

Electronic Supporting Information

Dummy Molecularly Imprinted Polymers Capped CdTe Quantum Dots for Fluorescent Sensing of 2,4,6-Trinitrotoluene

Shoufang Xu,^{abc} Hongzhi Lu,^a Jinhua Li,^b Xingliang Song,^a Aixiang Wang,^a Lingxin Chen,^{*b}
Shaobo Han^a

^a School of Chemistry & Chemical Engineering, Linyi University, Linyi 276005, China

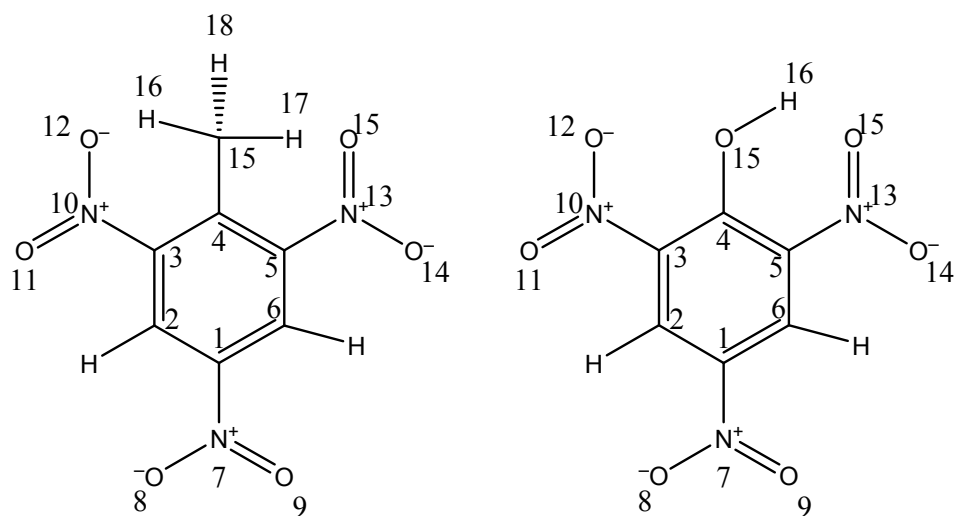
^b Key Laboratory of Coastal Zone Environmental Processes and Ecological Remediation,
Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, Yantai 264003,
China

^c University of Chinese Academy of Sciences, Beijing 100049, China

* Corresponding author.

E-mail: lxchen@yic.ac.cn; Fax/Tel: +86-535 2109130.

Figure S1. Bond length and bond angle of TNT and TNP.



	Bond length			Bond angle	
	TNT	TNP		TNT	TNP
C1-C2	1.38601	1.38602	C1-C2-C3	118.25739	118.25755
C2-C3	1.39052	1.39051	C2-C1-N7	119.28264	119.42376
C3-C4	1.41125	1.41126	C1-N7-O8	117.15488	117.10332
C4-C5	1.41127	1.41125	O8-N7-O9	125.68999	125.62312
C5-C6	1.39051	1.39052	C2-C3-N10	114.88034	115.83989
C1-N7	1.47500	1.47070	C3-N10-O11	116.90382	116.47112
C3-N10	1.48105	1.46457	O11-N10-O12	125.36949	125.75656
C5-N13	1.48107	1.47948			
N7-O8	1.22770	1.22855	C4-C15-H16	110.93805	
N7-O9	1.22770	1.22837	C4-C15-H17	110.93256	
N10-O11	1.22776	1.22991		Dihedral angle	
N10-O12	1.22837	1.22432		TNT	TNP
N13-O14	1.22776	1.21944	O7-N7-C1-C2	0.13723	1.13296
N13-O15	1.22836	1.25060	O11-N10-C3-C3	32.01427	30.02358
C4-C15	1.50795	1.31638	O15-N13-C5-C4	-33.18867	1.18657
C15-H16	1.08847	0.99323	H16-C15-C4-C3	26.96666	178.46113
C15-H17	1.08849		H17-C15-C4-C3	149.18025	
C15-H18	1.09347		H18-C15-C4-C3	-91.93290	
				Radius (Å)	
				TNT	TNP
				4.46	4.63

Figure S2. Fluorescence emission spectra of DMIP@QD prepared by reverse microemulsion method (A) and Stöber method (B) with increasing TNT concentration in ethanol solution.

