Supporting Information

Selective Detection of Fe³⁺ Ions based on Fluorescence MXene Quantum Dots via a Mechanism Integrating Electron Transfer and Inner Filter Effect

Qiuxia Zhang^{*a b*}, Yan Sun^{*a b*}, Meiling Liu*^{*b*}, Yang Liu*^{*a*}

^a Department of Chemistry, Beijing Key Laboratory for Analytical Methods and Instrumentation, Key Laboratory of Bioorganic Phosphorus Chemistry & Chemical Biology of Ministry of Education, Tsinghua University, Beijing 100084, China
^b Key Laboratory of Chemical Biology & Traditional Chinese Medicine Research (Ministry of Education, China), College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha 410081, P. R. China

* Corresponding author

E-mail address: liumeilingww@126.com, liu-yang@mail.tsinghua.edu.cn

1. The calculation of quantum yield.

Quantum Yield: using quinine sulfate (QY=0.55) in sulfuric acid (0.1 mol L⁻¹, η = 1.33) as the standard, 360 nm as the excitation wavelength as reference, the quantum yield (QY) of the MQDs was calculated. In the calculation of quantum yield, six concentrations of each compound had absorbance less than 0.1 at 380 nm. The MQDs sample was dissolved in water (η = 1.33). Their fluorescence spectra were recorded at excitation of 380 nm. quantum yield was estimated with equation 1.

$$\Phi_{x} = \Phi_{q} \left(F_{x}/F_{q} \right) \left(A_{q}/A_{x} \right) \left(\eta_{x}^{2}/\eta_{q}^{2} \right)$$
eq S1

 Φ , F, A, and η are the quantum yield of the standard sample, integrated fluorescence intensity, absorbance, and refractive index, respectively. The subscript "q" is quinine sulfate.



Fig. S1 (A) The nominalized FL intensity of MQDs in the presence of NaCl with different concentrations.



Fig. S2 Zeta potential of MQDs in the (a) absence and (b) presence of Fe^{3+} .



Fig. S3 The FL intensity of MQDs with different concentration of Fe^{3+} (0, 2.5, 5, 10, 15, 20, 25, 50, 100, 250, 500, 1000, 1500, 2000 μ M). (B) The linear relationship between FL intensity and concentration of Fe^{3+} .

Table S1 IFE of Fe³⁺ on the fluorescence of MQDs.Fe³⁺(mm) A_{EX} A_{EM} CF F_{obsd} F_{cor}

Fe ³⁺ (mm)	A _{EX}	$\mathbf{A_{EM}}$	CF	Fobsd	Fcor	$F_{cor/}F_{cor0}$
0	0.2765	0.2069	1.6712	3720	6216	1
5	0.2807	0.2139	1.6909	3425	5790	0.9315
10	0.288	0.2206	1.7152	3311	5679	0.9136
20	0.3188	0.2215	1.7715	3114	5516	0.8874
5	0.384	0.224	1.8954	2833	5369	0.8639

$$F_c/F_0 = 2.3 dA_{ex}/(1-10^{-dAex}) \cdot 10 gA_{em} \cdot 2.3 sA_{em}/(1-10^{-sAem})$$
 eq S2

The F_c is the corrected fluorescence intensity, F_0 is the measured fluorescence intensity; A_{ex} and A_{em} is the UV-vis absorbance intensity at the excitation wavelength (λ_{ex} =380 nm) and maximum emission wavelength (λ_{em} = 500 nm), respectively; d is the width of the cuvette(1.00 cm), g is the distance between the edge of the cuvette and the edge of the excitation beam (0.40 cm), s is the thickness of excitation beam (0.10 cm). The maximum value of the correction factor could not exceed 3; otherwise, the correction is not convincing.

Sample Number	Added (µM)	Found (µM)	Recovery
1	25	26.99	107.96%
2	50	48.10	96.20%
3	75	83.39	111.18%
4	100	104.20	104.20%
5	125	123.67	98.94%
6	200	205.41	102.71%

Table S2 The Fe³⁺ activity analysis in sea water using MQDs.