Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supporting information

Green Synthetic route for Surface-passivation of Carbon Dots as an Effective Multifunctional fluorescent sensor for Recognition of Toxic metal ions Detection from aqueous Solution

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ESI 1. XPS spectra of self-passivated and passivated CDs

The XPS analysis was performed to analysis the surface functionalization of Iy-CDs. The XPS survey spectra (Fig.S1 a) attributes the presence of C1s, N1s, and O1s elements. The C1s spectra (Fig.S1 b) shows three peaks at 284.2, 286.1 and 287.4 eV, which are recognized to C-C, C-O, and C=O/ C=N bands in Iy-CDs. The N1s spectra (Fig.S1 c) shows two peaks at 399.6 and 400.3 eV, which are recognized to C-N-C and N-C_3 bands in Iy-CDs. The O1s spectra (Fig.S1d) shows two peaks at 531.4, and 532.1 eV, which are attributed to C-OH/C-O-C and C=O bands in Iy-CDs.

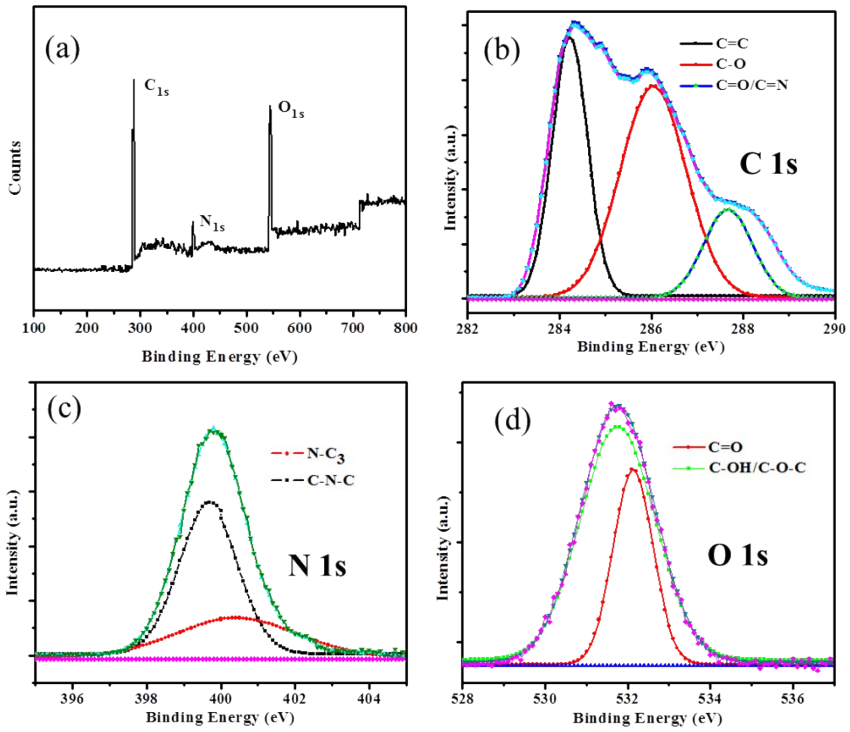

Fig.S1. The full range XPS spectra of (a) Iy-CDs. The Fig. c-d is high resolution XPS spectra of C1s, N1s and O 1s of Iy-CDs.

The XPS analysis of N,S/Iy-CDs exhibits the surface functionalization of C1s, N1s, O1s and S2p elements as shown in Fig.S2a. The C1s spectra (Fig.S2b) shows peaks at 283.7, 284.2, 285.4, 286.3, 287.4 and 289.0 eV, which are recognized to C=C, C-C, C-N, C-O, C=O/ C=N and O=C-O bands in N,S/Iy-CDs. The N1s spectra (Fig.S2 c) show peak at 400.1 eV, which are recognized to C-N band in N,S/Iy-CDs. The O1s spectra (Fig.S2d) shows a peak at 530.1, 531.1, and 532.3 eV, which are attributed to HO-C=O, C-OH/C-O-C and C=O bands in N,S/Iy-CDs. The S2p spectra (Fig.S2e) shows two peaks at 163.5 and 164.5 eV, which are attributed to C-S and C-SH bands in N,S/Iy-CDs.