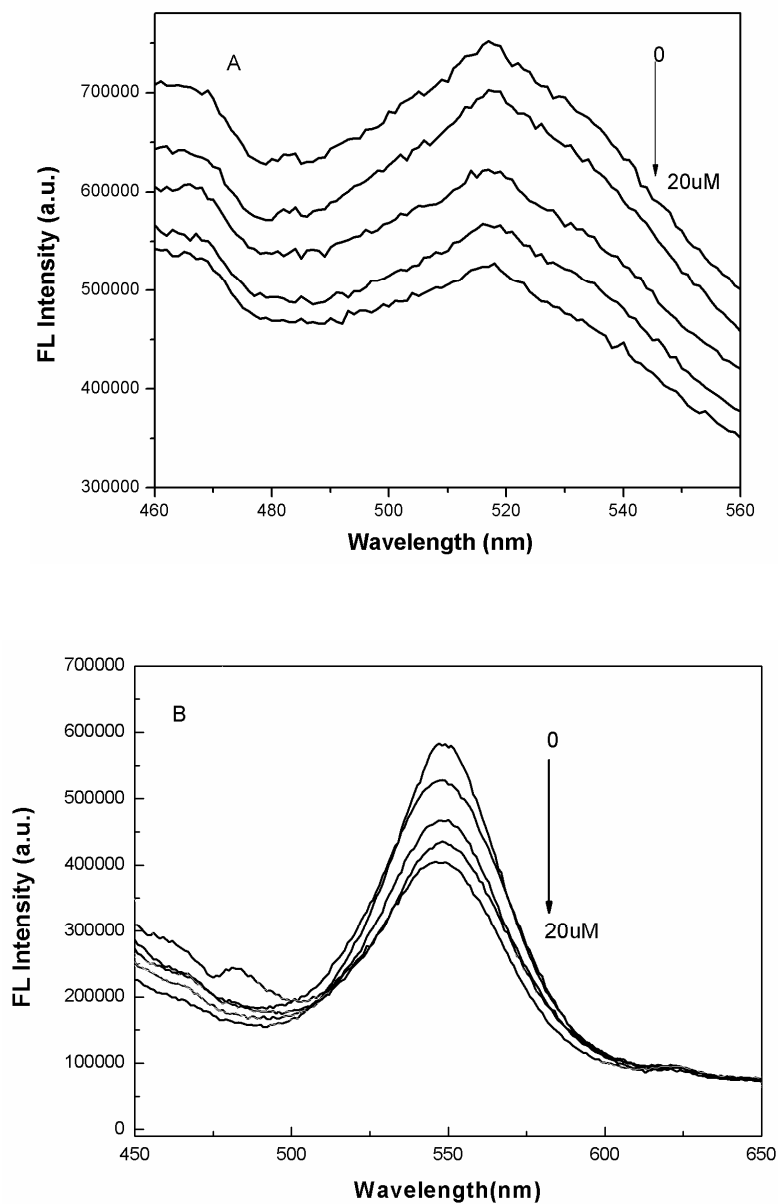


Figure S3. Fluorescence intensity change of DMIP@QDs within 7 days.

