Supporting Information

High selectivity in water soluble MoS₂ quantum dot for sensing nitroexplosives

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Figure S1:Energy dispersive X-ray spectroscopy (EDX) analysis of prepared MoS₂ quantum dot.



Figure S2: Zeta potential value (-1.04mV) of 1,4-diamminobutane functionalized MoS_2 quantum dot in water.



Figure S3: Zeta potential value (-17.4mV) of bare MoS₂ quantum dot in water.

Fluorescence quenching titration experiments:

We have also studied the fluorescence quenching experiments for different nitro explosives and different organic and inorganic acids but these shows very weak PL quenching to functionalized MoS₂ quantum dots compared to TNP. The quenching efficiency plots for those nitro compounds and different acids are given below;



Figure S4: PL quenching with the addition of 1 mM 2, 6-DNT solution pH = 7.



Figure S5: PL quenching with the addition of 1 mM 2-NT solution pH= 7.



Figure S6: PL quenching with the addition of 1 mM 4-NT solution pH= 7.



Figure S7: PL quenching with the addition of 1 mM 1, 2-DNB solution pH= 7.



Figure S8: PL quenching with the addition of 1 mM 1, 3-DNB solution pH= 7.



Figure S9: PL quenching with the addition of 1 mM 1,4-DNB solution pH= 7.



Figure S10: PL quenching with the addition of 1 mM NB solution pH= 7.



Figure S11: PL quenching with the addition of 1mM Benzoic Acid solution pH= 7.



Figure S12: PL quenching with the addition of 1 mM Formic Acid solution pH= 7.



Figure S13: PL quenching with the addition of 1mM Acetic Acid solution pH=7.



Figure S14: PL quenching with the addition of 1mM Phenyl Acetic Acid solution pH= 7.



Figure S15: PL quenching with the addition of 1mM Succinic Acid solution pH= 7.



Figure S16: PL quenching with the addition of 1mM Sulfuric Acid (H_2SO_4) solution pH= 7.



Figure S17: PL quenching with the addition of 1mM Ortho-Phosphoric acid (H_3PO_4)solution pH=7.



Figure S18: PL quenching with the addition of 1mM Hydrochloric acid (HCl) solution pH= 7.



Figure S19: PL quenching with the addition of 1mM Nitric acid (HNO₃) solution pH= 7.

7. Calculation of Detection Limit for TNP:

The detection limit for TNP is calculated from fluorescence quenching experiment of water soluble functionalized MoS₂ quantum dot with the addition of TNP. The intercept (log[TNP]) to X-axis is obtained by linear plot of the (Imax-I)/(Imax-Imin) vs. log[TNP], where Imax, I and Imin are the initial fluorescence intensity, intensity at different TNP concentration and intensity at saturation point respectively. Detection limit is calculated using formula, ([TNP] × MW_{TNP})/1000) and multiplying this with factor10⁹, we get the detection limit value in ppb¹. Here, MW_{TNP} is the molecular weight of TNP. The calculated detection limit for TNP is 204 ppb.



Figure S20: Detection limit of TNP by functionalized MoS_2 quantum dot.

Notes and References:

1. Roy B., Bar A. K., Gole B., Mukherjee, P. S., J. Org. Chem. 2013, 78, 1306-1310.