Supporting Information

Microwave Assisted Robust Aqueous Synthesis of Mn^{2+}-doped CdSe QDs with Enhanced Electronic Properties

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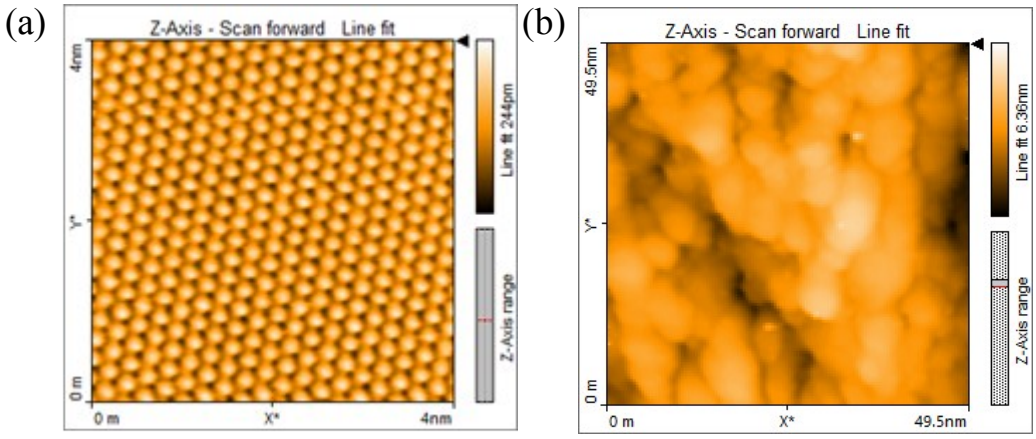

Fig. S1: STM topographic images of standard samples for calibration such as HOPG (a) and smooth Gold film (b). Topography images were recorded using set point current of 1nA and tip bias voltage 50mV.

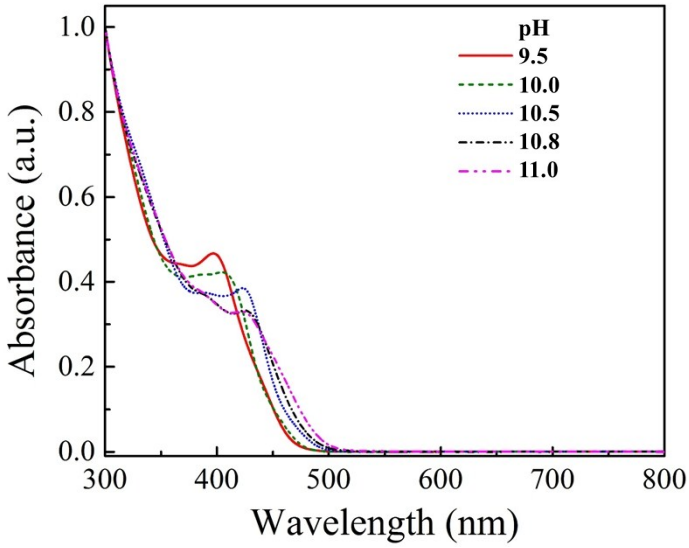

Fig. S2: Normalized electronic UV-vis absorbance spectra of 2% Mn-doped CdSe QD (SA5) for different pH values with microwave irradiation using 25% NH_4OH solution as pH adjusting reagent.

