

Electronic Supplementary Information

2-Hydroxy-naphthyl functionalized mesoporous silica for fluorescence sensing and removal of aluminum ion

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[#]Contributed equally

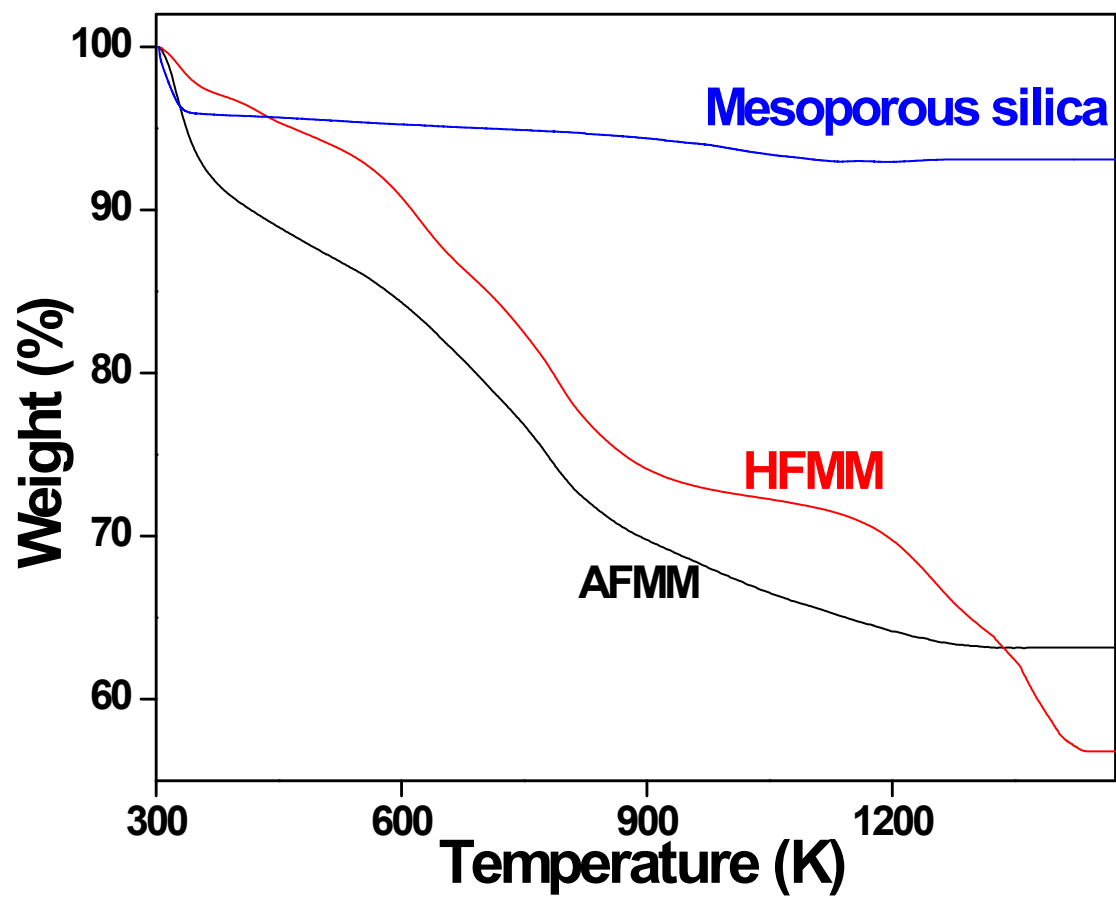


Fig. s1: Thermogravimetric analysis of mesoporous silica (blue), AFMM (black) and HFMM (red).

