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CORRECTION

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Correction: Towards predicting the power conversion efficiencies of organic solar cells from donor and acceptor molecule structures

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Correction for 'Towards predicting the power conversion efficiencies of organic solar cells from donor and acceptor molecule structures' by Yecheng Zhou *et al.*, *J. Mater. Chem. C*, 2018, **6**, 3276–3287.

There are errors in the equations on page 3279 of the article, under the heading '2.4 DOS determination.' The correct equations and related text are below.

DOSs are essential for the numerical simulations of CT in solar cells. However, we haven't found a theoretical method to estimate them for OSCs without any empirical or experimental parameters. Here, we put forward a method to estimate the DOS in OSCs. We assumed that each orbital can be occupied by two electrons, then DOS(E) can be calculated by $\mathrm{DOS}(E) = \sum_{\mathrm{LUMO}(E)} 2$, which is the summation over all LUMOs whose energies are E. The DOS(E) should be Gaussian-like due to the Gaussian distribution of LUMOs. Assuming the charge occupation in the semiconductor obeys the Fermi–Dirac distribution, then, the charge density of the OSCs is given by:

$$\begin{aligned} n &= \int_{E_f}^{\infty} \mathrm{DOS}(E) \frac{1}{1+\exp\left(\frac{E-E_f}{k_B T}\right)} \mathrm{d}E \\ &= \sum_{\mathrm{LUMO}(E)} 2 \times \frac{1}{1+\exp\left(\frac{E-E_f}{k_B T}\right)} \\ &\simeq \sum_{\mathrm{LUMO}(E)} 2 \times \exp\left(\frac{E-E_f}{-k_B T}\right) \\ &= \sum_{\mathrm{LUMO}(E)} 2 \times \exp\left(\frac{E-E_c}{-k_B T}\right) \times \exp\left(\frac{E_c-E_f}{-k_B T}\right) \\ &= N_c \times \exp\left(\frac{E_c-E_f}{-k_B T}\right) \end{aligned} \tag{8}$$

where E_c and E_f are the conduction band minimum (the LUMO energy level of $PC_{71}BM$) and the Fermi energy level, respectively. Since only LUMOs can be filled, $E - E_f$ is in the order of 0.1 eV which is several times higher than k_BT. The exponential term in Fermi–Dirac distribution

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is much larger than 1, then $\frac{1}{1+\exp\left(\frac{E-E_f}{kT}\right)} \simeq \exp\left(\frac{E-E_f}{-kT}\right)$. Therefore, the DOS of the conduction band can be expressed as:

$$N_c = \sum_{\mathrm{LUMO}(E)} 2 \times \exp\left(\frac{E-E_c}{-k_B T}\right). \quad (9)$$

The changes in the equations do not affect the interpretation of the results or the conclusions. The authors apologise for this oversight and for any confusion that it may have caused.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

