Electronic Supporting Information

Amphi-Functional Mesoporous Silica Nanoparticles for Dye Separation

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Effect of surface functional group on uptake of Nile Red dye from water

A similar selective functionalization protocol was applied to as synthesized SBA-15 materials[1] having slightly larger pores than MSN. Various materials were synthesized are as follows. The azide functionalized SBA-15 silica materials were subjected to Cu(I) catalyzed click reaction with – Propargyl alcohol, (2,5,8,11-tetraoxatridec-12-yne), propargyl terminated triethylene glycol monomethyl ether, propargyl terminated polyethylene glycol monomethylether (2000) to obtain these materials with different surface functionalities. The NR encapsulation experiments were performed very similar as mentioned in the main manuscript. It can be clearly observed from the PL spectra and relative intensities that when outer surface of silica is functionalized with bulky moieties the uptake of nile red was dramatically inhibited. The azide surface poses least hindrance to uptake process. It strongly suggests that presence of bulky surface groups like poly ethylene glycol acts as a barrier for the cargo molecules.

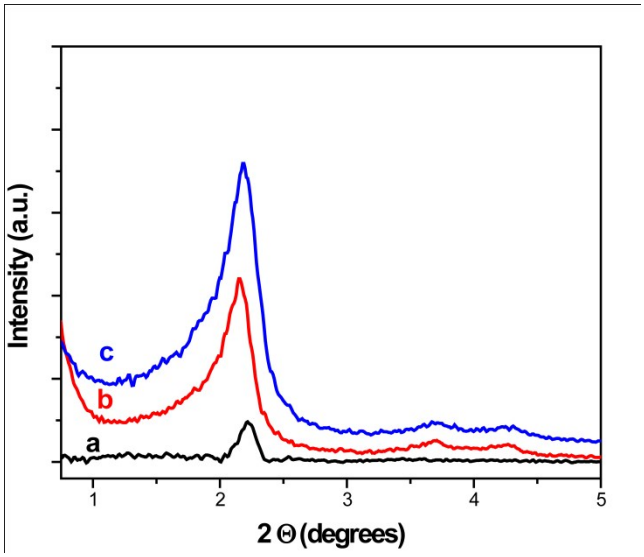
Separation of dye from the mixture of Nile Red with R6G or MB17 in dissolved water

NR was mixed withR6G/MB17 independently in water to have final concentrations of 0.05 mM for both dyes. To this a water dispersion of particles was added to give final particle concentration of 10mg/mL. This mixture was incubated on a rotovap for 6 hours at 50 RPM. After incubation the solutions were subjected to centrifuge and supernatant was analysed with UV-Vis spectroscopy to determine the uptake of R6G/MB17. The precipitate was dispersed in water by sonication and analysed with photoluminescence spectroscopy to determine the uptake of NR.

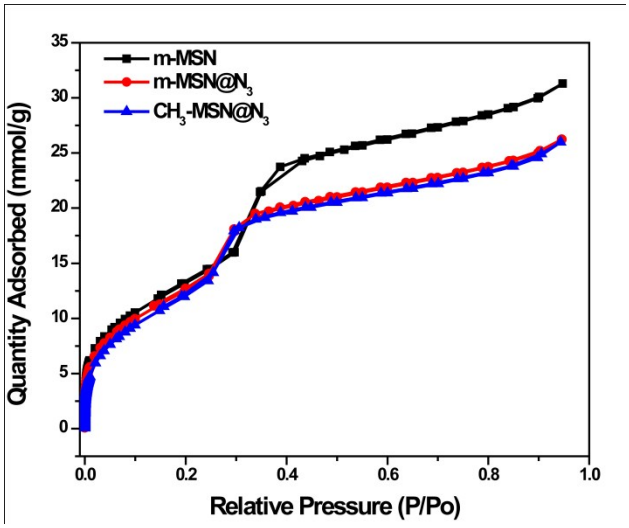
From the UV-Vis spectra of mixture of dyes before and after adsorption (SI 6 A and SI 7 A) with functionalized MSNs i.e. m-MSN@N_3 and CH_3-MSN@N_3; it can be seen that intensities of R6G (527 nm) and MB17 (broad peak from~ 460-635 nm with maxima at 530 nm) has decreased. This suggests the adsorption of these dyes from their mixture with NR by both m-MSN@N_3 and CH_3-MSN@N_3. Due to solubility issues of NR in water it does not show any absorption peak in water. To see the uptake of NR we analyzed the samples by PL. The precipitated solids were dispersed in water again and PL spectra were recorded (SI 6 B and SI 7 B). The PL spectra clearly show a strong emission peak at 640

nm in case of CH_3-MSN@N_3 which clearly indicates the presence of NR adsorbed with this material. There is also a peak at 547 nm which corresponds to emission of R6G in water.

