

Electronic Supplementary Information

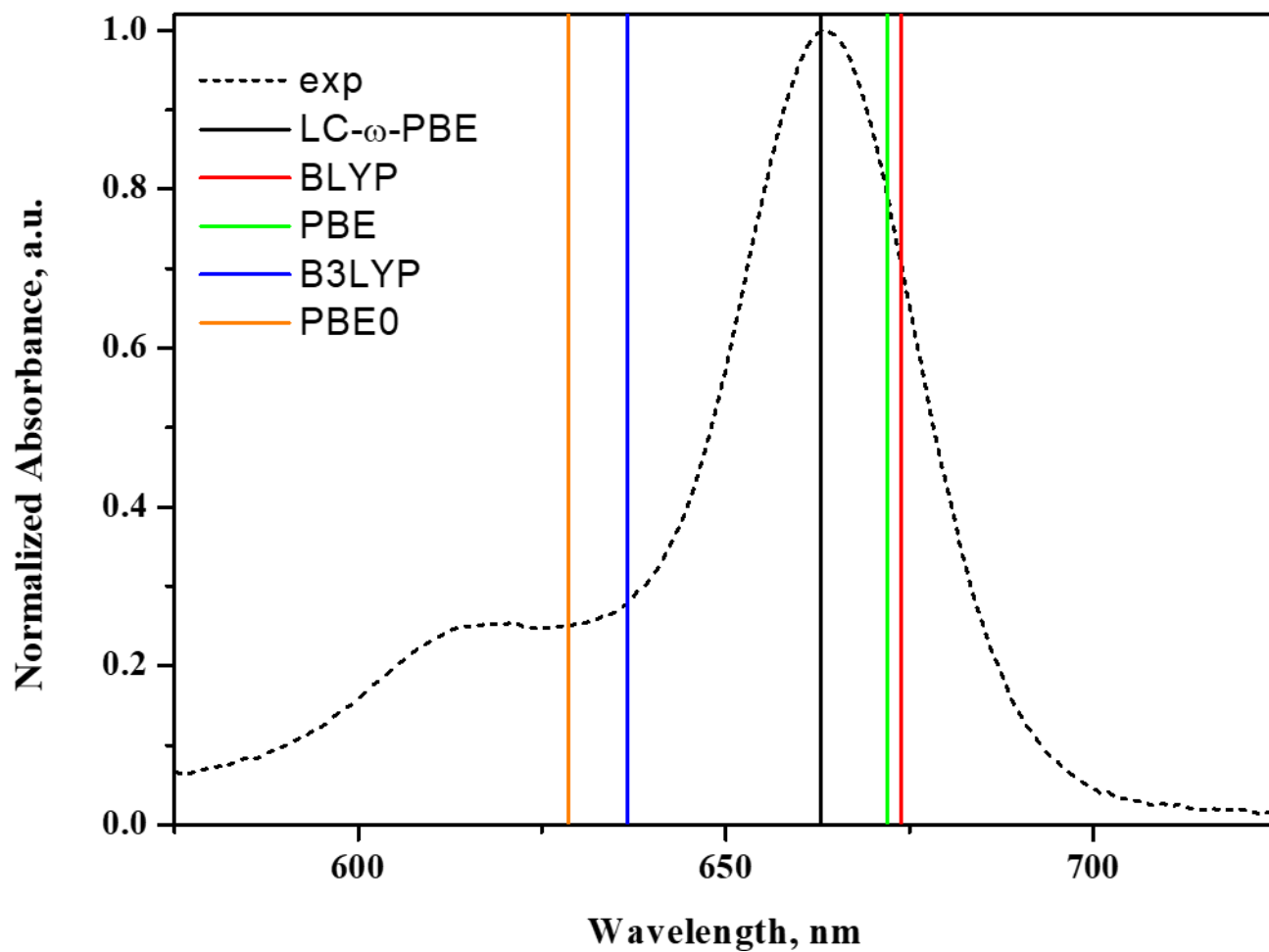
Mesoporous silica nanoparticles incorporating squaraine-based photosensitizers: a combined experimental and computational approach

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Table S1 – Average particle size obtained by DLS