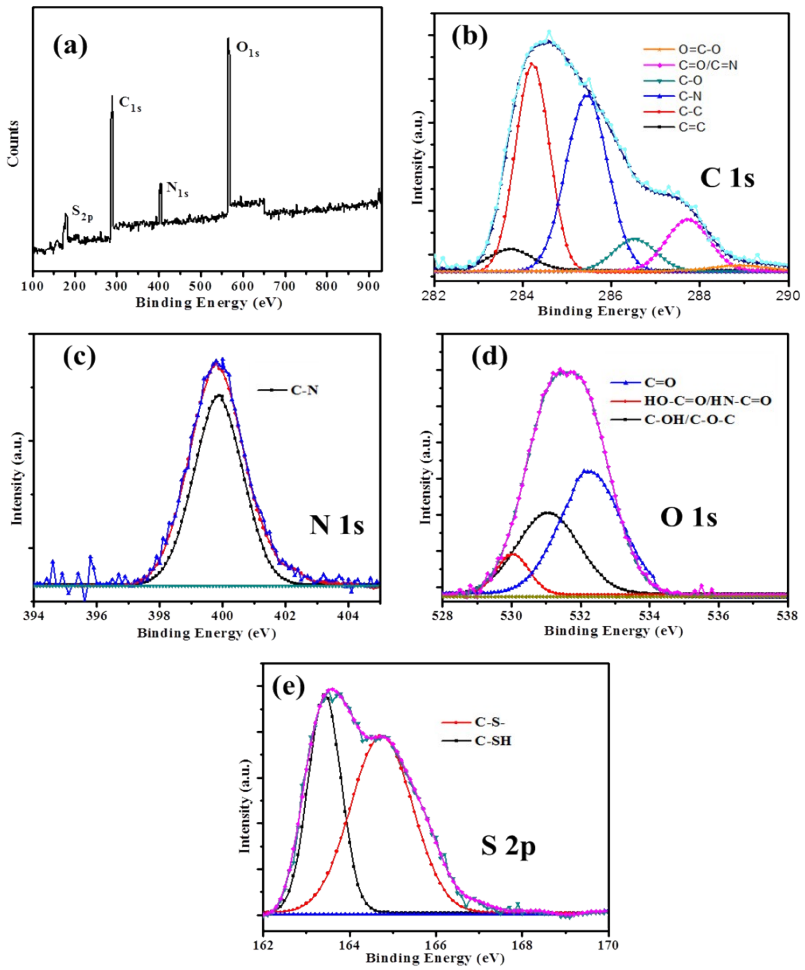

Fig.S2. The full range XPS spectra of (a) N,S/Iy-CDs. The Fig.c-e, is high resolution XPS spectra of C1s, N1s, O 1s, and S 2p of N,S/Iy-CDs.

The XPS analysis of N/Iy-CDs exhibits the surface functionalization of C1s, N1s, and O1s elements as shown in Fig.S3a. The C1s spectra (Fig.S3b) shows peaks at 284.3, 286.5 eV, which are recognized to C-C and C-N bands in N/Iy-CDs. The N1s spectra (Fig.S3c) show peak at 400.0 eV, which are recognized to C-N band in N/Iy-CDs. The O1s spectra (Fig.S3d) shows two peaks at 531.0, and 532.3 eV, which are attributed to C-OH/C-O-C and C=O bands in N/Iy-CDs.

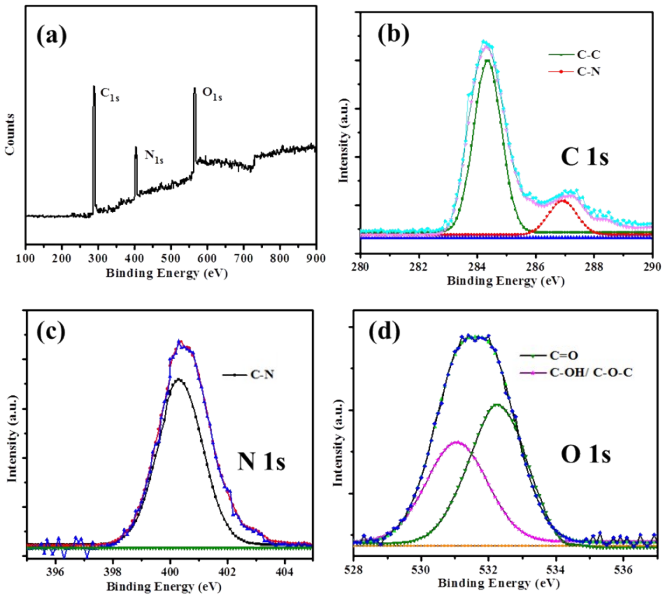

Fig.S3. The full range XPS spectra of (a) N/Iy-CDs. The Fig.c-d, is high resolution XPS spectra of C1s, N1s and O 1s of N/Iy-CDs.

