester (PCBM)"

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Supporting Information

Electronic coupling matrix elements (H_{ab}) reported in Tables 1 and 2 in the main text were not correctly calculated. In addition, the numerical values for the rates reported in Tables 1, 2, and S2 (Supporting Information) (k_{ET}) need to be multiplied by a factor of 2π. The tables with the correct electronic coupling values are given below. We also provide corrected versions of Figures 2 and 3, where coupling values were graphically illustrated. The correct electronic coupling values span a somewhat smaller range (73.9 to <0.1 meV) than originally reported (151 to <0.1 meV). This does not change any of the conclusions of the Letter. In the following, we summarize corrections to the original text in bold font.

Table 1. Electron-Transfer Parameter for Triclinic PCBM in the Minimum Energy Structure

ET direction	R (Å)	H_{ab} (meV)	λ (meV)	$\Delta E^{\ddagger}_{ad}$ (meV)	k_{ET} (Hz)
$[1\bar{1}1]^2_4$	9.87	15.2	137	21	3.03×10^{12}
$[010]^1_2$	9.88	48.4	138	1	1.39×10^{13}
$[0\bar{1}0]^3_4$	9.88	48.4	138	1	1.39×10^{13}
$[010]^1_3$	9.91	2.7	138	31	9.50×10^{10}
$[000]^1_3$	9.92	49.0	138	1	1.41×10^{13}
$[\bar{1}10]^1_2$	9.95	12.9	138	22	2.25×10^{12}
$[1\bar{1}0]^3_4$	9.95	12.9	138	22	2.25×10^{12}
$[000]^4_1$	10.00	50.0	138	1	1.43×10^{13}
$[000]^3_2$	10.00	50.0	138	1	1.43×10^{13}
$[01\bar{1}]^4_2$	10.08	16.8	138	20	3.57×10^{12}
$[000]^2_1$	10.11	40.0	138	5	1.15×10^{13}
$[000]^4_3$	10.11	40.0	138	5	1.15×10^{13}
$[\bar{1}\bar{1}1]^4_1$	10.18	5.1	138	30	3.50×10^{11}
$[00\bar{1}]^3_2$	10.18	5.1	138	30	3.50×10^{11}
$[100]^2_1$	13.20	0.2	146	36	4.31×10^{8}
$[100]^3_4$	13.20	0.2	146	36	4.31×10^{8}
$[100]^1_4$	13.42	0.5	146	36	2.71×10^{9}
$[100]^3_2$	13.42	0.5	146	36	2.71×10^{9}
$[\bar{1}10]^4_2$	13.68	5.8	147	31	4.11×10^{11}
$[100]^1_1$	13.83	0.3	147	36	9.60×10^{8}
$[100]^2_2$	13.83	0.3	147	36	9.60×10^{8}
$[100]^3_3$	13.83	0.0	147	37	$<1.06 \times 10^{8}$
$[100]^4_4$	13.83	0.0	147	37	$<1.06 \times 10^{8}$
$[00\bar{1}]^3_1$	14.19	1.6	148	35	2.83×10^{10}
$[00\bar{1}]^4_2$	14.51	0.1	148	37	1.04×10^{8}
$[1\bar{1}0]^3_1$	14.53	0.1	148	37	1.04×10^{8}

Table 2. Electron-Transfer Parameter for Monoclinic PCBM in the Minimum Energy Structure

ET direction	R (Å)	H_{ab} (meV)	λ (meV)	$\Delta E^{\ddagger}_{ad}$ (meV)	k_{ET} (Hz)
$[010]^4_1$	9.99	3.8	138	31	1.92×10^{11}
$[010]^3_2$	9.99	3.8	138	31	1.92×10^{11}
$[010]^3_1$	10.10	28.7	138	12	7.91×10^{12}
$[011]^2_1$	10.18	14.0	139	22	2.59×10^{12}
$[000]^1_2$	10.18	14.0	139	22	2.59×10^{12}
$[00\bar{1}]^4_2$	10.22	31.1	139	10	8.71×10^{12}
$[100]^2_3$	12.97	1.0	145	35	1.11×10^{10}
$[000]^1_4$	12.97	1.0	145	35	1.11×10^{10}
$[00\bar{1}]^4_3$	13.15	1.5	146	35	2.54×10^{10}
$[010]^3_4$	13.15	1.5	146	35	2.54×10^{10}
$[010]^2_2$	13.76	0.0	147	37	$<1.06 \times 10^{8}$
$[010]^4_4$	13.76	0.0	147	37	$<1.06 \times 10^{8}$

