Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Modelling quenching mechanisms of disordered molecular systems in presence of molecular aggregates.

Giacomo Fanciullo,[a] Irene Conti,[a] Pascal Didier,[b] Andrey Klymchenko,[b] Jérémie Léonard,[c] Marco Garavelli[a] and Ivan Rivalta*[a,d]

[a.] *Dipartimento di Chimica Industriale "Toso Montanari", ALMA MATER STUDIORUM, Università di Bologna, Viale del Risorgimento 4, 40126 Bologna, Italia*
[b.] *Laboratoire de Bioimagerie et Pathologies, UMR 7021 CNRS, Université de Strasbourg, 74 Route du Rhin, 67401 Illkirch, France*
[c.] *Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67000 Strasbourg, France*
[d.] *Université de Lyon, École Normale Supérieure de Lyon, Université Lyon 1, CNRS UMR 5182, Laboratoire de Chimie, 46 allée d'Italie, F69364 Lyon, France*

Table of content

S.1 – The influence of initial exciton density

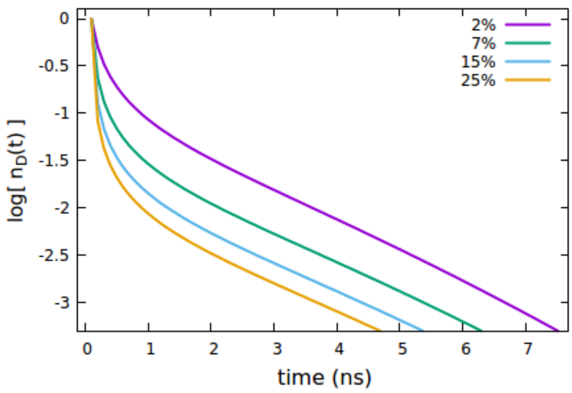

Figure S1. Effect of the initial exciton density $n_d(0)$ (expressed as % of C_d^{TOT}) on the (normalized) exciton density decay. Fixed parameters are: R_{d*d*}= 4 nm; R_{d*d}= 5 nm; R_{d*q}= 2 nm; τ_q= 4 ns; C_q = 0.25 % of C_d^{TOT}.

S.2 – The influence of parameters at higher initial exciton density

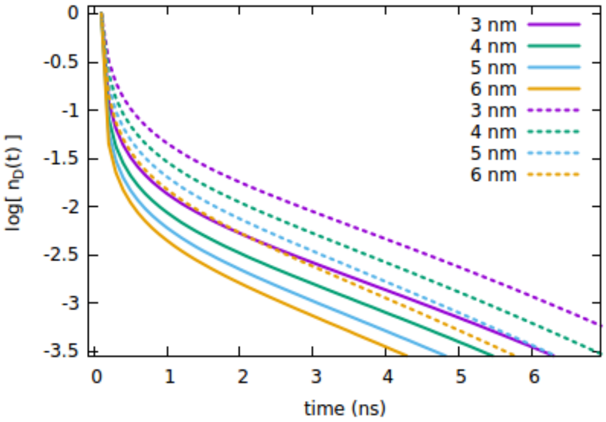

Figure S2. Effect of the R_{d*d*} radius governing the direct EEA mechanism on the (normalized) exciton density decay. Solid line: $n_d(0)$ = 25 % ; Dashed lines: $n_d(0)$ = 7 % (see Figure 4 in the main text). Fixed parameters are: R_{d*d} = 5 nm; R_{d*q} = 2 nm; τ_q = 4 ns; C_q = 0.25 % of C_d^{TOT}.

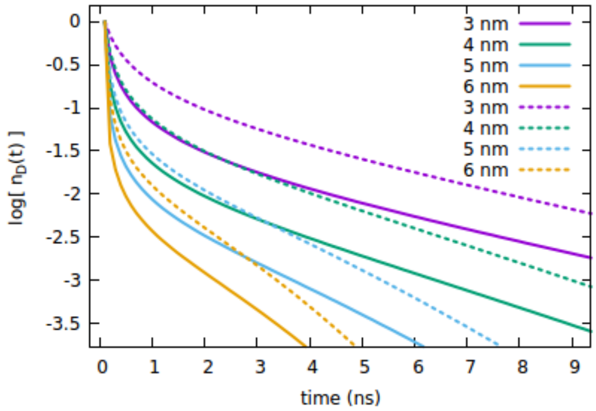

Figure S3. Effect of the R_{d*d} radius governing the diffusive EEA mechanism on the (normalized) exciton density. Solid line: $n_d(0)$ = 25 % ; Dashed lines: $n_d(0)$ = 7 % (see Figure 5 in the main text). Fixed parameters are: R_{D*D*}= 4 nm; R_{d*q}= 2 nm; τ_q= 4 ns; C_q = 0.25 % of C_d^{TOT}.