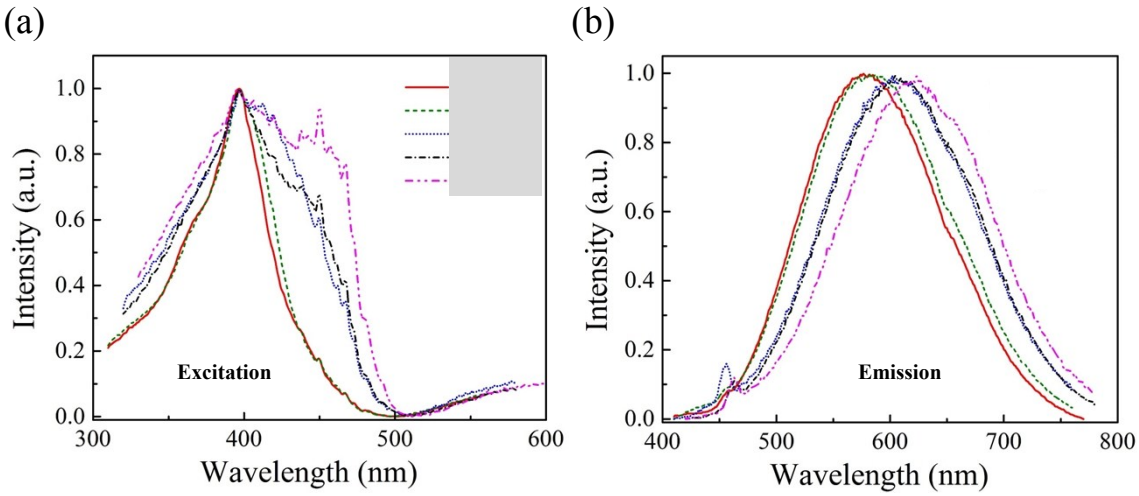

Fig. S3: Normalized Photoluminescence (a) excitation and (b) emission spectra of microwave irradiated 2% Mn-doped CdSe QD (SA5) samples synthesised using different pH values as indicated in legends with different coloured lines. Excitation spectra were recorded by fixing emission peak at 580 nm and emission spectra were recorded by fixing excitation peak at 395 nm.

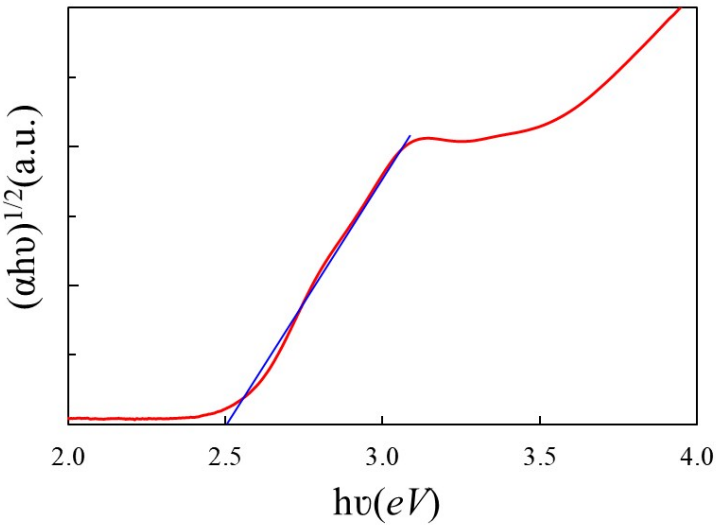

Fig. S4: Tauc plot showing the band gap energy 2.5 eV derived from the UV-vis absorption spectrum of the microwave irradiated 2% Mn^{2+}-doped CdSe QD (SA5) sample.