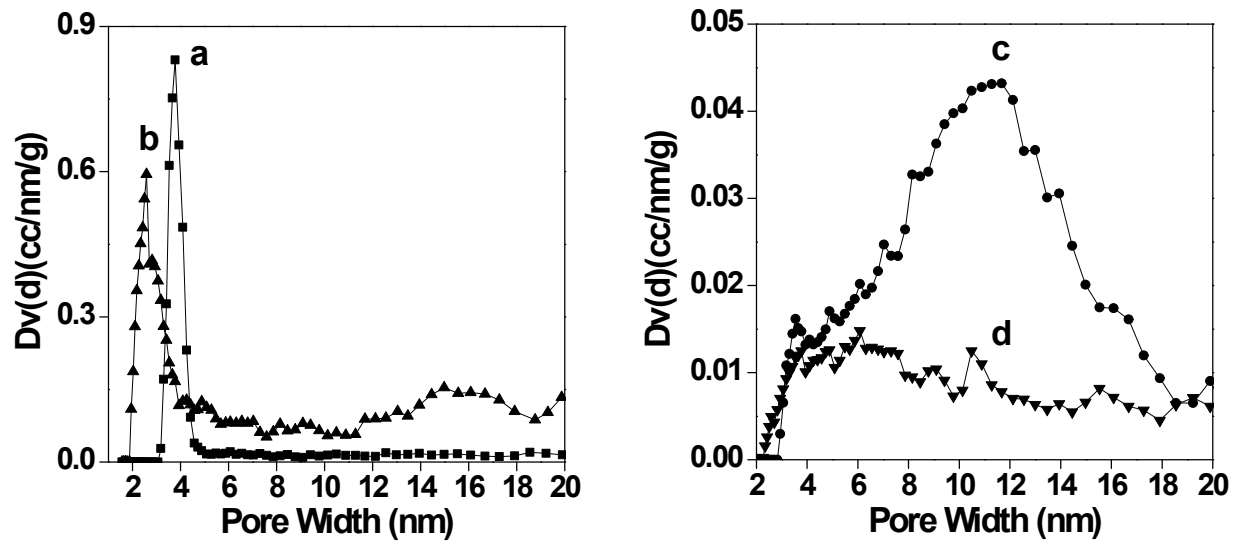
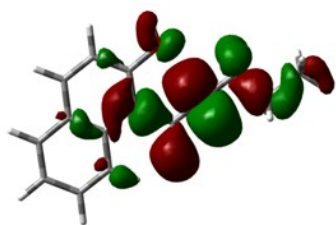
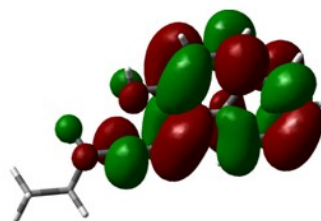


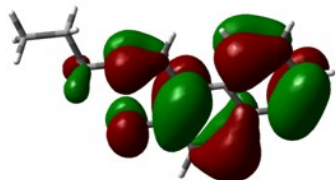
Fig. s2: Pore size distribution of mesoporous silica (a), AFMM (b), HFMM (c) and Al bound HFMM (d).



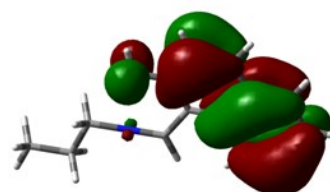
HOMO (-4.5236eV)



LUMO(-1.2161eV)

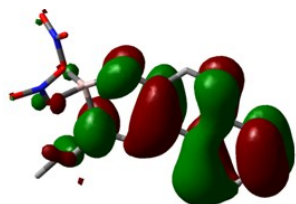


HOMO-1 (-5.6096eV)

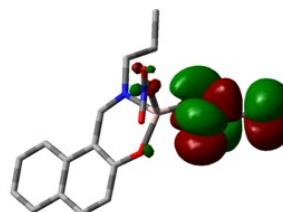


HOMO-2 (-6.4339eV)

