Supporting Information for

Examining Förster energy transfer for semiconductor nanocrystalline quantum dot donors and acceptors

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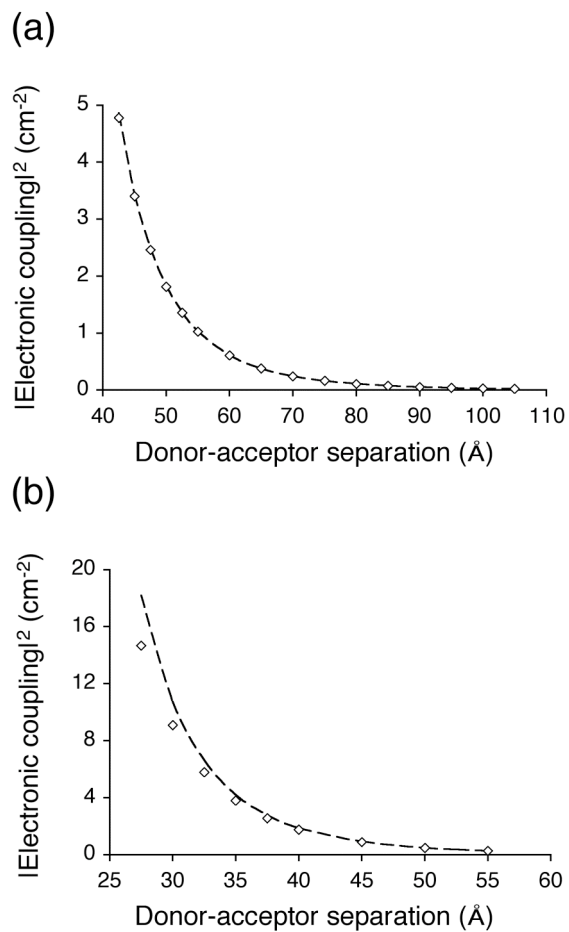2 National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Figure SI-1. Squared electronic couplings predicted by the full 3D expression (diamonds) and by the point-dipole approximation (dashed lines) for donor-acceptor pairs in the DL orientation as a function of their center-to-center separation. (a) Two 3.9 nm CdSe QDs. (b) A 3.9 nm CdSe QD and a chlorophyll molecule.

Table SI-1. Components in the crystallographic axis of the complex transition dipole moment (in Debye) of the CdSe QD considered in this work.

	X	Y	Z
μ	4.4-i·2.9	-1.2+i·6.2	0.0

Table SI-2. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between two 3.9 nm CdSe QDs in the FF orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, an experimental spectral overlap $J = 10^{-4}$cm as obtained in Ref [1], and a screening factor s=1. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
42.5	10.09	10.11	0.84	0.84
45.0	7.16	7.18	1.18	1.18
47.5	5.18	5.19	1.63	1.63
50.0	3.81	3.82	2.22	2.21
52.5	2.84	2.85	2.97	2.97
55.0	2.15	2.16	3.93	3.92
60.0	1.27	1.28	6.63	6.61
65.0	0.79	0.79	10.72	10.68
70.0	0.51	0.51	16.72	16.67
75.0	0.33	0.34	25.29	25.22
80.0	0.23	0.23	37.24	37.15
85.0	0.16	0.16	53.58	53.46
90.0	0.11	0.11	75.51	75.34
95.0	0.08	0.08	104.44	104.22
100.0	0.06	0.06	142.08	141.81
105.0	0.04	0.04	190.40	190.08

Table SI-3. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between two 3.9 nm CdSe QDs in the HT orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, an experimental spectral overlap $J=10^{-4}$cm as obtained in Ref [1], and a screening factor $s=1$. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
42.5	31.44	32.15	0.27	0.26
45.0	22.31	22.78	0.38	0.37
47.5	16.13	16.45	0.52	0.51
50.0	11.86	12.07	0.71	0.70
52.5	8.85	9.00	0.95	0.94
55.0	6.69	6.80	1.26	1.24
60.0	3.97	4.03	2.13	2.10
65.0	2.46	2.49	3.44	3.40
70.0	1.57	1.59	5.36	5.31
75.0	1.04	1.05	8.12	8.04
80.0	0.71	0.71	11.95	11.85
85.0	0.49	0.49	17.20	17.07
90.0	0.35	0.35	24.23	24.07
95.0	0.25	0.25	33.52	33.32
100.0	0.19	0.19	45.60	45.35
105.0	0.14	0.14	61.11	60.80