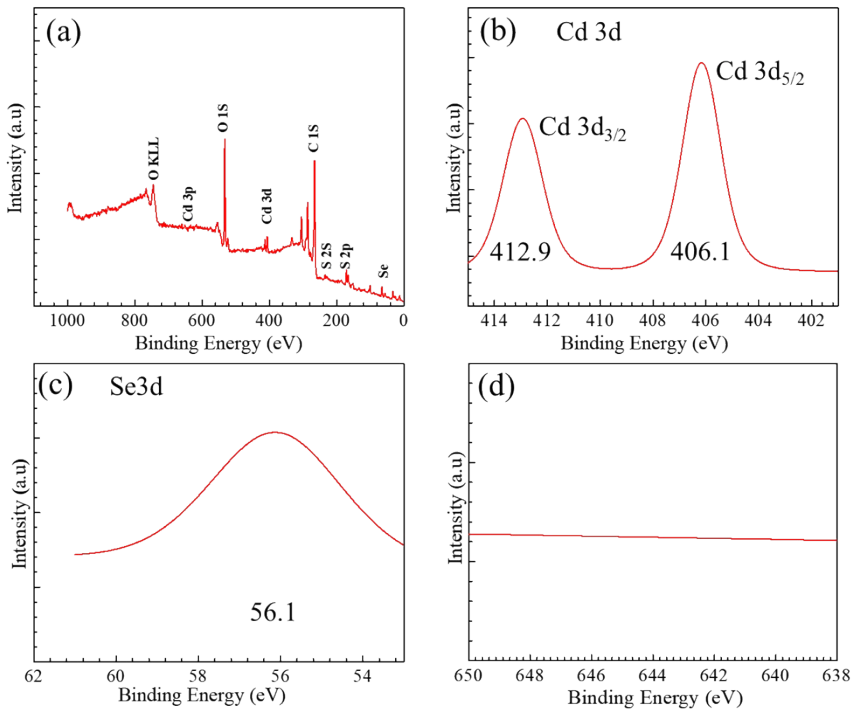

Fig. S5: (a) Survey X-ray photoelectron spectrum of undoped CdSe QDs (SA1). (b) & (c) High-resolution spectrum of Cd3d electrons showing doublet splitting with binding energy separated by 6.8 eV and Se3d respectively. (d) High-resolution spectrum recorded from binding energy 638 eV to 650 eV for Mn2p core electrons peaks but no peaks detected in this region.

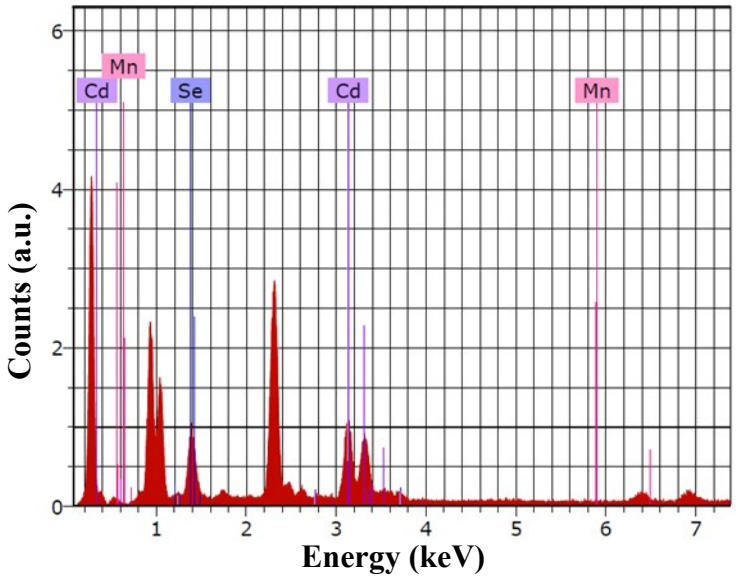

Fig. S6: EDS spectrum showing the composition of 2% Mn^{2+}-doped 3-MPA capped CdSe Quantum Dots (SA5).

Elements in CdSe QDs	Atomic weight %				
	SA1	**SA2**	**SA3**	**SA4**	**SA5**
Cd	63.42	62.64	62.27	61.88	60.33
Se	36.58	37.11	37.42	37.48	38.48
Mn	0.00	0.25	0.31	0.64	1.19

Table S1: Elemental composition of undoped and all Mn^{2+} doped CdSe QDs samples from EDS analysis.

CdSe QDs samples	Cd	Se	Mn
SA1: Undoped	1134.85	397.562	0.018
SA5: 2% Mn^{2+}-doped	1150.57	435.236	9.947

Table S2: Elemental composition of undoped (SA1) and 2% Mn^{2+} doped CdSe QDs (SA5) from ICP Atomic Emission Spectrometer. All values are in ppm.

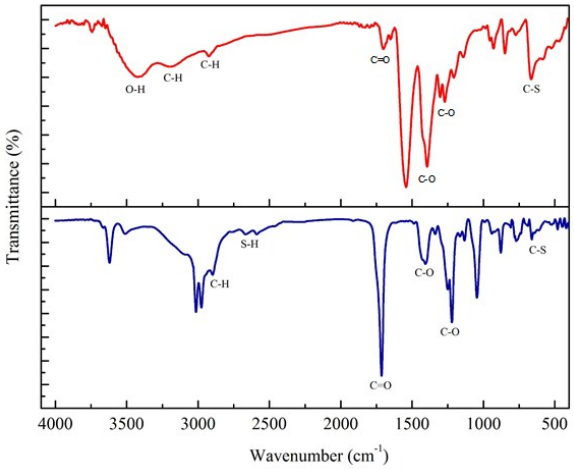

Fig. S7: Comparison between the FTIR spectrum of the ligand molecule 3-MPA (solid blue line, bottom) and 3-MPA capped CdSe QDs (solid red line, top). The chemical bonds corresponding to each vibrational absorption peak arec also indicated.