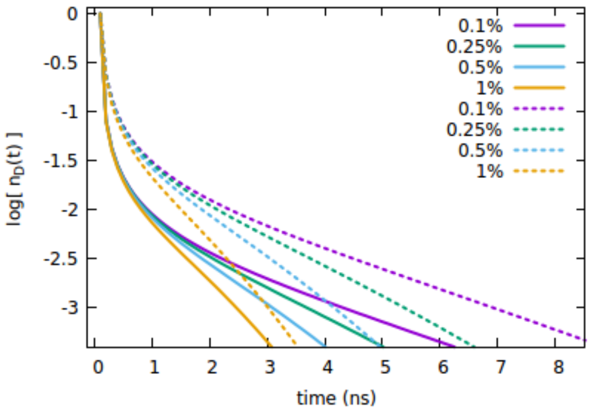

Figure S4. Effect of the quencher concentration C_q (expressed as % of C_d^{TOT}) on the (normalized) exciton density decay. Solid line: $n_d(0)$ = 25 % ; Dashed lines: $n_d(0)$ = 7 % (see Figure 6 in the main text). Fixed parameters are: R_{d*d} = 5 nm; R_{d*d*} = 4 nm; R_{d*q} = 2 nm; τ_q = 4 ns.

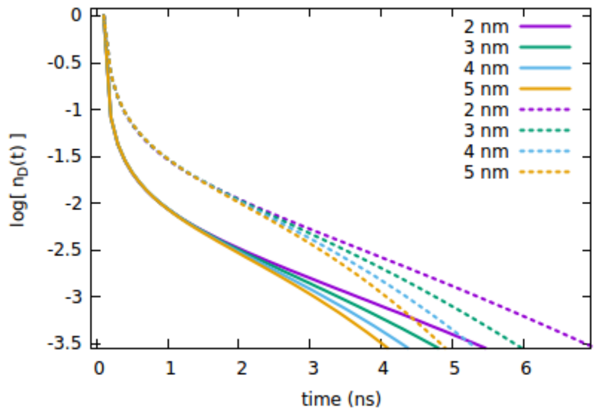

Figure S5. Effect of the R_{d*q} radius (entering the expression for the diffusion coefficient) on the (normalized) exciton density decay. Solid line: $n_d(0)$ = 25 % ; Dashed lines: $n_d(0)$ = 7 % (see Figure 7 in the main text). Fixed parameters are: R_{d*d}= 5 nm; R_{d*d*}= 4 nm; τ_q= 4 ns; C_q = 0.25 % of C_d^{TOT}.

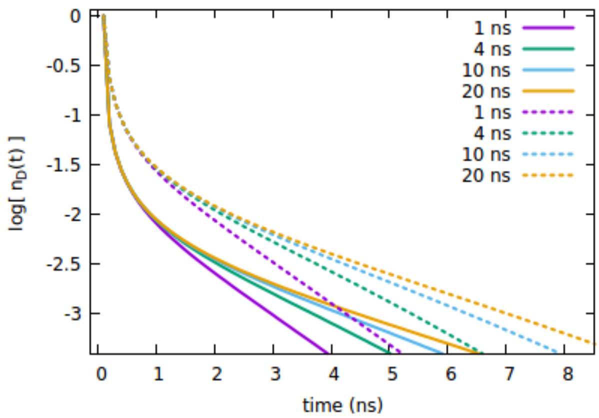

Figure S6. Effect of the quencher lifetime on the (normalized) exciton density decay . Solid line: $n_d(0)$ = 25 % ; Dashed lines: $n_d(0)$ = 7 % (see Figure 8A in the main text). Fixed parameters are: R_{d*d}= 5 nm; R_{d*d*}= 4 nm; R_{d*q}= 2 nm; C_q = 0.25 % of C_d^{TOT}

