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Enhancing silicon solar cells with singlet fission: the case for Förster resonant energy transfer using a quantum dot intermediate (Erratum)

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This article [*J. Photonics for Energy*, 8(2), 022008 (2018), doi: 10.1117/1.JPE.8.022008] was originally published online on 10 May 2018 with an error in the formula for the FRET efficiency (Eqs. 5 and 6). The authors neglected to include the dipole density in silicon, which lead to false units for the FRET rate. The authors have shared the Mathematica 11.3 file used for the calculations (https://github.com/HybridSolarCells/FRETQDtoSilicon), following Stavola et al.[1] and Lakowicz[2] for the dipole density.

The correction affects multiple parts of the paper, outlined in the following six points.

1. On page 2, the distance has been corrected in the following sentence.
   "We find that FRET can be efficient when the QDs are within 1.5 nm to the surface of Si, even for QDs with a bandgap close to the Si bandgap" was replaced with, "We find that FRET can be efficient when the QDs are within 3.5 nm to the surface of Si, even for QDs with a bandgap close to the Si bandgap."

2. Equation 5 was corrected as follows.
   Original:

$$k_{\mathrm{FRET}} = \frac{R_0^6}{\tau_{D,0}} \iint_{0,0}^{\infty,2\pi} \frac{r}{(R_{\mathrm{DA}}(r_{\mathrm{DA}}, r))^6} \mathrm{d}r\, \mathrm{d}\phi = \frac{R_0^6}{\tau_{D,0}} \iint_{0,0}^{\infty,2\pi} \frac{r}{\left(\sqrt{r_{\mathrm{DA}}^2 + r^2}\right)^6} \mathrm{d}r\, \mathrm{d}\phi = \frac{R_0^6}{\tau_{D,0}} * \frac{\pi}{2r_{\mathrm{DA}}^4},$$

   where $R_{\mathrm{DA}}(r_{\mathrm{DA}}, r)$ is the distance from the donor dipole to an infinitesimal acceptor dipole.
   Corrected:

$$k_{\mathrm{FRET}} = \sigma_{\mathrm{Si}} \frac{R_0^6}{\tau_{D,0}} \iint_{0,0}^{\infty,2\pi} \frac{r}{(R_{\mathrm{DA}}(r_{\mathrm{DA}}, r))^6} \mathrm{d}r\, \mathrm{d}\phi = \sigma_{\mathrm{Si}} \frac{R_0^6}{\tau_{D,0}} \iint_{0,0}^{\infty,2\pi} \frac{r}{\left(\sqrt{r_{\mathrm{DA}}^2 + r^2}\right)^6} \mathrm{d}r\, \mathrm{d}\phi = \sigma_{\mathrm{Si}} \frac{R_0^6}{\tau_{D,0}} * \frac{\pi}{2r_{\mathrm{DA}}^4},$$

   where $R_{\mathrm{DA}}(r_{\mathrm{DA}}, r)$ is the distance from the donor dipole to an infinitesimal acceptor dipole, and σ_{Si} is the density of silicon atoms on a <111> silicon surface ($\sigma_{\mathrm{Si}} = 7.8/\mathrm{nm}^2$).

3. Equation 6 and subsequent text was corrected as follows.
   Original:

$$k_{\mathrm{FRET}} = \frac{\pi R_0^6}{2\tau_{D,0}} \int_0^{-\infty} \frac{1}{(z'(z, r_{\mathrm{DA}}))^4} \mathrm{d}z = \frac{\pi R_0^6}{2\tau_{D,0}} \int_0^{-\infty} \frac{1}{\left(z\left(\frac{n_{\mathrm{Si}}}{n}\right) + r_{\mathrm{DA}}\right)^4} \mathrm{d}z = \frac{\pi R_0^6}{6\tau_{D,0}} \left(\frac{n}{n_{\mathrm{Si}}}\right) \frac{1}{r_{\mathrm{DA}}^3}.$$

   For the integration $z'(z, r_{\mathrm{DA}})$ is split into the integration variable for the half space z and the distance from the donor to the surface of the bulk acceptor r_{DA}.