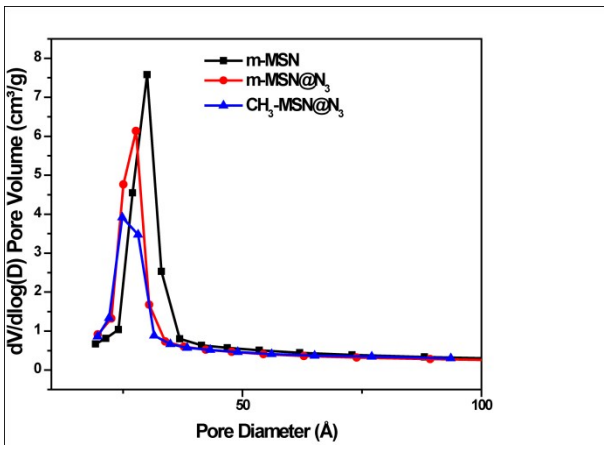
The above observations clearly indicate that NR has been absorbed by CH_3-MSN@N_3 from its mixtures with R6G as well as MB17. The UV data indicates that MB17 and R6G were absorbed by both m-MSN@N_3 and CH_3-MSN@N_3. This can be because of non-specific adsorption of dyes on silica surface since there is no observable difference between with and without trimethyl silyl functional groups. On contrary, the difference seen in case of NR uptake is very prominent. We could not perform a quantitative estimation of uptake because of the experimental issues especially the solubility of NR in water. So to conclude it seems that in this case of competitive adsorption on functionalized MSN with NR and MB17/R6G, NR is being adsorbed on hydrophobic functionalized surface.



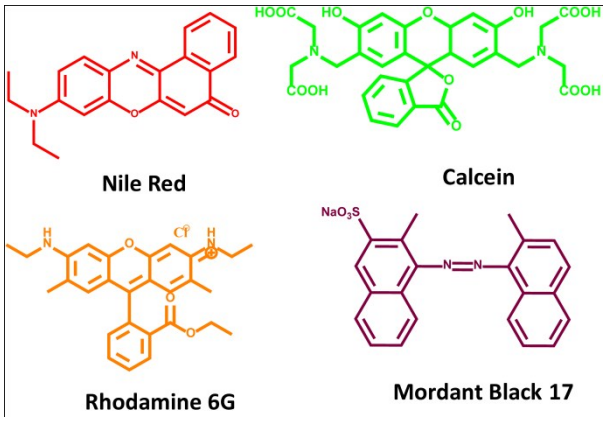
SI 1 Low angle PXRD pattern of a) MSN b) m-MSN@N_3 and c) CH_3-MSN@N_3



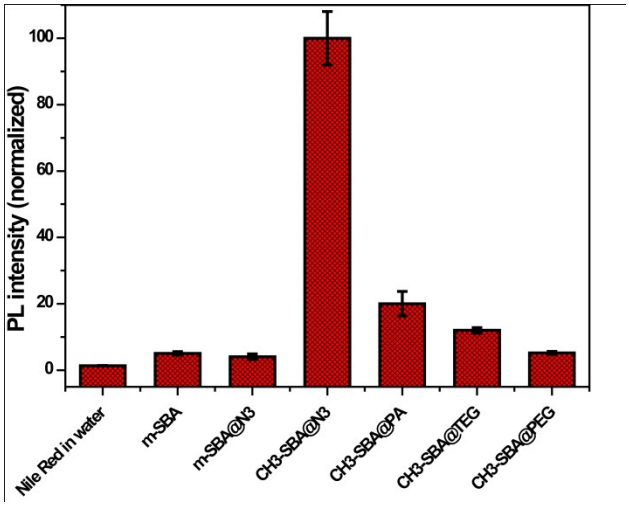
SI 2 Nitrogen adsorption-desorption Isotherm of Various functionalized silica. Surface area was calculated by BET method