The XPS analysis of N,O/Iy-CDs exhibits the surface functionalization of C1s, N1s, and O1s elements as shown in Fig.S4a. The C1s spectra (Fig.S4b) shows peaks at 284.06, 85.5, 287.6 and 290.1 eV, which are recognized to C-C/C=C/C-H, C-OH/C-N, C-O-C/C=O and HO-C=O/HN-C=O bands in N,O/Iy-CDs. The N1s spectra (Fig.S4c) show peak at 398.0 and 400.0 eV, which are recognized to C-N-C and N-C_3 band in N,O/Iy-CDs. The O1s spectra (Fig.S4d) shows peaks at 530.1, 531.1, and 532.0 and 534.1 eV, which are attributed to HO-C=O, C-OH/C-O-C, C=O and H-O-H bands in N,O/Iy-CDs.

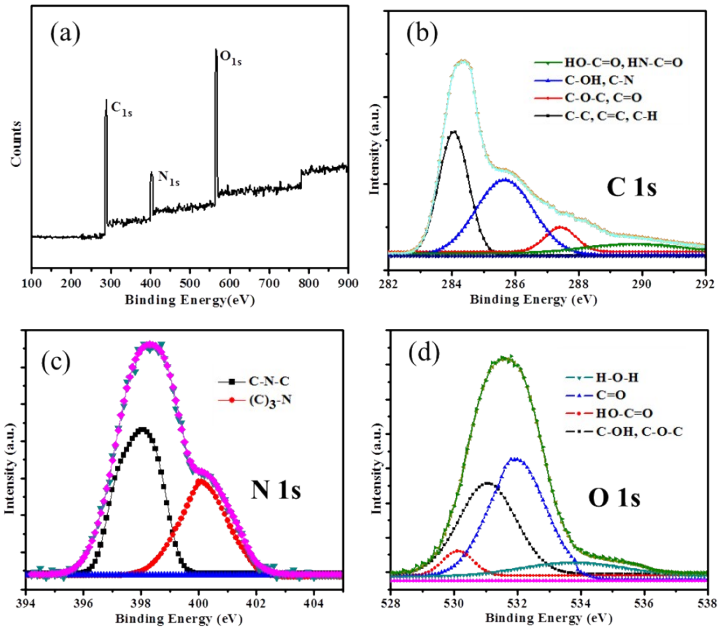

Fig.S4. the full range XPS spectra of (a) N,O/Iy-CDs. The Fig.c-d, is high resolution XPS spectra of C1s, N1s and O 1s of N,O/Iy-CDs.

ESI 2. Optimization of reaction time

The time-dependent fluorescence quenching response rate between CDs with metal ions were estimated. As shown in Fig. S5, when Hg^{2+} ions (50 µM), Cu^{2+} ions (30 µM), Pb^{2+} (10 µM) and Fe^{3+} (60 µM), respectively are spiked into self-passivated and passivated CDs solution, the quenching in fluorescence intensity was observed with reference to time. The quenching response of Iy-CDs for Hg^{2+} ions (50 µM), and N,O/Iy-CDs for Fe^{3+} (60 µM) occurs immediately in 1 min of contact time, and the steady state attained within 2 min. Furthermore, the N,S/Iy-CDs for Cu^{2+} ions (30 µM) and N/Iy-CDs for Pb^{2+} (10 µM), the fluorescence intensity was quenched within 2 min of the contact time and the reaches the steady state in 3 min. the fluorescence intensity of the CDs remain constant with further increase in contact time.

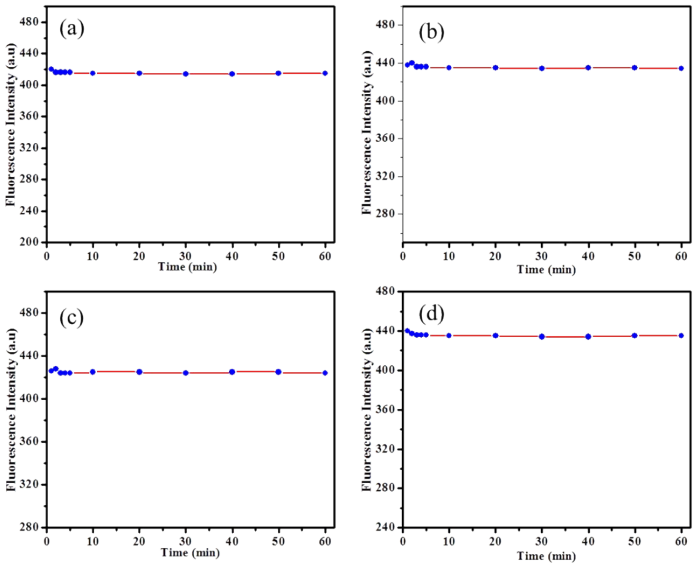

Fig.S5. The time-dependent fluorescence quenching response of CDs (a) self-passivated Iy-CDs and the surface passivated absorption spectra of (b) N,S/Iy-CDs, (c) N/Iy-CDs, and (d) N,O/Iy-CDs.

