Supplementary Material (ESI) for *Nanoscale*

Two-photon excited fluorescence of silica nanoparticles loaded with fluorene-based monomer and its cross-conjugated polymer: their application to cell imaging

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Charge transfer (CT) character of M1 and P1

Figure S1 shows the model used for **M1** in DFT calculations and the most important molecular orbitals involved in the electronic transitions. The long wavelength absorption maxima ($S_0 \rightarrow S_1$) resulted to be λ_{max}=397 nm (415 nm experimentally). This transitions shows a significant charge transfer (CT) character, where the charge is transferred from π orbitals of fluorene fragment to π* orbitals of benzothiadiazole moiety. Broad and intense absorption maxima for **M1** in the range 280-340 nm can be attributed to $S_0 \rightarrow S_2$ and $S_0 \rightarrow S_3$ transitions. In the case of $S_0 \rightarrow S_3$, the transition has high oscillator strength (1.22) and involves π orbitals extended over entire molecule (HOMO→ LUMO+1). On the other hand, the weaker $S_0 \rightarrow S_2$ transition (HOMO-1 →LUMO) has CT character similar to $S_0 \rightarrow S$.

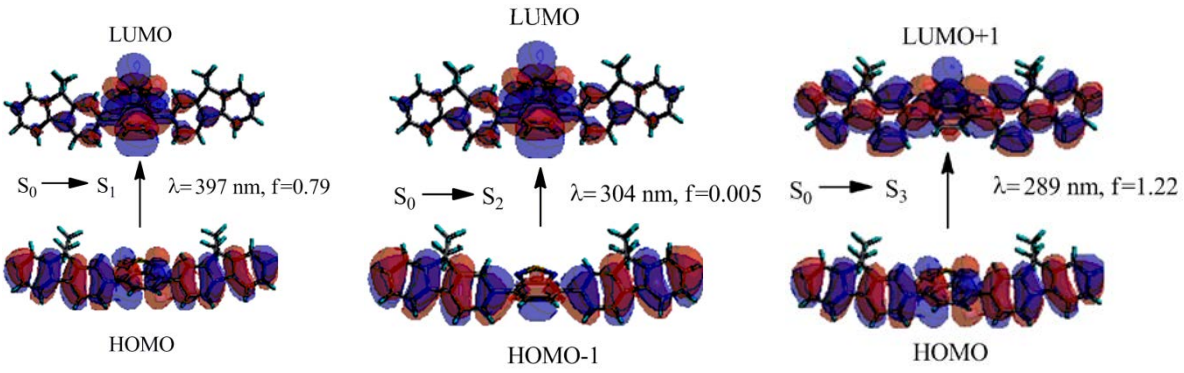

Figure S1. The most important excitations contributing to the transitions in **M1**.

Figure S2 shows the model used for **P1** in DFT calculations. In this case **P1** was modelled using an oligomer as depicted in the figure. The long wavelength absorption maxima ($S_0 \rightarrow S_1$) involves mostly four molecular orbitals (HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2 and LUMO+3) as it has a charge transfer (CT) character similar to **M1**. It is noteworthy to note than $S_0 \rightarrow S_2$ transition also has CT character and lies very close to $S_0 \rightarrow S_1$ (395 mn), contributing to the long wave absorption of **P1**, but with very weak oscillator strength. For short wavelength absorption, the most intense transition is S_0-S_5 (λ_{max}=291, oscillator strength 2.40), corresponding to a combination of HOMO-1→LUMO+3 and HOMO→LUMO+2, with no CT character.