S.3 – The influence of parameters at different energy transfer timescales

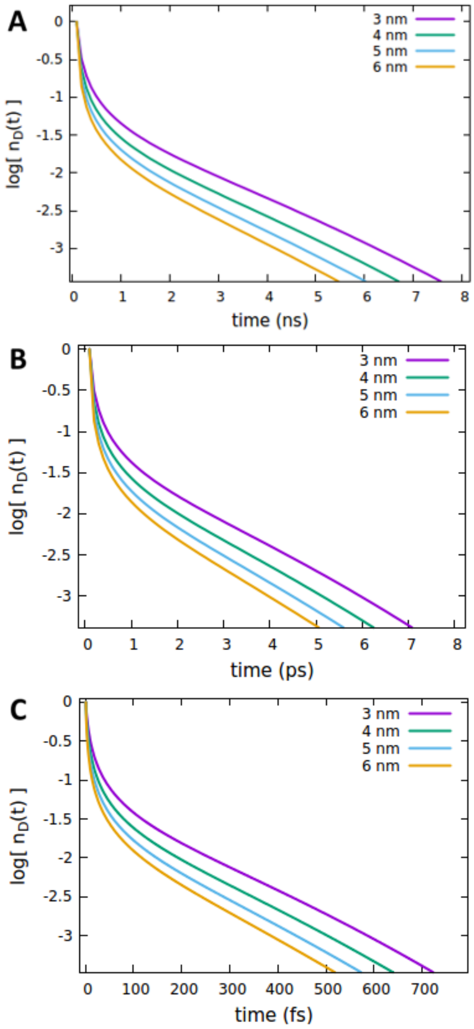

Figure S7. Effect of the R_{d*d*} radius governing the direct EEA mechanism on the (normalized) exciton density decay at different energy transfer timescales. A: τ_d = τ_q = 4 ns; B: τ_d = τ_q = 4 ps ; C: τ_d = τ_q = 400 fs. Fixed parameters are: R_{d*d}= 5 nm; R_{d*q}= 2 nm; C_q = 0.25 % of C_d^{TOT}; $n_d(0)$ = 7 % of C_d^{TOT}.

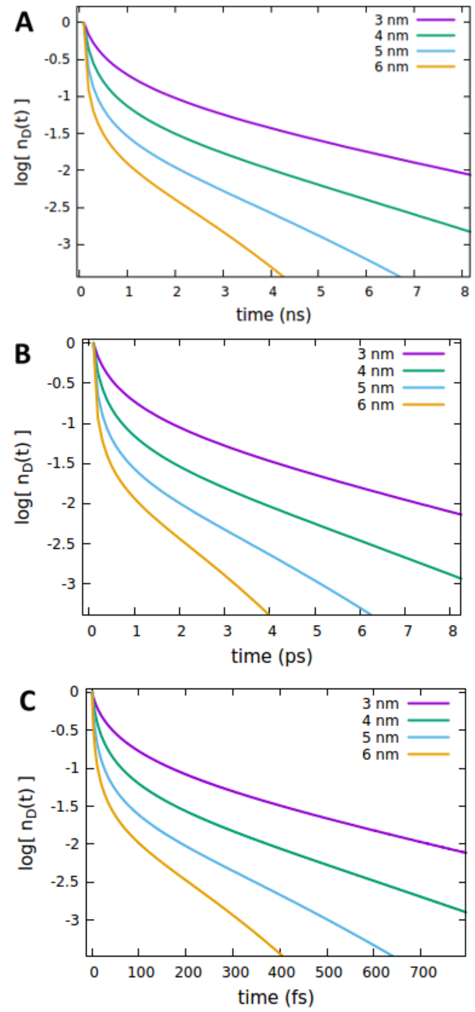

Figure S8. Effect of the R_{d*d} radius governing the diffusive EEA mechanism on the (normalized) exciton density decay at different energy transfer timescales. A: τ_d = τ_q = 4 ns; B: τ_d = τ_q = 4 ps ; C: τ_d = τ_q = 400 fs. Fixed parameters are: R_{d*d*}= 4 nm; R_{d*q}= 2 nm; C_q = 0.25 % of C_d^{TOT}; $n_d(0)$ = 7 % of C_d^{TOT}.

