Supporting Information:

Chlorine-Doped MoS_2 Quantum Dots Embedded in Molecularly Imprinted Polymer for Highly Selective and Sensitive Optosensing of Quercetin

Fengyi Wu*, Jiliang Yang, Yousheng Ye, Rong Wu, Haiyan Wang

Water environment research center, College of Chemistry and Material Engineering, Chaohu University, Hefei 238000, China

Water Environment Research Center, College of Chemistry and Material Engineering, Chaohu University, Hefei 238000, China; yangjiliang1984@126.com (J.Y.); yysheng@chu.edu.cn (Y.Y.); wurong@chu.edu.cn (R.W.); haiyan681108@163.com (H.W.)

* Correspondence: wfy@chu.edu.cn; Tel.: +86-551-82362251

Contents

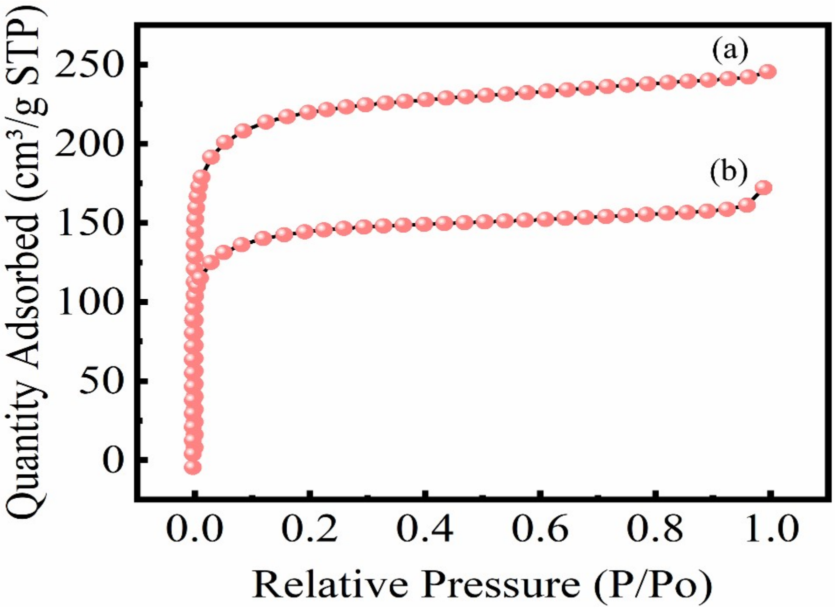


Figure and Table：

Fig.S1 BET surface area of Cl-MoS_2 QDs @ SiO_2 @ QR (a) and Cl-MoS_2 QDs @ SiO_2 @ MIP(b)

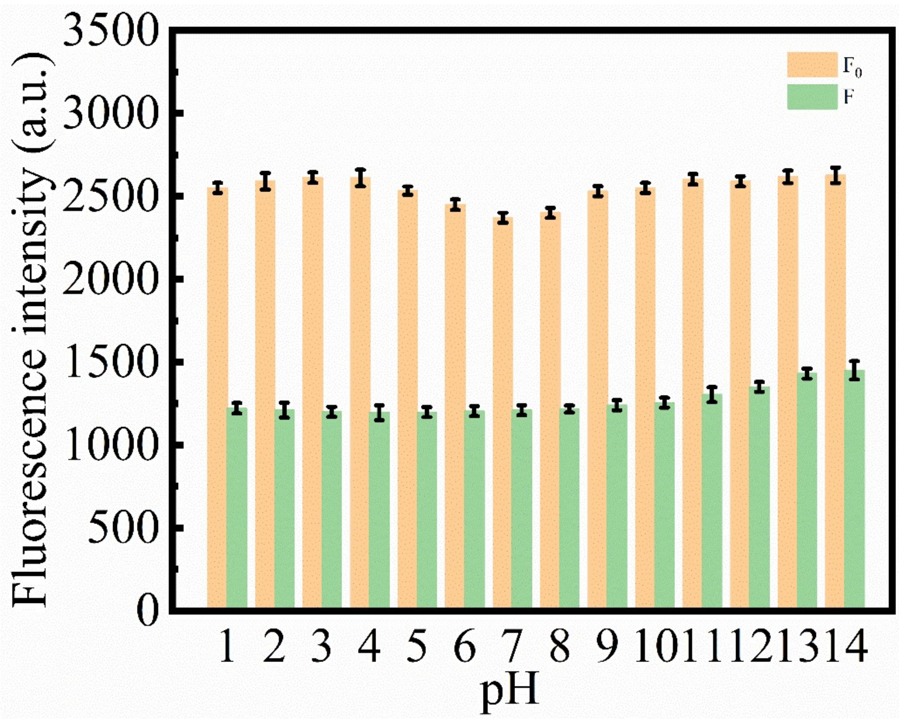
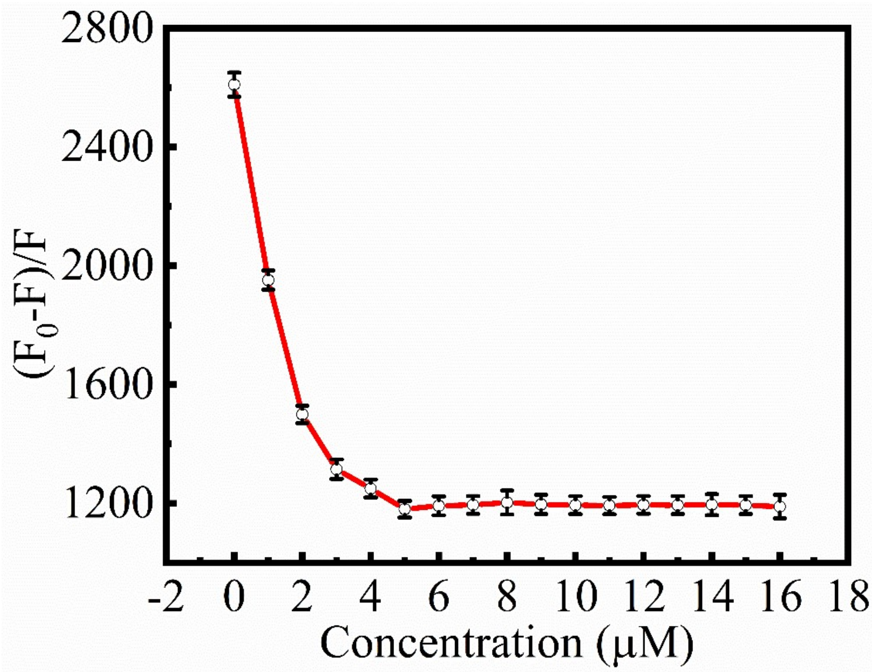