ESI 3. Optimization of pH

The fluorescence quenching response CDs were investigated upon regulating the pH values. As shown in Fig. S6, fluorescence intensity of the self-passivated and passivated CDs are significantly analyzed in an acidic to a basic medium. The emission response of CDs remains stable in acidic to basic range, upon addition of metal ions high quenching efficiency was noted in neutral medium (pH=7), this supports the potential application of synthesized CDs in neutral medium.

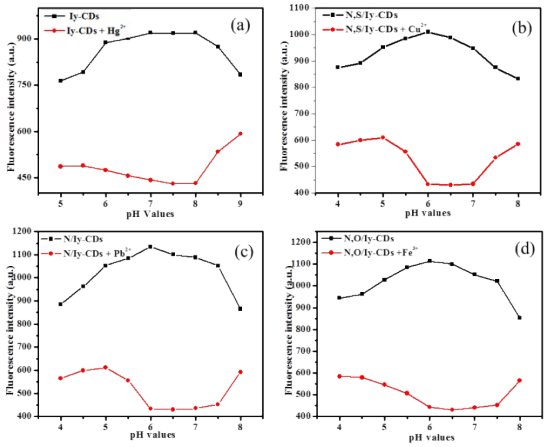

Fig. S6. The fluorescence quenching response of CDs (a) self-passivated Iy-CDs and the surface passivated absorption spectra of (b) N,S/Iy-CDs, (c) N/Iy-CDs, and (d) N,O/Iy-CDs at different pH values and in presence of Hg^{2+} ions (50 µM), Cu^{2+} ions (30 µM), Pb^{2+} (10 µM) and Fe^{3+} (60 µM) respectively

ESI 4. Optimization of CDs concentration

The concentrations of carbon dots are significantly affect the efficiency of the analysis. The blank experiment were performed at different concentration of CDs 20, 50, 100, 150, 200, 250, 300, µg/mL. The fluorescence intensity was measured for different concentration of CDs (self-passivated Iy-CDs and surface passivated (b) N,S/Iy-CDs, (c) N/Iy-CDs, and (d) N,O/Iy-CDs) as shown in Fig. S7. The fluorescence intensity increases with increase in concentration of CDs till 200 µg/mL for Iy-CDs, 100 µg/mL for N,S/Iy-CDs and 150 µg/mL for N/Iy-CDs, and N,O/Iy-CDs. Furthermore increase in concentration of CDs has decrease the fluorescence intensity. At higher concentration non-specific interaction occurs between CDs to quench the emission intensity. Thus, the optimized concentration of 0.2 mg/mL for Iy-CDs, 0.1 mg/mL for N,S/Iy-CDs and 0.15 mg/mL for N/Iy-CDs, and N,O/Iy-CDs are prepared as stock solution and 10 µL are used for the experimental analysis.

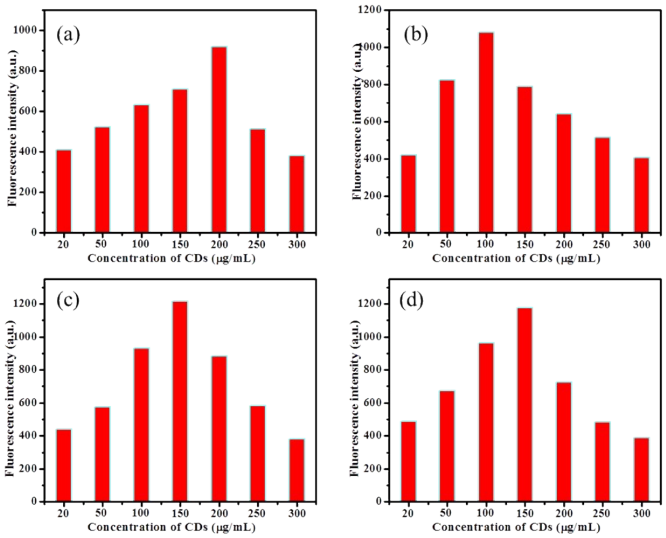

Fig.S7. The effect of different concentration CDs (a) self-passivated Iy-CDs and the surface passivated absorption spectra of (b) N,S/Iy-CDs, (c) N/Iy-CDs, and (d) N,O/Iy-CDs.