Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supporting information

Probing the interactions between disulfide based ligands and gold nanoparticles using a functionalised fluorescent perylene-monoimide dye†

Julien R. G. Navarro[1,2], Marcel Plugge[3], Matthieu Loumaigne[4], Angel Sanchez Gonzalez[5], Benedetta Mennucci[5], Anne Débarre[4], Albert M. Brouwer[3], Martinus H. V. Werts[1,2]*

[1] *Ecole Normale Supérieure de Cachan/Bretagne, Laboratoire SATIE (UMR 8029), Campus de Ker Lann, F-35170 Bruz, France*

[2] *CNRS, Laboratoire SATIE (UMR 8029), ENS Cachan/Bretagne, Campus de Ker Lann, F-35170 Bruz, France*

[3] v*an 't Hoff Institute for Molecular Sciences, Nieuwe Achtergracht 129, NL-1018 WS Amsterdam, The Netherlands*

[4] *CNRS, Laboratoire Aimé Cotton (UPR 3321), Université Paris Sud, Bâtiment 505, F-91405 Orsay, France*

[5] *Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Via Risorgimento 35, I-56126 Pisa, Italy*

† Part of the special issue dedicated to Jan W. Verhoeven

* Corresponding author. E-mail: martinus.werts@bretagne.ens-cachan.fr

Figure SI-1

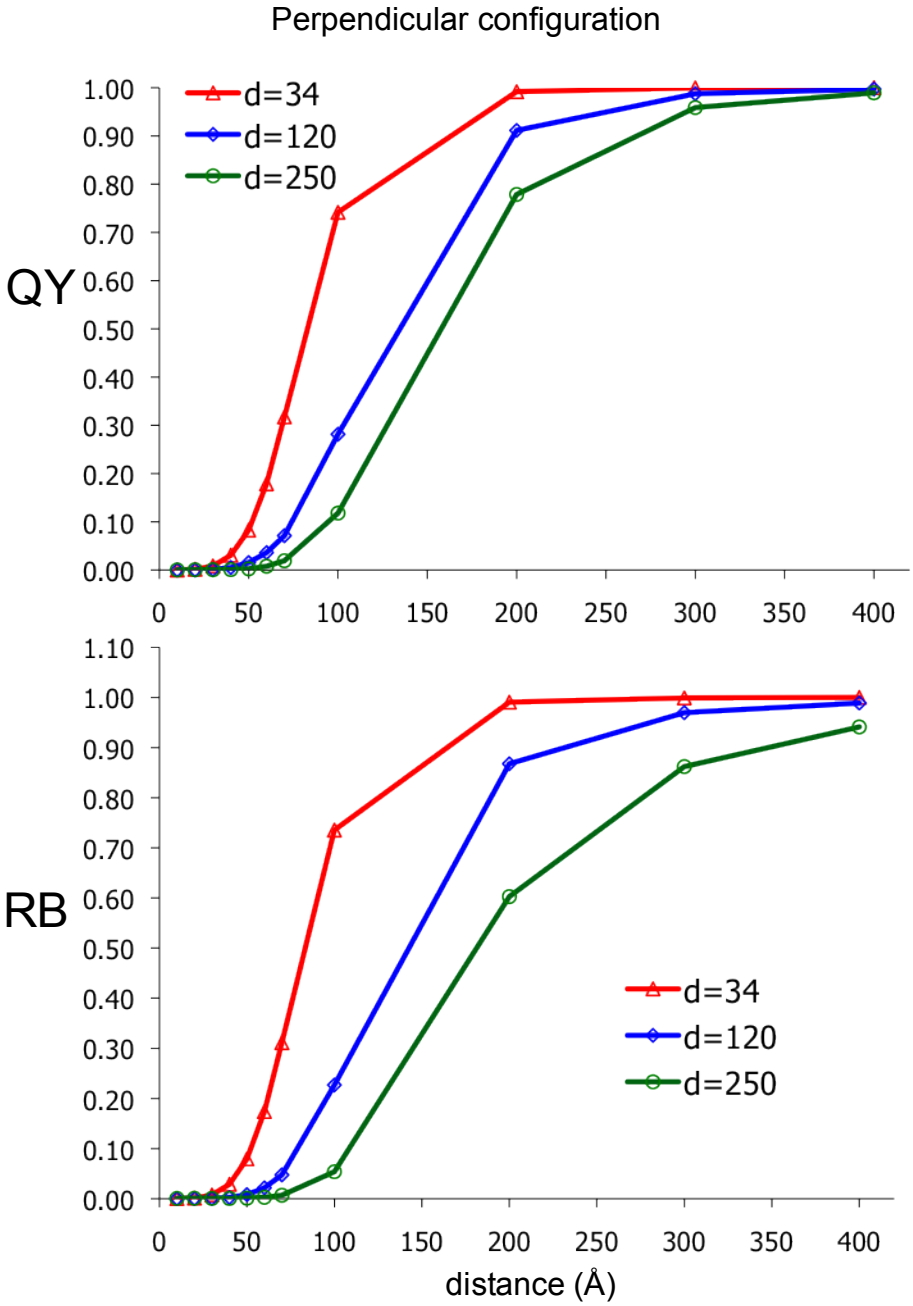

Figure SI-1. Quantum chemical predictions of fluorescence quantum yield and relative brightness of PMI near a gold nanoparticle in DMF in perpendicular configuration (transition moment parallel to the particle surface). Top: fluorescence quantum yield vs distance, Bottom: relative brightness vs distance, for three different AuNP diameters: 34 Å, 120 Å and 250 Å.