Fig.S2 Fluorescence intensity of Cl-MoS_2 QDs @SiO_2@ MIP with (F_0) and without (F) the quercetin under different pH. The results show that the fluorescence intensity of Cl-MoS_2 QDs @SiO_2@ MIP first decreases and then increases as the pH value increases. This fluorescence trend is related to the stability of Cl-MoS_2 QDs @SiO_2@ MIP. In acidic and alkaline solutions, Cl-MoS_2 QDs @SiO_2@ MIP has good stability ,thereby exhibiting relatively strong fluorescence. However, under alkaline conditions,



quercetin undergoes partial decomposition,which affect the reliability of testing results.Overall consideration. The optimal pH value is 4 for detection of quercetin using Cl-MoS_2 QDs @SiO_2@ MIP sensor.

Fig. S3 Effect of incubation time on fluorescence intensity of Cl-MoS_2 QDs@SiO_2@ MIP. The results revealed a rapid and significant decrease in fluorescence intensity of Cl-MoS_2 QDs@SiO_2@ MIP within a 5-minute interval upon addition of quercetin. Afterward, the fluorescence intensity of Cl-MoS_2 QDs@SiO_2@ MIP remained relatively constant. As a result, the optimal incubation time for quercetin detection using Cl-MoS_2 QDs@SiO_2@ MIP is determined to be 5 minutes.

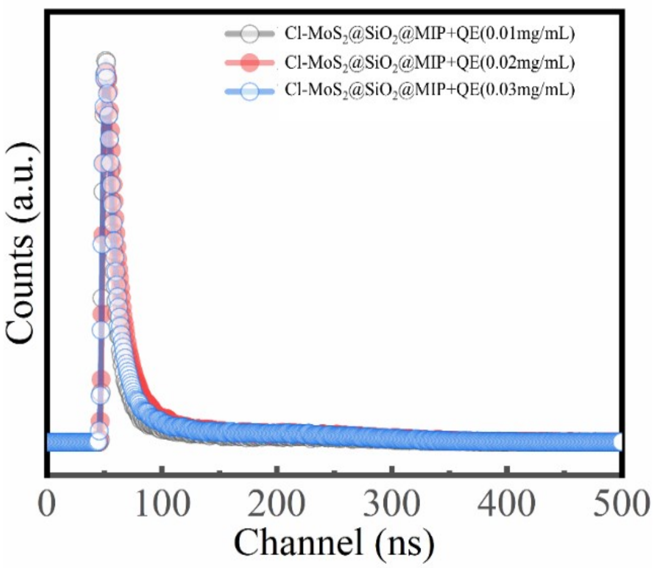


Fig. S4 Transient photoluminescence spectra of Cl-MoS_2 QDs @ SiO_2 @ MIP with the additon of different concentrations quercetin (QR).