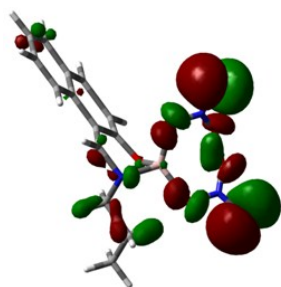
Frontier MOs of OF



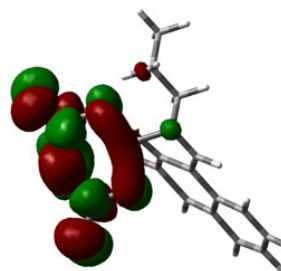
HOMO (-5.0387eV)



LUMO (-4.1247eV)



HOMO-5 (-7.9713eV)



LUMO+1(-2.7870eV)

Frontier MOs of OF-Al Complex

Fig. s3: Frontier MOs of OF and its aluminum complex, OF-Al.

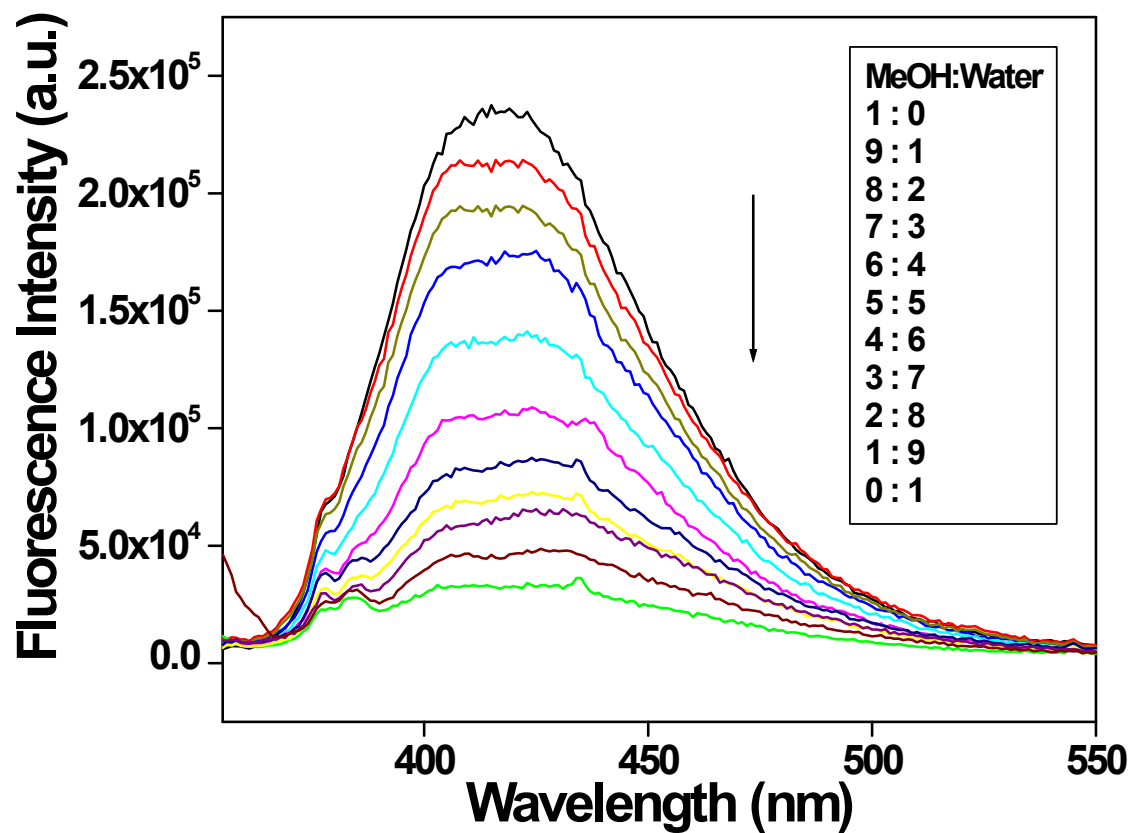


Fig. s4: Emission intensity of HFMM (0.7 mg/l) in the presence of 800 μM of Al³⁺ in various ratio of methanol/water.