Corrected:

$$k_{\mathrm{FRET}} = \rho_{\mathrm{Si}} \frac{\pi R_0^6}{2\tau_{D,0}} \int_0^{-\infty} \frac{1}{(z'(z, r_{\mathrm{DA}}))^4} \mathrm{d}z = \rho_{\mathrm{Si}} \frac{\pi R_0^6}{2\tau_{D,0}} \int_0^{-\infty} \frac{1}{\left(z\left(\frac{n_{\mathrm{Si}}}{n}\right) + r_{\mathrm{DA}}\right)^4} \mathrm{d}z$$
$$= \rho_{\mathrm{Si}} \frac{\pi R_0^6}{6\tau_{D,0}} \left(\frac{n}{n_{\mathrm{Si}}}\right) \frac{1}{r_{\mathrm{DA}}^3}.$$

For the integration $z'(z, r_{\mathrm{DA}})$ is split into the integration variable for the half space z and the distance from the donor to the surface of the bulk acceptor r_{DA}, and ρ_{Si} is the density of silicon atoms ($\rho_{\mathrm{Si}} = 50/\mathrm{nm}^3$).

4. In Section 3, the following corrections were made.

- The percentage was corrected in the following passage from the 5th paragraph.

"[. . .] the FRET efficiencies are improved considerably up to around 50% for the dipole—infinite plane model in the relevant region [. . .]"
was replaced with, " [. . .] the FRET efficiencies are improved considerably up to around 85% for the dipole—infinite plane model in the relevant region [. . .]."

- Also in the 5th paragraph of Section 3, the sentence, "This occurs due to the different distance dependencies in different models, as shown in Fig. 5," was replaced with, "This occurs due to the different distance dependencies and acceptor dipole densities (ρ_{Si} and σ_{Si}) in different models, as shown in Fig. 5."

- The following passage, from the 4th sentence of the 5th paragraph through the 7th paragraph, was corrected as follows.

Original: "In contrast to the improvement from the sixth to fourth power distance dependence, the change from fourth to third power leads to lower efficiency values for donor–acceptor distances below around 4 nm. This observation can also be made by comparing the top and bottom panel of Fig. 4. Each of the three models exhibits the highest FRET efficiency in a certain region of distances. Figure 5 illustrates the improved FRET efficiency over most of the range shown in the case of the "dipole-infinite plane model." However, at small distances, the point dipole–point dipole model shows the highest efficiencies and the "dipole—bulk model" takes over at distances beyond 5 nm, which is not shown in the figure. It is worth noting that the regions defined here have the same limits for any value of R0, which means that in the case of larger Förster distances, the bulk-model would be the dominant one. This arises because the difference between the models at short distances rDA becomes marginal for large R0 and with increasing donor–acceptor separation, the bulk-model FRET efficiency decreases the slowest.

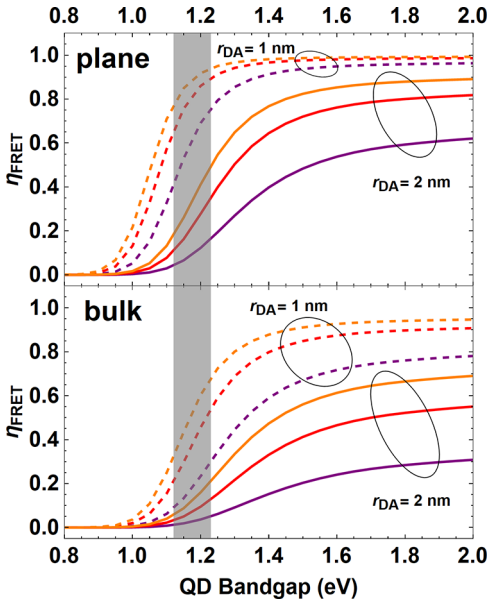
At small distances, FRET always out-competes other decay channels. For distances up to about 0.8 nm, the point-dipole model yields marginally higher efficiencies as in the plane dipole model, the fraction of dipoles at larger lateral distance outweigh the gain by the weaker D-A distance dependence. For distances between 0.8 and 4 nm, the infinite plane model yields the highest efficiency, whereas the bulk model only yields higher efficiency when the distance is very large (and overall efficiency low). This is again due to the fact that the dipoles in the bulk are on average further away from the donor, which is only compensated for at larger distances."

Corrected: "Figure 5 shows that the point model shows the steepest distance dependency, which is relaxed in the planar geometry, and the efficiency drop with distance in the bulk model is the most shallow. The efficiency is unity for small separations r_{DA} for all models and drops of to zero at 2 nm for the point model, 8 nm for the plane model, and is nonzero even for separations exceeding 10 nm for the bulk model.