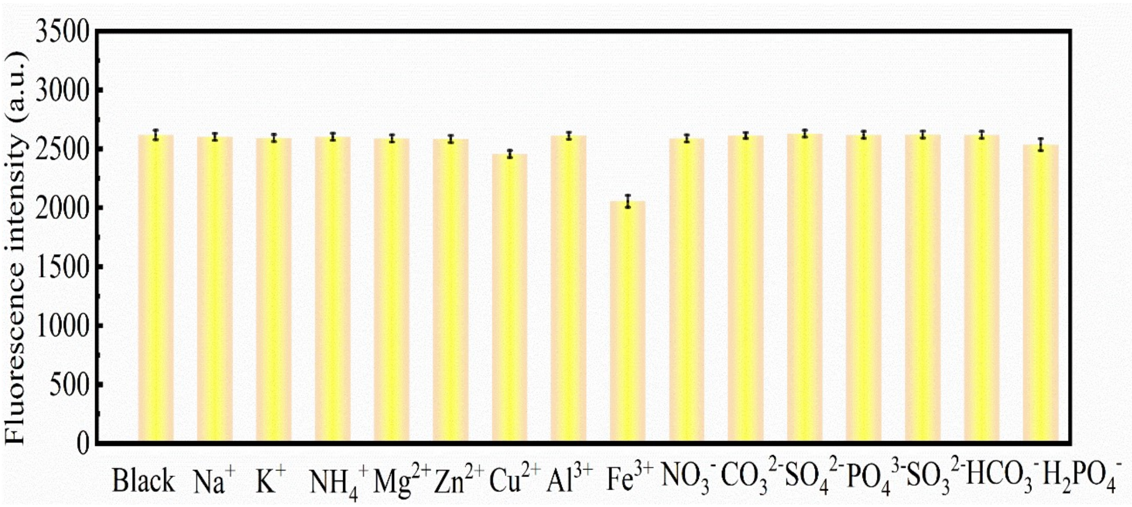


Fig. S5 Fluorescence of the Cl-MoS_2 QDs @ SiO_2 @ MIP with diverse interfering ions.

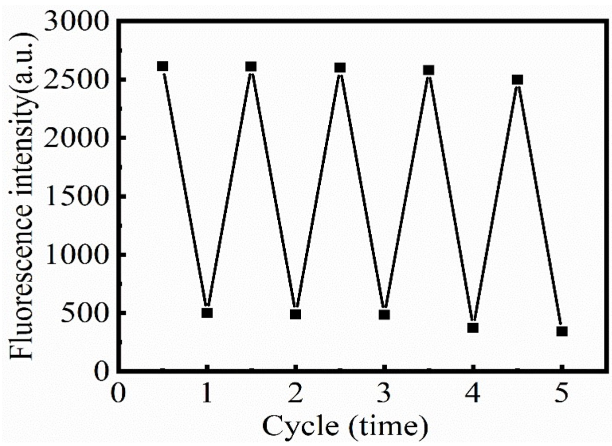
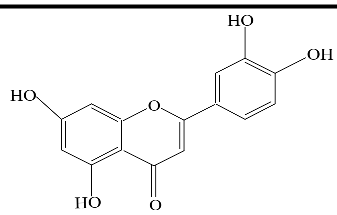
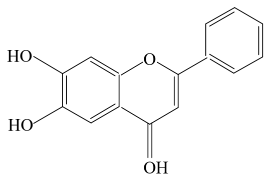
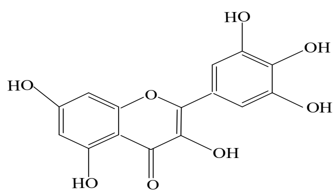
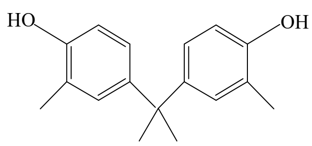


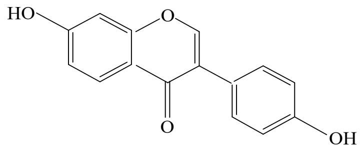
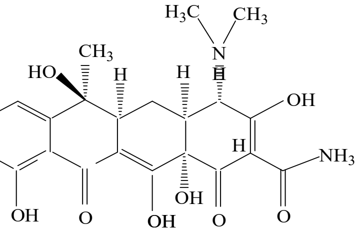
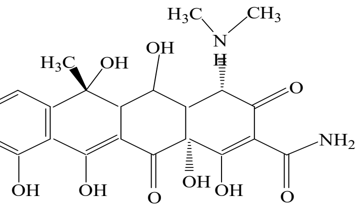
Fig. S6 Recyclablility test of quercetin with Cl-MoS_2 QDs @SiO_2@ MIP. In order to reuse Cl-MoS_2 QDs @ SiO_2 @ MIP, the fluorescent probe was collected by centrifugation after the latest detection. Then, the obtained fluorescent probe was reflowed with acetone and vacuum dried for the next use.