Calculation of the detection limit (LOD)

Detection limit of HFMM for Al^{3+} was determined from 3σ method by following

equation: $\text{LOD} = K \cdot \text{Sb1}/S$

Where $K = 3$ in this case; Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. vs $[\text{Al}^{3+}]$.

$\text{Sb1} = 780.17267$

$S = 131.21192$

$\text{LOD} = (3 \times 780.17267)/131.21192 = 17.84 \mu\text{M}$

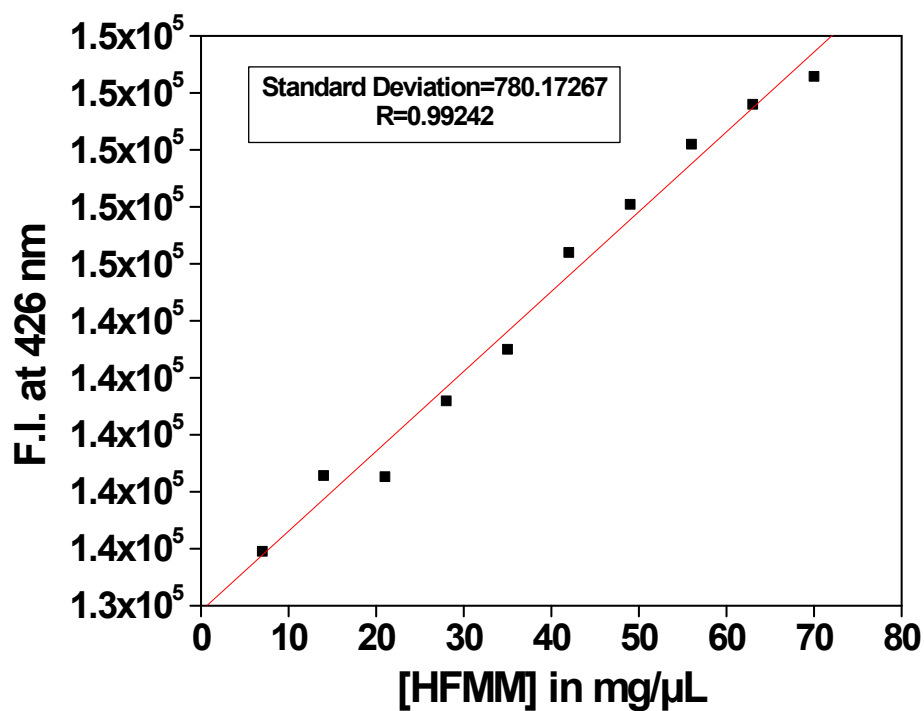


Fig. s5: Determination of Sb1 of the blank, HFMM solution

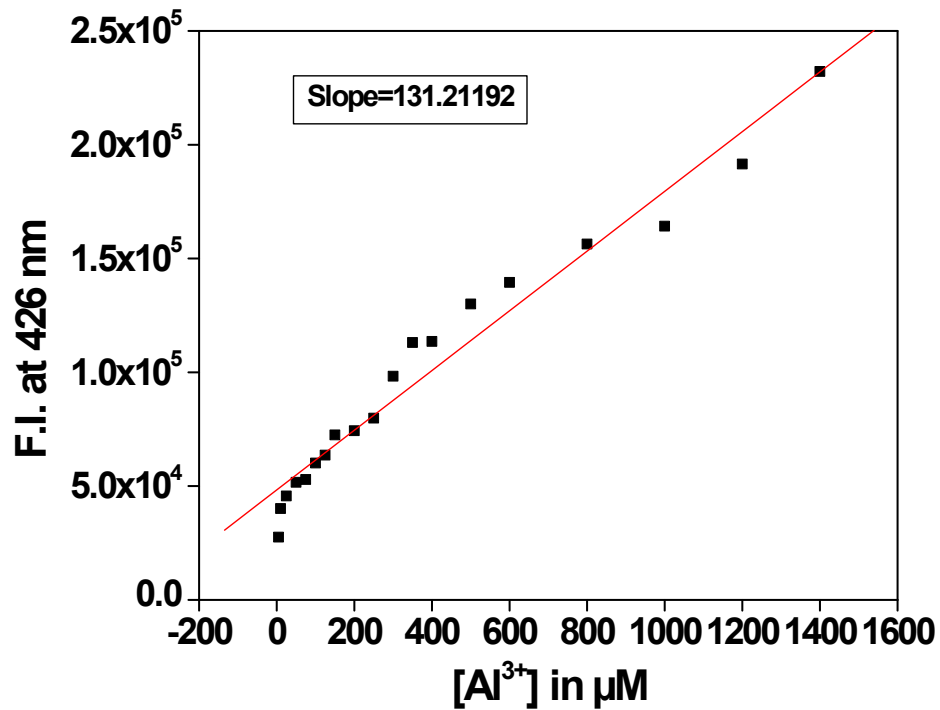