Table SI-4. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between two 3.9 nm CdSe QDs in the DL orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, an experimental spectral overlap $J=10^{-4}$cm as obtained in Ref [1], and a screening factor $s=1$. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
42.5	4.86	4.78	1.74	1.77
45.0	3.45	3.40	2.45	2.49
47.5	2.49	2.46	3.39	3.43
50.0	1.83	1.81	4.61	4.66
52.5	1.37	1.36	6.18	6.23
55.0	1.03	1.03	8.16	8.23
60.0	0.61	0.61	13.76	13.84
65.0	0.38	0.38	22.25	22.35
70.0	0.24	0.24	34.70	34.83
75.0	0.16	0.16	52.50	52.66
80.0	0.11	0.11	77.32	77.52
85.0	0.08	0.08	111.25	111.49
90.0	0.05	0.05	156.75	157.04
95.0	0.04	0.04	216.83	217.17
100.0	0.03	0.03	294.97	295.37
105.0	0.02	0.02	395.28	395.76

Table SI-5. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between a chlorophyll molecule and a 3.9 nm CdSe QD in the FF orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, a standard value for the spectral overlap $J=10^{-4}$cm, and a screening factor $s=1$. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
22.5	226.88	193.59	0.04	0.04
25.0	121.07	106.38	0.07	0.08
27.5	68.57	61.63	0.12	0.14
30.0	40.80	37.31	0.21	0.23
32.5	25.30	23.46	0.33	0.36
35.0	16.25	15.23	0.52	0.55
37.5	10.76	10.18	0.79	0.83
40.0	7.32	6.97	1.15	1.21
45.0	3.62	3.48	2.33	2.42
50.0	1.93	1.87	4.38	4.52
55.0	1.09	1.06	7.75	7.95

Table SI-6. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between a chlorophyll molecule and a 3.9 nm CdSe QD in the HT orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, a standard value for the spectral overlap $J=10^{-4}$cm, and a screening factor $s=1$. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
27.5	279.76	306.69	0.03	0.03
30.0	166.04	179.44	0.05	0.05
32.5	102.76	109.73	0.08	0.08
35.0	65.90	69.69	0.13	0.12
37.5	43.57	45.72	0.19	0.18
40.0	29.59	30.85	0.29	0.27
45.0	14.60	15.07	0.58	0.56
50.0	7.76	7.96	1.09	1.06
55.0	4.38	4.47	1.93	1.89

Table SI-7. Squared electronic couplings obtained from the full 3D expression and the point-dipole approximation between a chlorophyll molecule and a 3.9 nm CdSe QD in the DL orientation as a function of the center-center separation. EET times ($\tau = 1/k_{EET}$) estimated from the corresponding couplings, a standard value for the spectral overlap $J=10^{-4}$cm, and a screening factor $s=1$. Distances, squared couplings, and time constants are in Å, cm^{-2} and ns, respectively.

R	$|V_{dip\text{-}dip}|^2$	$|V_s^{(3D)}|^2$	$\tau_{dip\text{-}dip}$	τ_{3D}
27.5	18.20	14.67	0.46	0.58
30.0	10.74	9.09	0.79	0.93
32.5	6.62	5.81	1.28	1.46
35.0	4.23	3.81	2.00	2.22
37.5	2.79	2.56	3.03	3.30
40.0	1.89	1.76	4.48	4.79
45.0	0.93	0.89	9.12	9.54
50.0	0.49	0.48	17.22	17.76
55.0	0.28	0.27	30.59	31.25

References.

(1)　　Scholes, G. D.; Andrews, D. L. *Phys. Rev. B* **2005**, *72*, 125331.