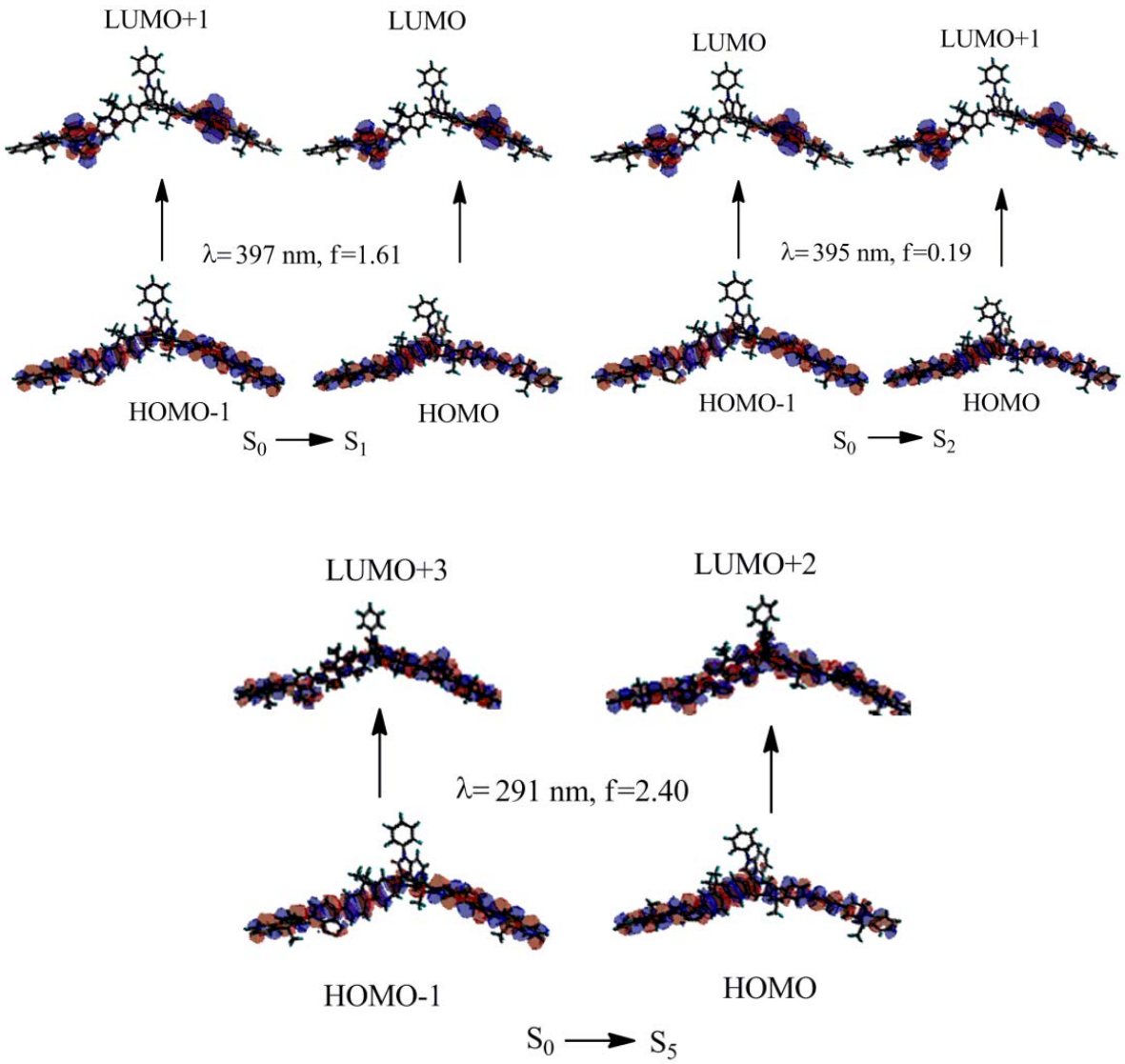

Figure S2. The most important excitations contributing to the transitions of an oligomer structure used a s model for **P1**.