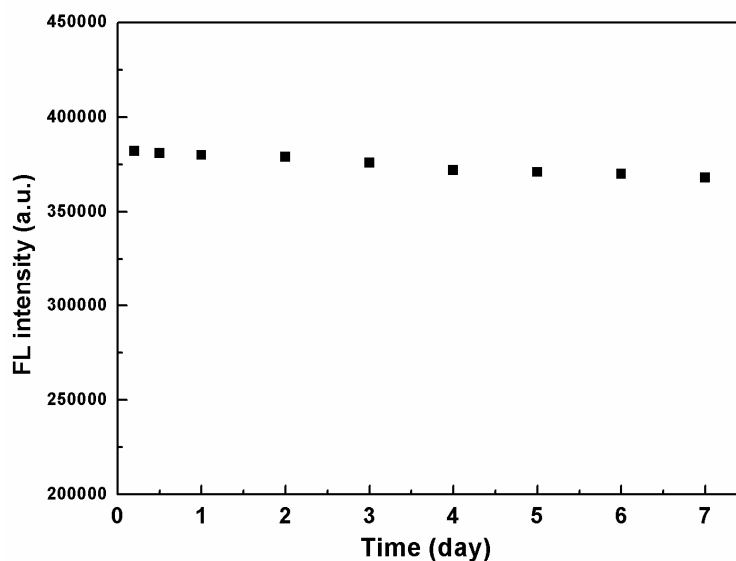


Figure S4. Effect of disperse medium on quenching efficiency. During the experiment, the concentration of TNT was fixed as 10 μ M, changing the disperse medium for water (black line), water/ethanol (8:2) (green line), water/ethanol (7:3) (blue line), and ethanol (red line). The lines of A, B, C, D were DMIP@QDs without TNT, and the line of a, b, c, d were those DMIP@QDs in the present of 10 μ M TNT.

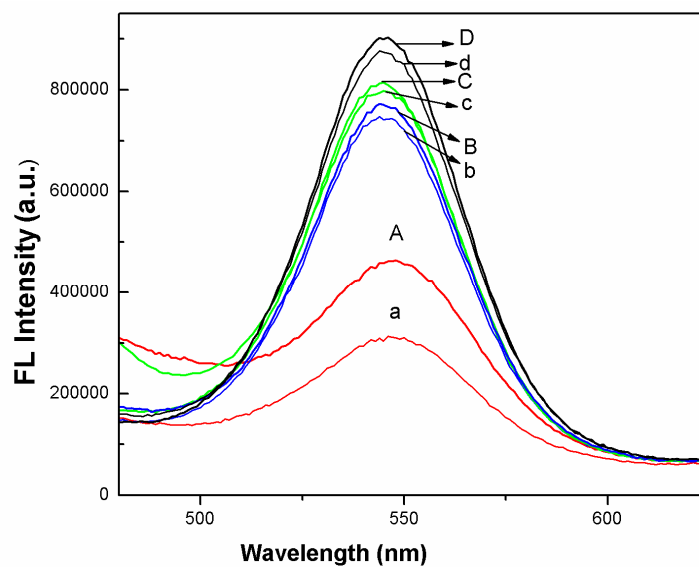


Figure S5. Effect of amount of DMIP@QDs on quenching efficiency. During the experiment, the concentration of TNT was fixed as 10 μ M, changing the amount of DMIP@QDs from 10mg/L (green line), 30 mg/L (red line), 50 mg/L (black line) and 70 mg/L (blue line). The lines of A, B, C, D were DMIP@QDs without TNT, and the line of a, b, c, d were those DMIP@QDs in the present of 10 μ M TNT.

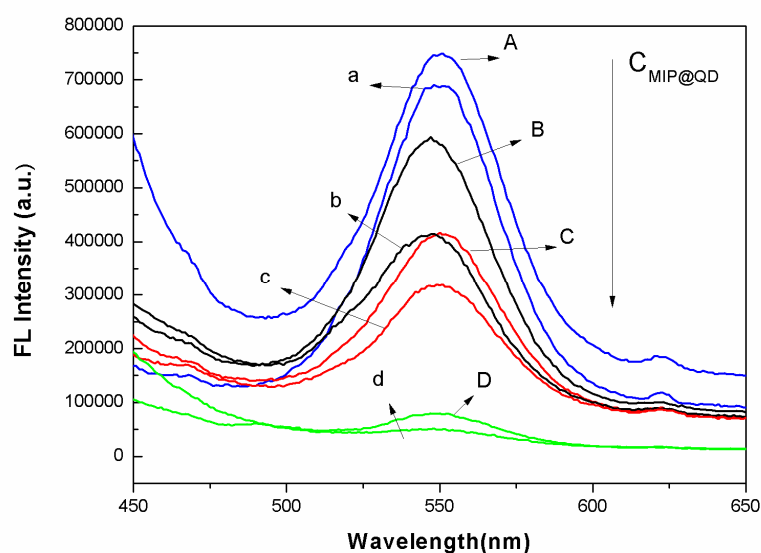


Figure S6. Recovery of FL intensity of DMIP@QDs after removal of TNT. (Experimental condition: DMIP@QD: 50 mg, C_{TNT} : 10 μ M)