Fig. s6: Linear dynamic plot of F.I. (at 426 nm) vs. $[Al^{3+}]$ for the determination of S (slope); Concentration of HFMM = 0.7 mg/l.

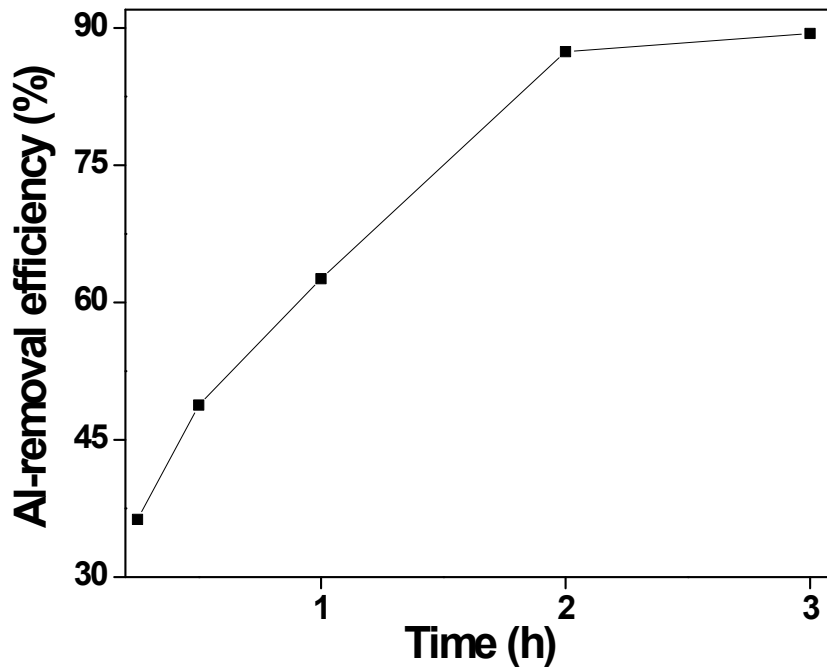


Fig. s7: Plot of aluminum removal efficiency of HFMM in 9:1 methanol/water against time

Table s1: Selected bond lengths and bond angles of OF-Al complex.

Bond lengths (Å)			
C5-O16	1.3396	Al17-O16	1.7811
C11-N12	1.3200	Al17-O18	1.8398
C13-N12	1.4926	Al17-O22	1.9673
Al17-N12	1.9466		
Bond angles (°)			
O16-Al17-O22	118.41	N12-Al17-O18	95.24
O16-Al17-O18	131.14	N12-Al17-O16	93.37
N12-Al17-O22	96.26	C5-O16-Al17	132.91
C11-N12-Al17	123.26	C11-N12-C13	117.94