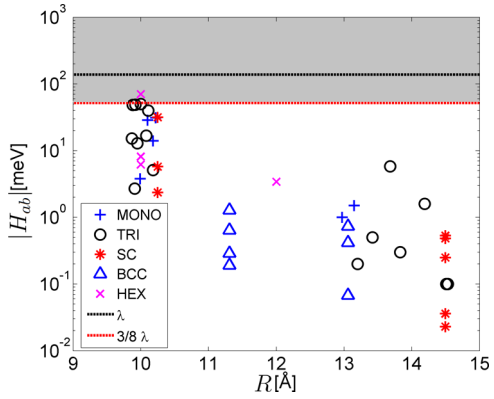

Figure 2. Electronic coupling matrix element (H_{ab}) as a function of the distance (R) between the centers of mass of two PCBM molecules. Each data point corresponds to a unique electron transfer direction in the tc, mc, sc, bcc, and hex crystals. The reorganization energy (λ) is shown in black lines and the coupling value $H_{ab} = (3/8)\lambda$, for which the activation energy for electron transfer vanishes ($\Delta E^{\ddagger}_{ad} = 0$), in red lines.

- On page 1014, the last sentence of the first paragraph should read "Overall, the data for H_{ab} span **four** orders of magnitude, ranging from **73.9 meV for the [100] direction in the hex structure** (R = 10 Å) to **<0.1 meV** for the [$\bar{1}$10] direction in the sc structure (R = 14.5 Å)".

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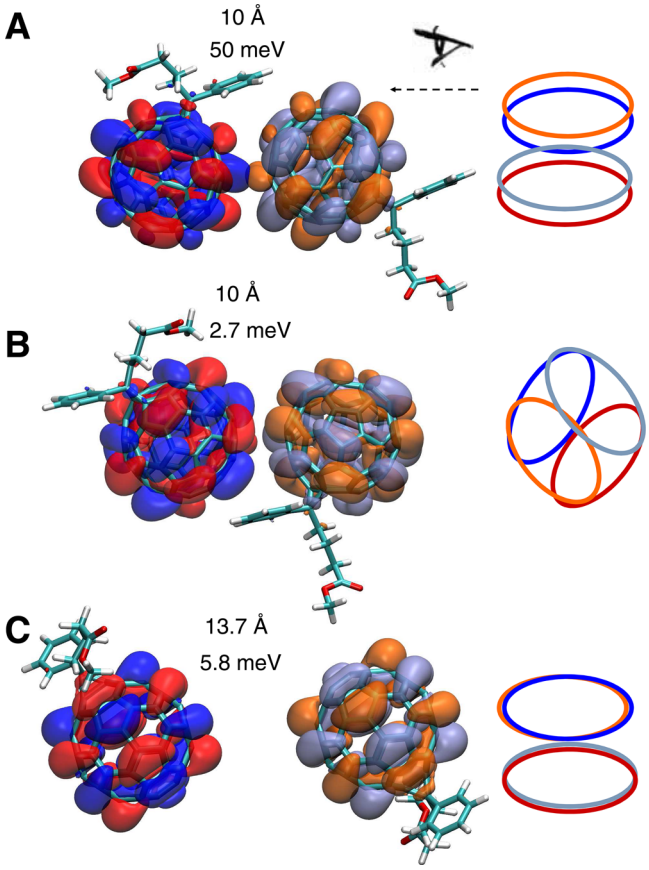

Figure 3. Interpretation of electronic coupling values by consideration of orbital symmetry. The isosurfaces for the SOMO of the $PCBM^-$ donor molecule are shown in red/blue and the ones for the acceptor molecule in orange/silver. The symmetry of the lobes of the orbitals where the interaction is the greatest, that is, between donor and acceptor, is indicated in the panel to the right. The distance between the centers of mass of the PCBM donor and acceptor molecules and the corresponding electronic coupling values are indicated for each pair.

- On page 1014, the third sentence of the second paragraph should read "In the configurations shown in panels A and B of Figure 3, H_{ab} takes values of **50 and 2.7 meV** although the donor−acceptor distance is the same, R = 10 Å."
- On page 1014, the third to last sentence of the second paragraph should read "Consequently, the overlap is destructive and H_{ab} drops by about a factor of **∼20**."
- On page 1015, the fourth and fifth sentences of the second paragraph should read "Importantly, we find that in the **hex structure** there is at least one direction where the activation energy is negative. Similarly, also in the **tc**, mc, and sc structures there exist directions where the activation energy almost vanishes."

■ ASSOCIATED CONTENT

Supporting Information

Supporting results (computational methods, electronic level structure of C_{60} and PCBM, Figure S1, and Tables S1−S2). This material is available free of charge via the Internet at http://pubs.acs.org.

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