Table S1. Detection of quercetin with different fluorescense sensors

Material	linear range	LOD	Recovery	Referenc
C QDs	0-40 μM	79 nM		[1]
Au QDs	0.089-180 μM	0.018 μM		[2]
Ag-Au QDs	0.9-100 μM	0.65 μM		[3]
CdSe/ZnS QDs	0.576–184 mg/L	0.14 mg/L		[4]
C NPs	3.3-41.2 μM	0.175 μM		[5]
C dots	1-47μM	172.4 nM		[6]
Ni-CQDs	0.5-300 μM	0.137 μM	97.3-101.9%	[7]
[Tb_4] MOF	0−993 μM	0.76 μM	-	[8]
C_3N_4 QDs@MIP	10–1000 ng/mL	2.5 ng/mL	90.7-94.1%	[9]
C QDs@MOF@MIP	0−50 μM	2.9 nM		[10]
N-C QDs	0.5-80 μg/mL	0.21 μg/mL		[11]
MoS_2QDs@SiO_2@MIP	2-200ng/mL	1.2 ng/mL	91.2%-104.2%	This is work

Table S2. The structure formula of small organic molecules

Chemicals	molecular formula	structural formula
Quercetin (QE)	$C_{15}H_{10}O_7$	
Baicalein (BE)	$C_{15}H_{10}O_5$	
Myricetin (ME)	$C_{15}H_{10}O_8$	
Bisphenol C (BC)	$C_{17}H_{20}O_2$	

Daidzein (DE)	$C_{15}H_{10}O_4$	
Tetracycline (TC)	$C_{22}H_{24}N_2O_8$	
Oxytetracycline (OC)	$C_{22}H_{24}O_9N_2$	

The Stern-Volmer equation:

$$\frac{F_0 - F}{F} = K_{SV}C_q = K_q\tau_0 C_{q,}$$

where F_0 and F are the fluorescence (FL) intensity of Cl-MoS_2 QDs @ SiO_2 @ MIP in the absence and presence of quercetin, respectively; Cq is the concentration of quercetin, and the dynamic quenching constant Ksv is 4.79 $\times 10^6$ $(mol/L)^{-1}$ by taking the slope of the regression line in Figure 6 (b). Here, term τ_0 is the average fluorescence lifetime of Cl-MoS_2 QDs @ SiO_2 @ MIP (τ_0 = 8.10 ns).

References

1. Y. Zou, F. Y. Yan, T. C. Zheng, D. C.Shi, F. Z. Sun, N. Yang and L. Chen, *Talanta*, 2015, **135**, 145-148.
2. Z. G. Chen, S. H. Qian, J. H. Chen and X. Chen, *J. Nanopart. Res.*, 2012, **14**, 1-8.
3. Z. Chen, G. Zhang, X. Chen, J. Chen and Z. Fu, *Plasmonics*, 2013, **8**, 201-207.
4. W.-P. Hu, G.-D. Cao, W. Dong, H.-B. Shen, X.-H. Liu and L.-S. Li, *Anal. Methods*, 2014, **6**, 1442-1447.
5. P. L. Zuo, D. L. Xiao, M. M.Gao, J. Peng, R. F. Pan, Y. Xia and H. He, *Microchim.*

Acta, 2014, **181**, 1309-1316.
6. F. F. Du, S. M. Shuang, Z. H. Guo, X. J. Gong, C. Dong, M. Xian and Z. H. Yang, *Talanta*, 2020, **206**, 120243-120250.
7. Y.-F. Gao, X. Jin, F.-Y. Kong, Z.-X. Wang and W. Wang, *Analyst*, 2019, **144**, 7283-7289.
8. T.-Q. Song, K. Yuan, W.-Z. Qiao, Y. Shi, J. Dong, H.-L. Gao, X.-P. Yang, J.-Z. Cui and B. Zhao, *Anal. Chem.*, 2019, **91**, 2595-2599.
9. S. N. Xu, L.G. Chen and L. Ma, *Microchim. Acta*, 2018, **185**, 1-9.
10. L. H. Xu, M. F. Pan, G. Z.Fang and S. Wang, *Sens. Actuators, B-Chem.*, 2019, **286**, 321-327.
11. B. H. Gao, Y. Sun, Y. C.Miao, H.H. Min, L. Xu and C. B. Huang, *Aust. J. Chem.*, 2018, **71**, 882-889.