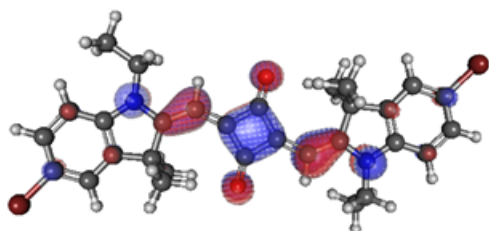
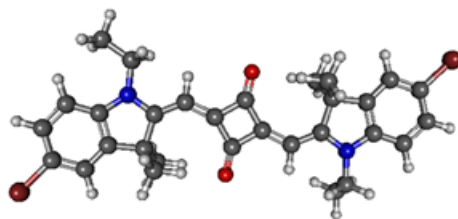
SAMPLE	Average diameter (nm)
MSNs	181±18
Br-NH/MSN	185±23
Br-C2/MSN	184±19
Br-C4/MSN	180±22



exp	LC-ω-PBE	BLYP	PBE	B3LYP	PBE0
663 nm	663.00 nm	673.92 nm	672.02 nm	636.61 nm	628.59 nm

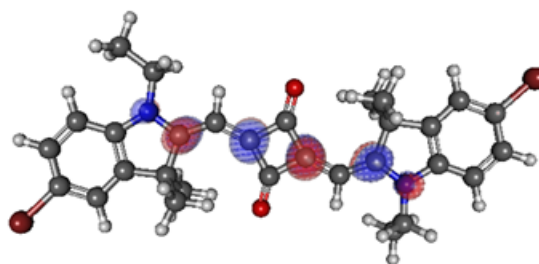
Figure S1 Experimental UV-Vis absorption spectrum (dashed line) and simulated UV-Vis absorption spectra calculated with different hybrid and pure functionals.

A

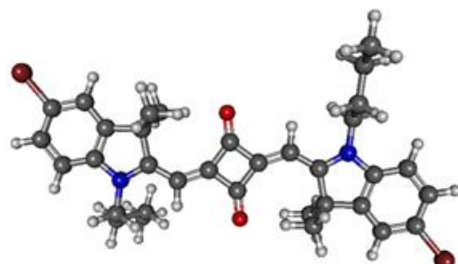


HOMO

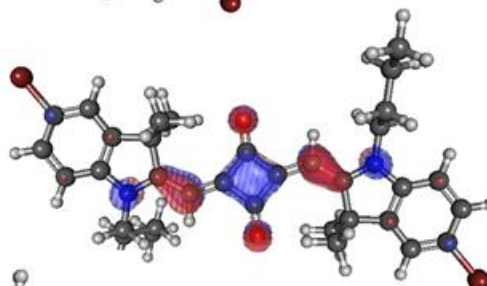
LUMO



B



HOMO



LUMO

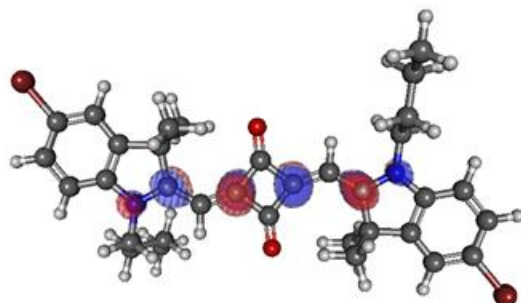
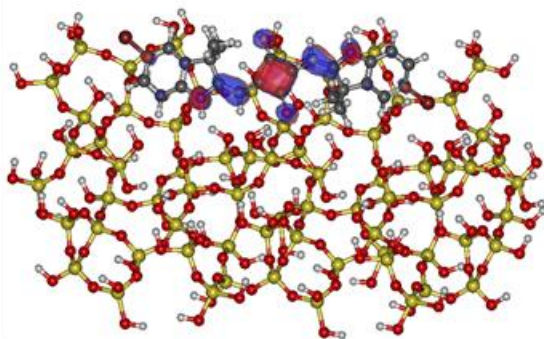


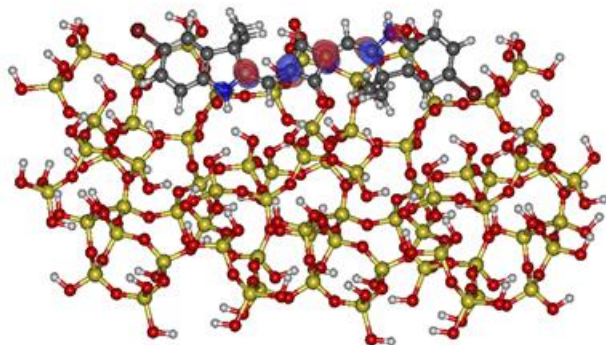
Figure S2 Optimized structure of Br-C2 (**A**) and Br-C4 (**B**) molecules in DMF solution