Figure SI-2

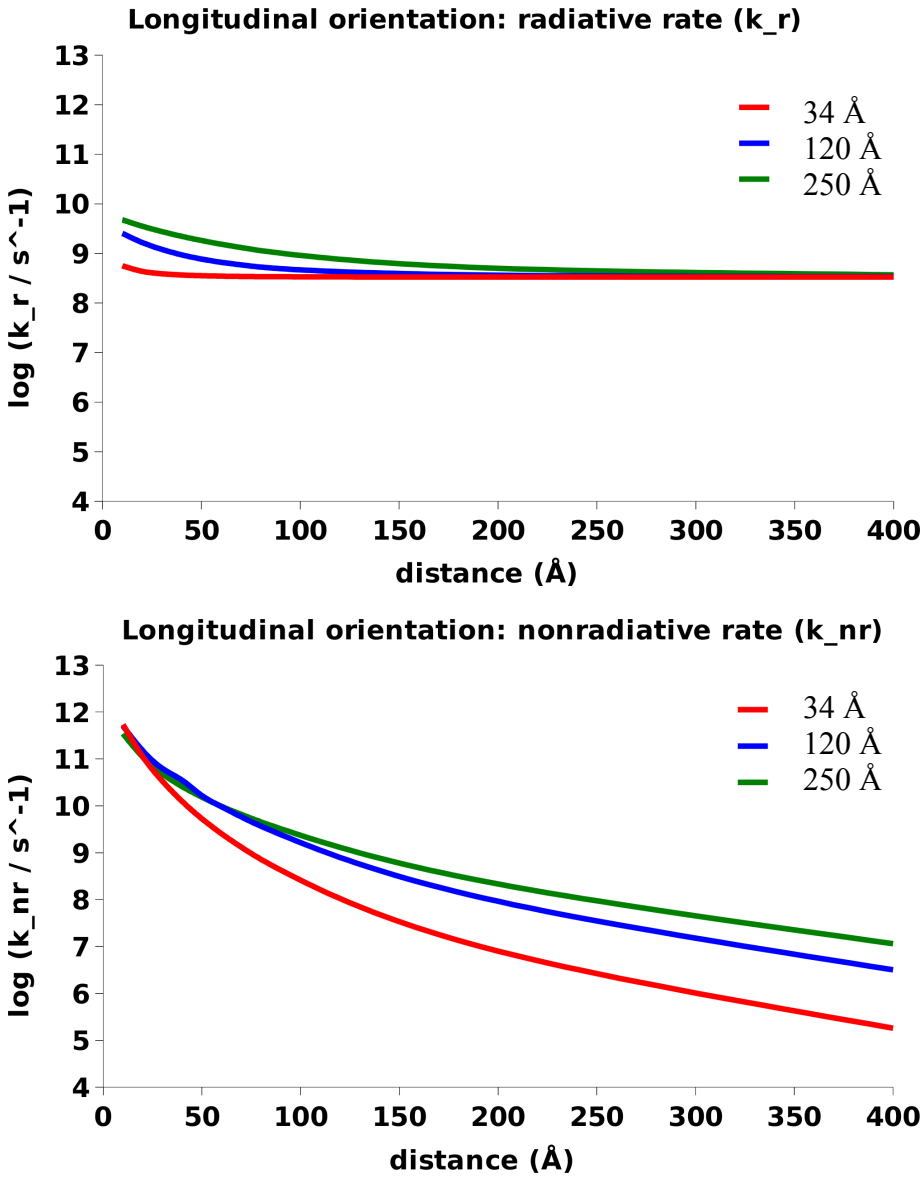

Figure SI-2. Quantum chemical predictions of the radiative rate k_r (top) and nonradiative rate k_{nr} (bottom) of PMI near a gold nanoparticle in DMF in longitudinal configuration (transition moment perpendicular to the particle surface) as a function of chromophore-particle surface distance, for three different AuNP