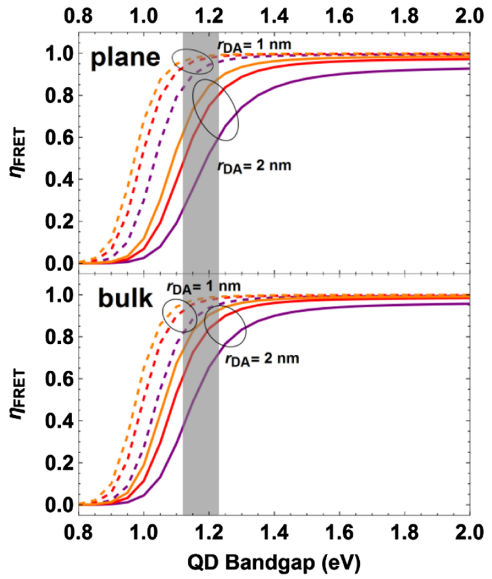
Usually the characteristic length for FRET, the distance at which the transfer efficiency is 50%, is in the order of 10 nm (QD-QD FRET of 8 nm,[13,15]) which is considerably longer than in the case of QD-silicon energy transfer which we discuss in this paper. However, the FRET distance becomes larger going from point (1.8 nm) to plane (2.5 nm) to bulk (3.5 nm) model. The slope is mainly determined by the distance dependence of the FRET rate [Eq. (1)] which changes from r^{-6} (point model) to r^{-4} (plane model) to r^{-3} (bulk model). The absolute efficiencies going from point to plane to bulk model are larger because the FRET rate is dominant compared to base rate $k_{D,0}$ [(Eq. 1)]. The underlying reason for the larger efficiencies is that there are more acceptors available in bulk (ρ_{Si}) compared to plane (σ_{Si}) and point (one acceptor) models."

5. Figure 4 was corrected as follows.

Original:

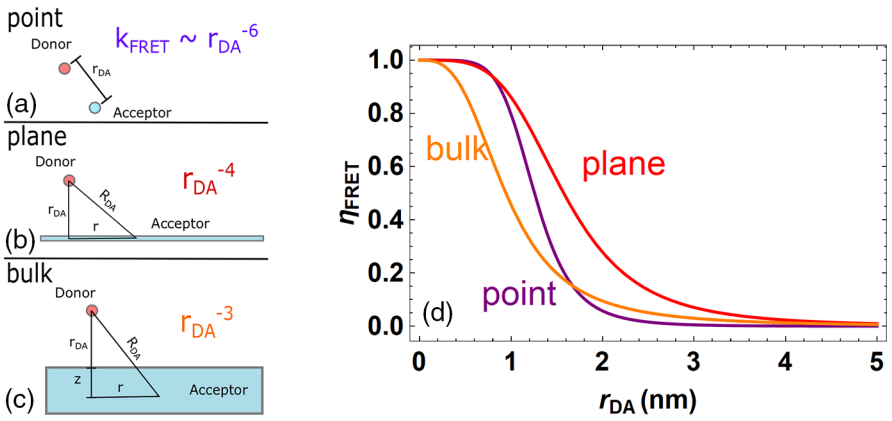


Corrected:

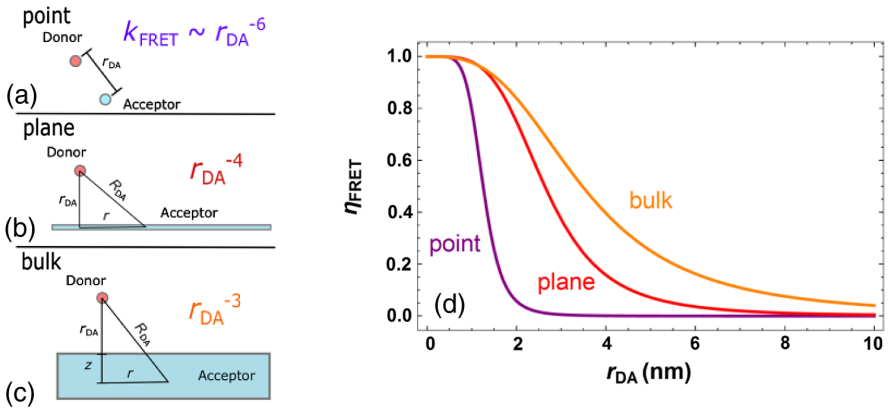


6. Figure 5 was corrected as follows.

Original:



Corrected:



The paper was corrected online on 10 August 2019. The following references were added as Refs. 32 and 33.

References

1. M. Stavola, D. L. Dexter, and R. S. Knox, "Electron-hole pair excitation in semiconductors via energy transfer from an external sensitizer," *Phys. Rev. B* **31**, 2277–2289 (1985).
2. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd ed., Springer-Verlag, Boston, Massachusetts (2006).