A

HOMO

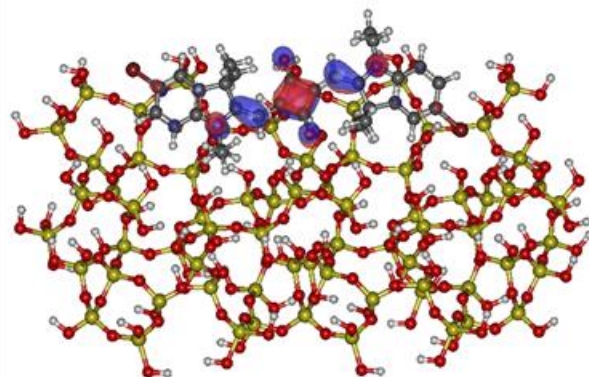


LUMO

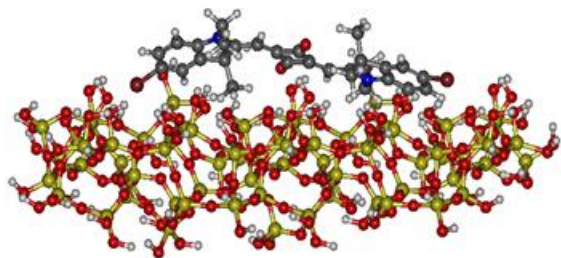
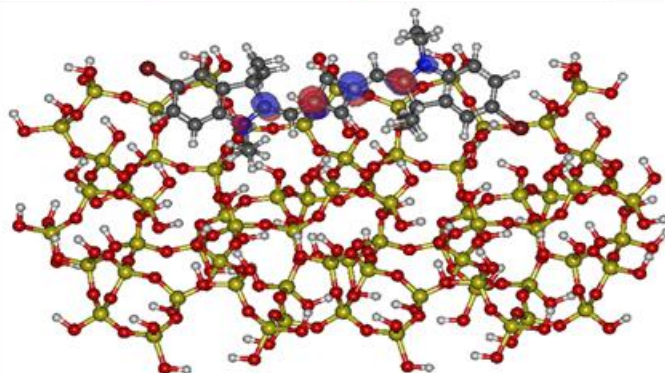


B

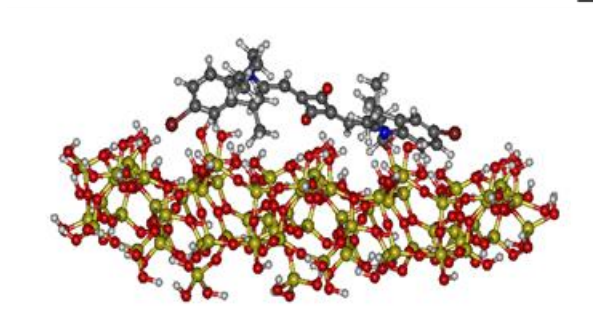
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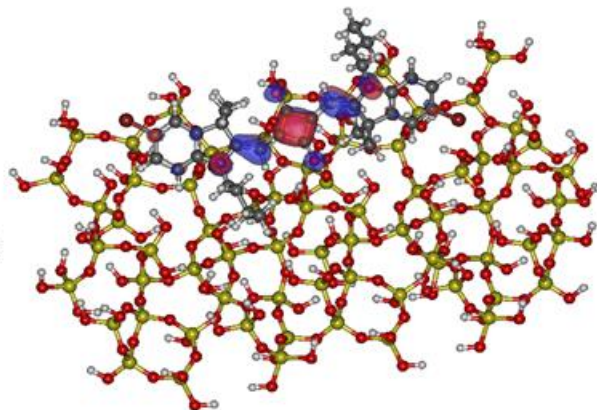
LUMO