diameters: 34 Å, 120 Å and 250 Å. The extinction coefficient ε is proportional to k_r.[1-3]

Figure SI-3

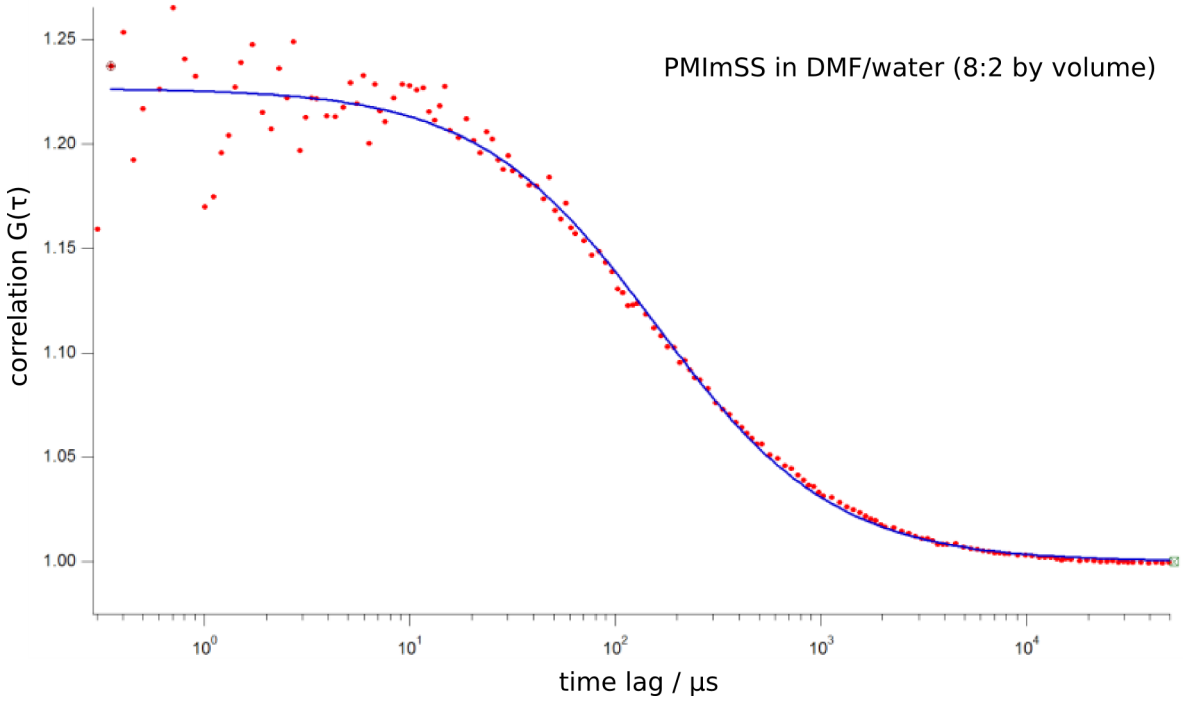

Figure SI-3. Fluorescence correlation trace (red dots) of fPMImSS in DMF/water 8:2 (by volume), excitation wavelength 488 nm. The blue line is a fit according to Eqn.6, corresponding to an experimental diffusion time τ_D = 0.16 ms.