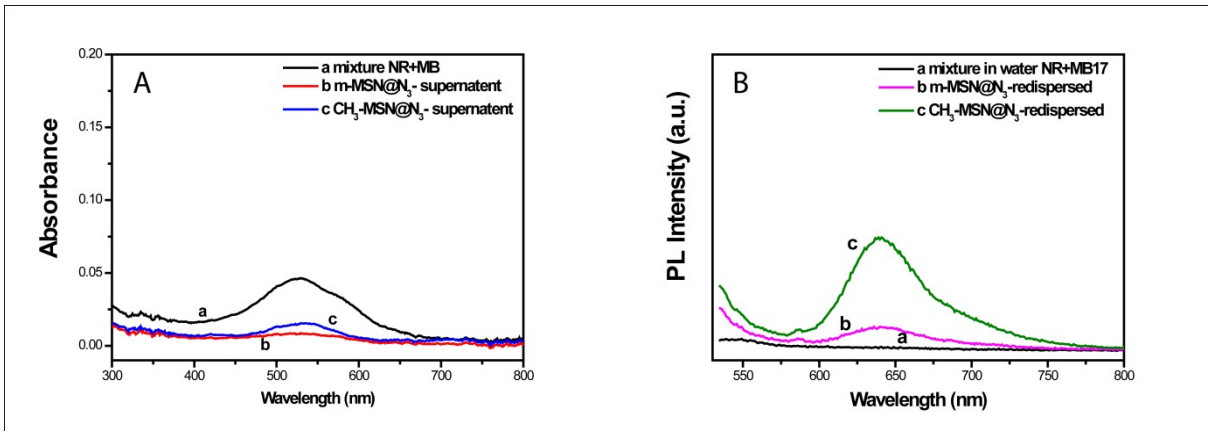
SI 3 Pore size distribution for MSN at various stages of functionalization obtained by BJH method



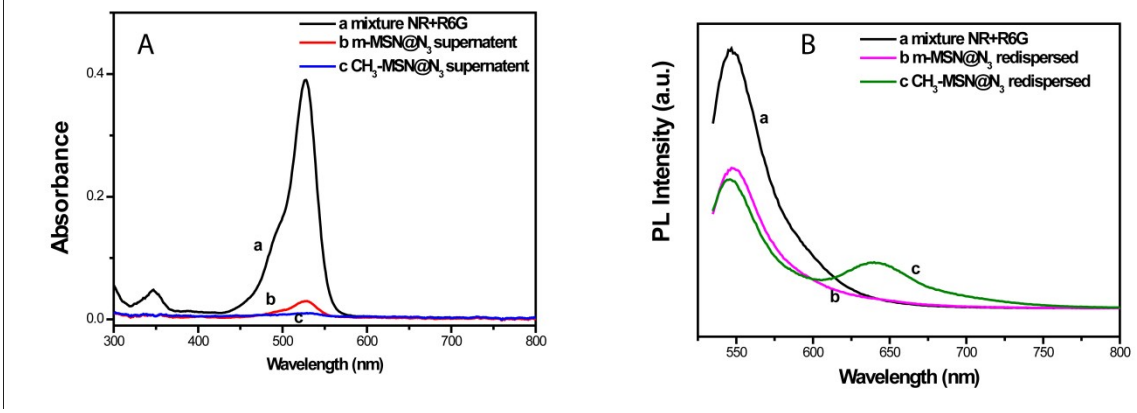
SI 4 Chemical structures of various dyes used in the study.



SI 5 Normalized PL intensities of Nile red when incubated with various functionalized SBA particles in water.



SI 6 Spectrophotometric analysis of dye adsorption by functionalized MSN from aqueous mixture of NR and MB 17 (0.05 mM each). A) UV-Vis spectra of a) mixture of dyes, supernatant solution after separation with b) m-MSN@N_3 and c) CH_3-MSN@N_3 . B) PL intensities after excitation at 525 nm a) mixture and dispersion in water incubated with various functionalized MSN particles after separation of unabsorbed dyes b) with b) m-MSN@N_3 and c) CH_3-MSN@N_3.



SI 7 Spectrophotometric analysis of dye adsorption by functionalized MSN from aqueous mixture of NR and R6G (0.05 mM each). A) UV-Vis spectra of a) mixture of dyes, supernatant solution after separation with b) m-MSN@N_3 and c) CH_3-MSN@N_3 . B) PL intensities after excitation at 525 nm a) mixture and dispersion in water incubated with various functionalized MSN particles after separation of unabsorbed dyes b) with b) m-MSN@N_3 and c) CH_3-MSN@N_3.

References

1. B. Singh, K. R. Mote, C. S. Gopinath, P. K. Madhu and V. Polshettiwar, *Angew.Chem.Int.Ed.*, 2015, **127**, 6083-6087.