C



HOMO



LUMO

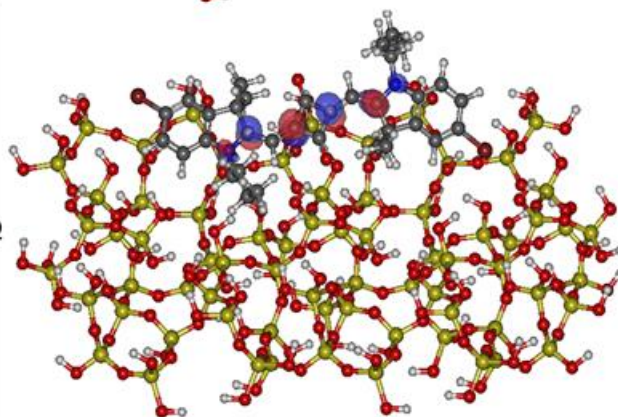


Figure S3 Models of Br-NH (**A**), Br-C2 (**B**) and Br-C4 (**C**) adsorbed on silica surface

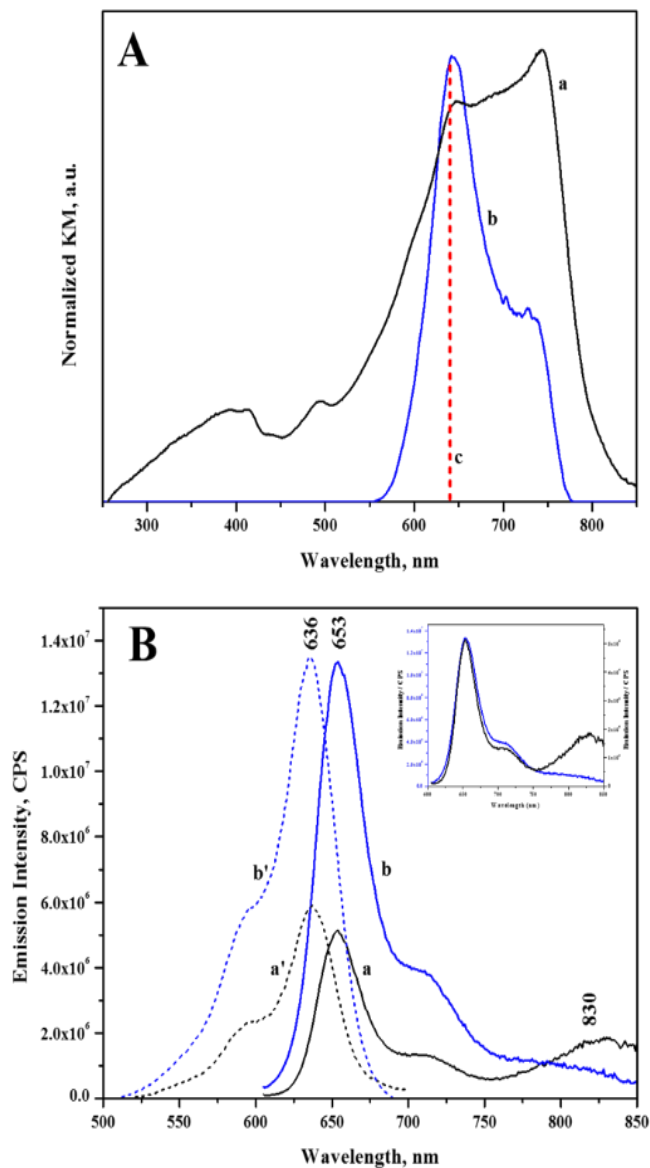


Figure S4. A. DR-UV-Vis spectra of the as prepared Br-NH/MSN hybrid (a, black curve), washed Br-NH/MSN (b, blue curve) and simulated absorption (c, red dashed line). **B.** Emission (solid curves) and excitation (dashed curves) spectra of the as prepared (a, a', black curves) and washed (b, b', blue curves) Br-NH/MSNs. The emission spectra are reported in the inset with normalized y scales for the sake of comparison.

DR-UV-Vis spectrum of the as-prepared sample is dominated by a signal at ca. 730 nm which intensity decreased significantly after the washing procedure. In parallel, the intensity of the large emission band at 830 nm decreased after the washing procedure. Noticeably, the overall emission intensity of the washed sample is about thrice the emission of the as-prepared sample, suggesting that the washing procedure lead to both the removal of most of the aggregated squaraine molecules and a re-distribution of the dyes, leading to a beneficial effect on the emission properties