

Optical sensors based on functionalized mesoporous silica SBA-15 for the detection of multianalyte (H^+ and Cu^{2+}) in water

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1. The ^{13}C MAS-NMR spectrum of 2-MPT-SBA-15

As shown in Figure S1, the detail analysis of the ^{13}C MAS-NMR spectrum of 2-MPT-SBA-15 directly verifies the presence of the intermediate, trimethoxysilane-derivative of 2-MPT, and its successful immobilization.^{S1}

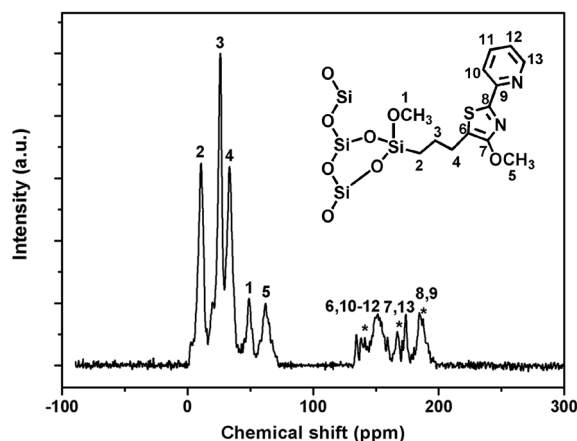
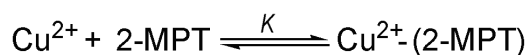


Fig. S1 Detail analysis of the ^{13}C MAS-NMR spectrum of 2-MPT-SBA-15

2. The formation constant for the interaction of 2-MPT-SBA-15 with Cu(II)

In this work, we applied the similar method reported in the previous literatures (ref. S2) to determine the formation constant for the interaction of 2-MPT-SBA-15 with Cu(II).

When 2-MPT-SBA-15 and Cu(II) coexisted, there should be the coordination equilibrium in the solution as follows:



Assuming the initial concentration of ligand 2-MPT is $[L]_0$, the concentration of the uncomplexed ligand [2-MPT] in the solution is $[L]$, and the concentration of Cu^{2+} is $[M]$, the binding constant could be represented as Eq. 1.

$$K = (1 - \alpha) / (\alpha [Cu^{2+}]) \quad (1)$$

The introduced α (Eq. 2, defined as the ratio between $[L]$ and $[L]_0$), could be directly related to the measured fluorescence intensity values F , where F_0 and F_1 are the limiting fluorescence values for $\alpha = 1$ (in the absence of Cu^{2+}) and $\alpha = 0$ (fully complexed 2-MPT).

$$\alpha = (F - F_1) / (F_0 - F_1) \quad (2)$$

In Figure S2, α is given as a function of the logarithm of Cu^{2+} ion concentration. The curve fitting for the experimental data points was calculated from Yang's equations with $\log K = 4.42$.^{S2a} The curve can serve as the calibration curve for the detection of Cu^{2+} .

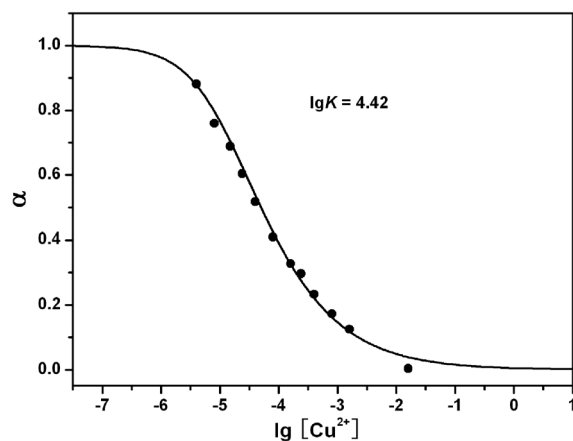


Fig. S2 Response parameter values (α) as a function of the logarithm of Cu^{2+} concentration. α is defined as the ratio between the free ligand concentration and the initial concentration of ligand.

References

- S1. (a) C. D. Nunes, A. A. Valente, M. Pillinger, A. C. Fernandes, C. C. Romão, J. Rocha and I. S. Gonçalves, *J. Mater. Chem.*, 2002, **12**, 1735; (b) D. Pérez-Quintanilla, I. Hierro, M. Fajardo and I. Sierra, *J. Mater. Chem.*, 2006, **16**, 1757.
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