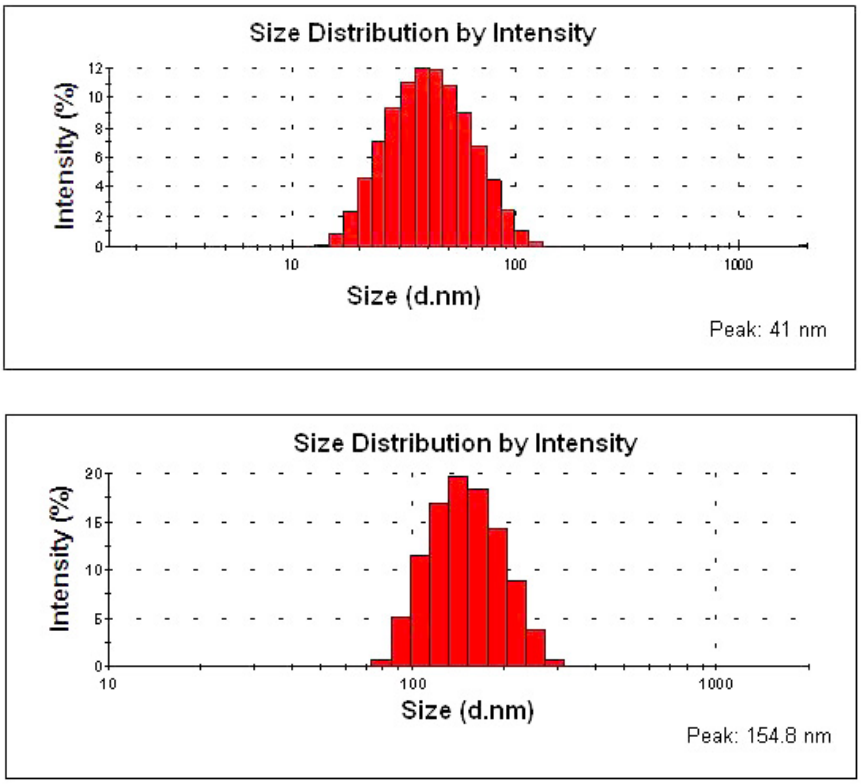

Figure S3. Nanoparticles size distribution obtained through DLS for: upper) **P1**-NPs suspension with CTAB concentration of 0.08 mM, bottom) **P1**-SNPs suspension processed with aerosol-OT at concentration of 50 mM.

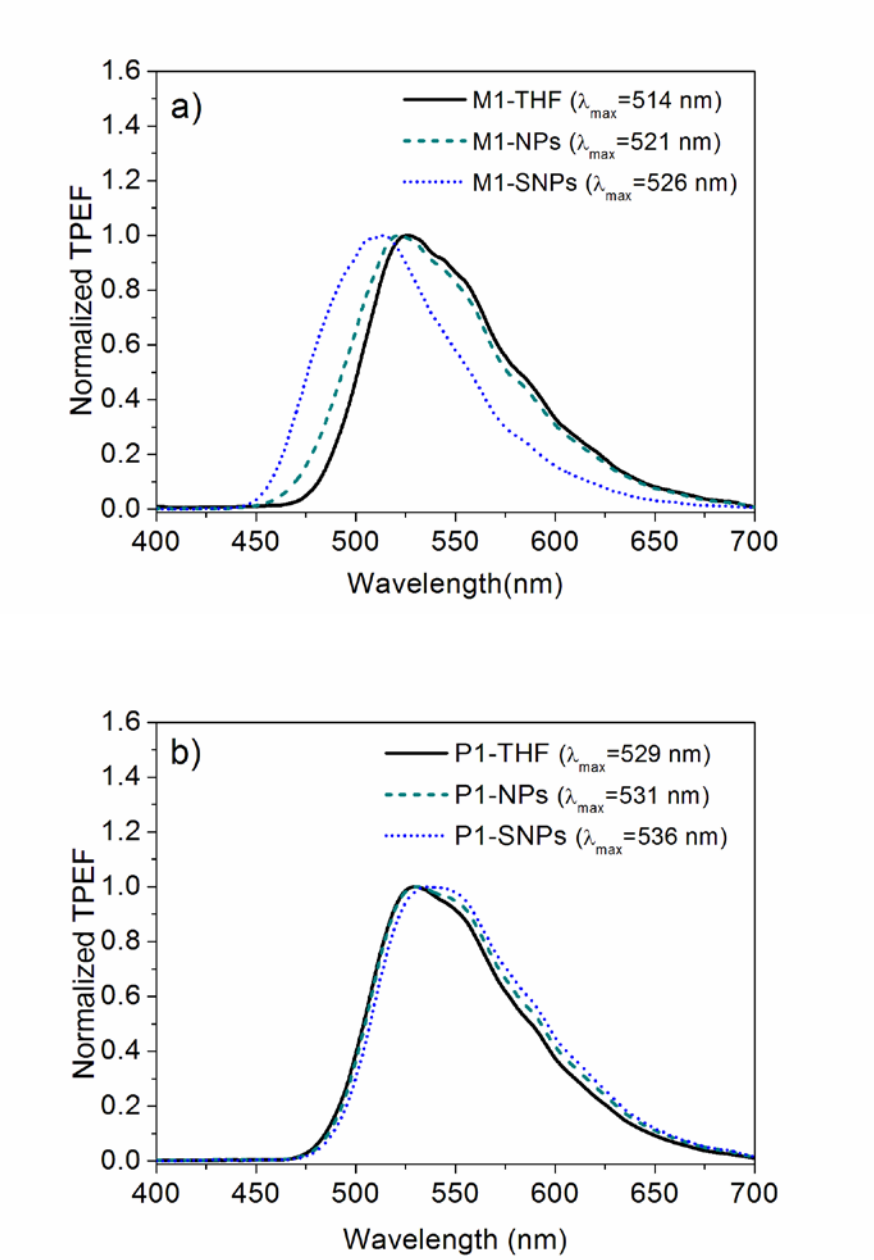

Figure S4. Normalized TPEF spectra for a) monomer **M1** and b) polymer **P1** in solutions and aqueous suspensions. Excitation: femtosecond pulses at 750 nm