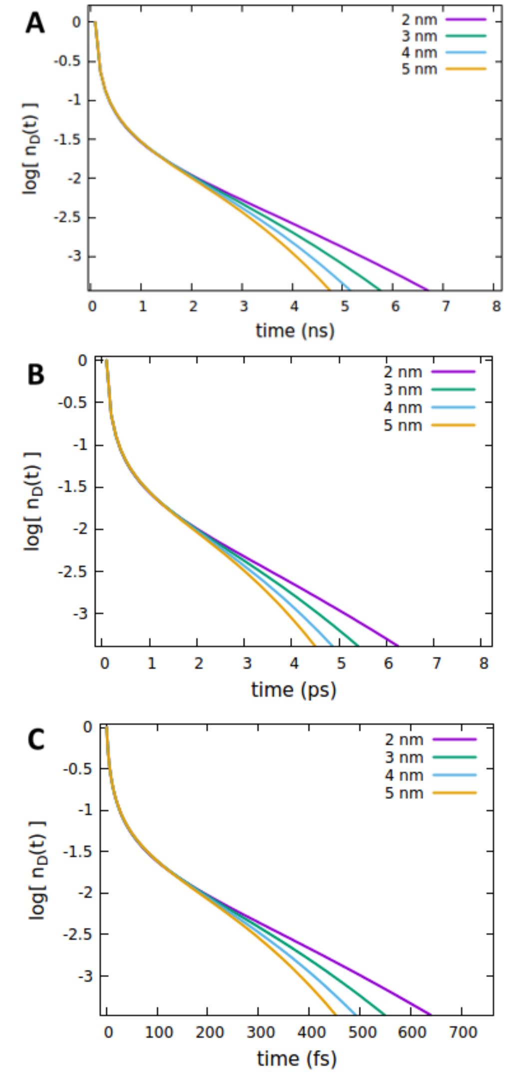

Figure S9. Effect of the R_{d*q} radius governing the direct quenching mechanism on the (normalized) exciton density decay at different energy transfer timescales. A: τ_d = τ_q = 4 ns; B: τ_d = τ_q = 4 ps ; C: τ_d = τ_q = 400 fs. Fixed parameters are: R_{d*d*}= 4 nm; R_{d*d}= 5 nm; C_q = 0.25 % of C_d^{TOT}; $n_d(0)$ = 7 % of C_d^{TOT}.

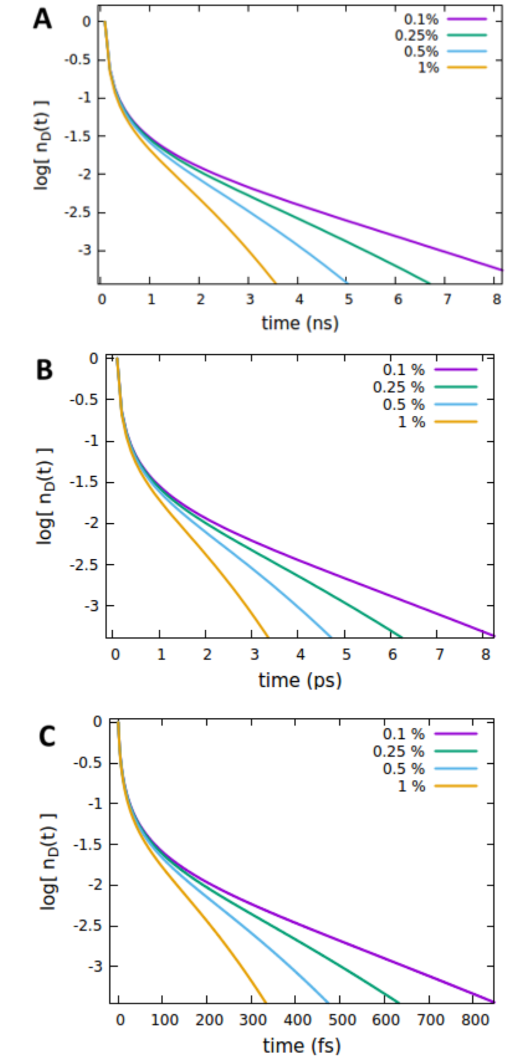

Figure S10. Effect of the quencher concentration C_q (expressed as % of C_d^{TOT}) on the (normalized) exciton density decay at different energy transfer timescales. A: τ_d = τ_q = 4 ns; B: τ_d = τ_q = 4 ps ; C: τ_d = τ_q = 400 fs. Fixed parameters are: R_{d*d*}= 4 nm; R_{d*d}= 5 nm; R_{d*q}= 2 nm; $n_d(0)$ = 7 % of C_d^{TOT}.