Figure SI-4

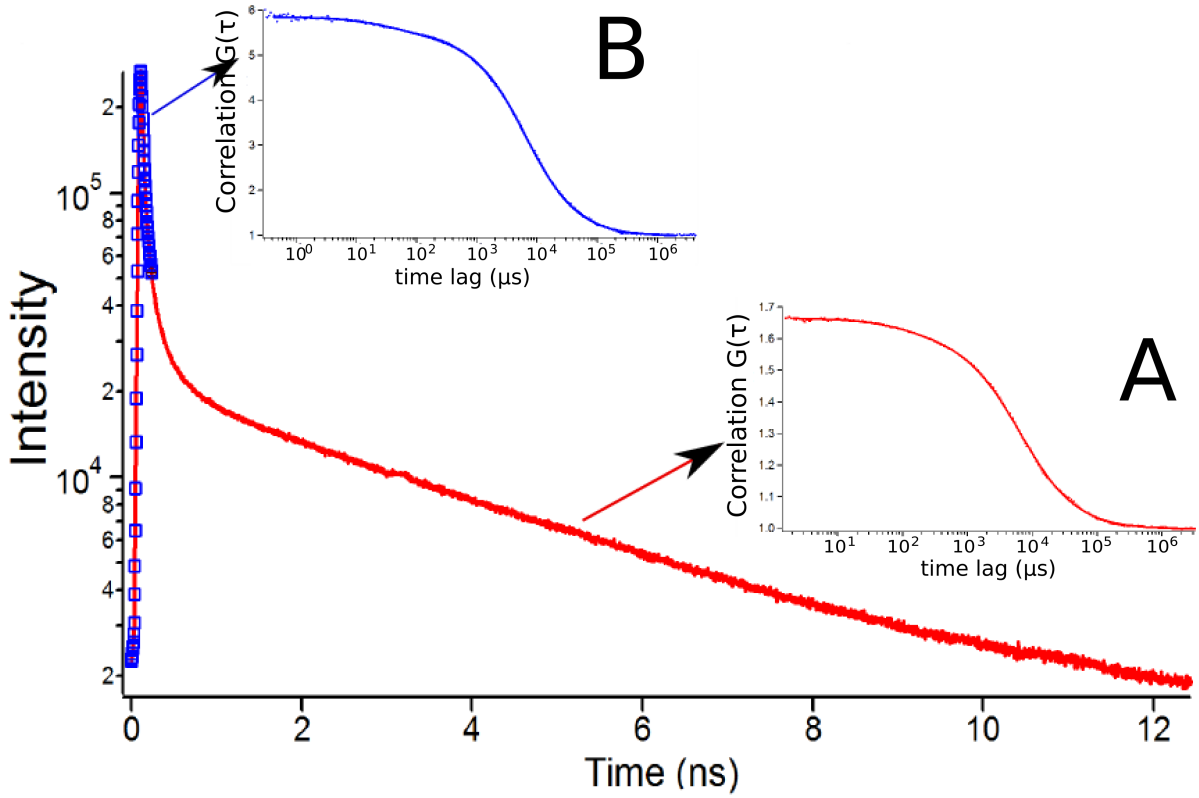

Figure SI-4. Main graph: Fluorescence decay of a one-day old sample of PMImSS-AuNP in DMF. The decay curve was obtained from the 'microtime' of the time-tagged time-resolved (TTTR) photon arrival time data. Inset A, red curve: fluorescence correlation trace of the total signal. The FCS curve can be fitted by the sum of free ligands (τ_{diff} = 130 µs) and large diffusing fluorescent objects (τ_{diff} = 6500 µs). Inset B, blue curve: correlation curve of the quenched part of the luminescence obtained by time gating the lifetime trace in order to keep only the photons emitted within the impulse response of the detector. The resulting FCS curve can be fitted with only one component of large diffusing fluorescent objects with a blinking component of 50 µs that has an amplitude of 0.08.

References

1 A. Einstein, Zur Quantentheorie der Strahlung, *Physik. Z*, 1917, **18**, 121-128.

2 G. Lewis and M. Kasha, Phosphorescence in fluid media and the reverse process of singlet-triplet absorption, *J. Am. Chem. Soc*, 1945, **67**, 994-1003.

3 S. J. Strickler and R. A. Berg, Relationship between absorption intensity and fluorescence liftetime of molecules, *J. Chem. Phys.*, 1962, **37**, 814-822.