Note: The bonds originated by the interaction of the thiol group in the capping ligands 3-MPA with the metal atom Cd (II) can be analysed from the FT-IR spectrum. The dried undoped sample SA1 was ground with KBr to make pellet for transmission mode FTIR. FTIR of 3-MPA was taken by mixing it with chloroform ($CHCl_3$). The Fig. S7 above shows the FT-IR Spectrum obtained from 3-MPA (Blue) and 3-MPA capped CdSe QD (Red). The absorption bands at 2663 cm^{-1} and 2561 cm^{-1} which correspond to the S-H bond in the capping agent is absent in the CdSe spectrum which indicates that the capping agent binds to the metal ion through the sulphur atom. The strong band at 1713 cm^{-1} for the ligand refers to the C=O stretching. This band in 3-MPA capped CdSe QD spectra is clearly visible. This carboxylate ions resulted from the deprotonating of the carboxylic acid group at pH 9.5 during QDs growth. The peak at 2925 cm^{-1} corresponds to C-H bond of CH_2 group in 3-MPA. All other characteristic peaks of 3-MPA are clearly visible in CdSe QDs spectra like C-O and C-S bonds as shown in Fig. above. This result confirms the presence of capping ligand 3-MPA on CdSe QDs surface.

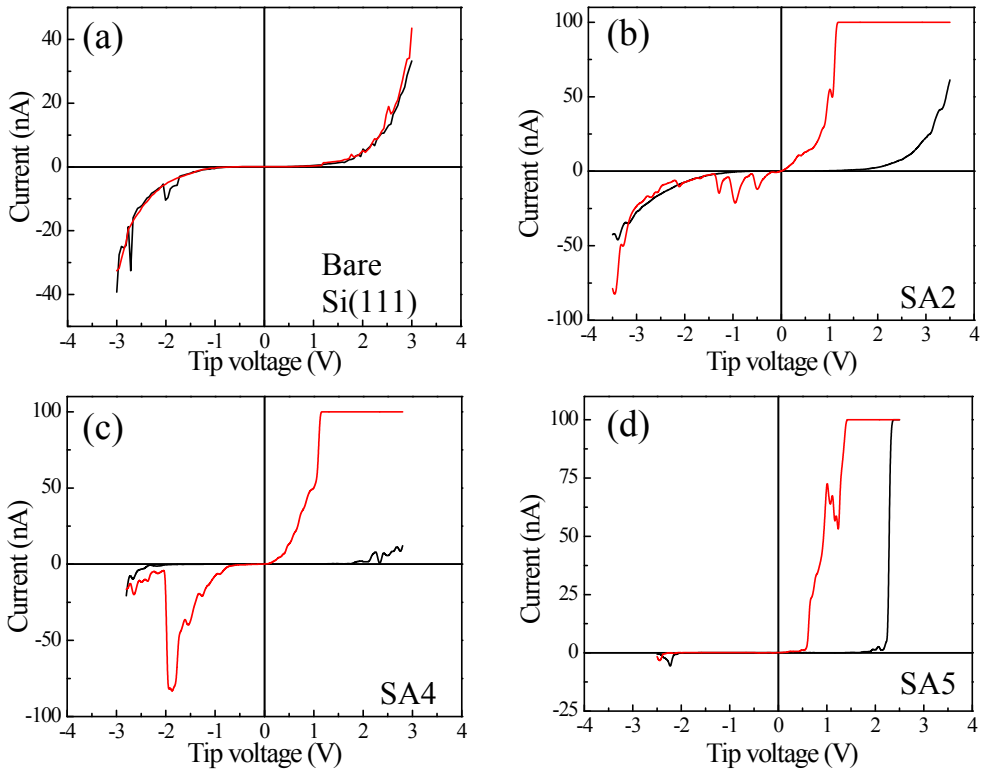

Fig. S8: Current-voltage (*I-V*) characteristics of the monolayer of quantum dots devices with a STM tip for both sweep directions between $-V_{Max}$ and $+V_{Max}$: (a) cleaned bare Si(111) with V_{Max}= 3.0 V, (b) 0.1 % doped CdSe QDs with V_{Max}= 3.5 V, (c) 1.0 % doped CdSe QDs with V_{Max}= 3.0 V, and (d) 2.0 % doped CdSe QDs with V_{Max}= 2.5 V.

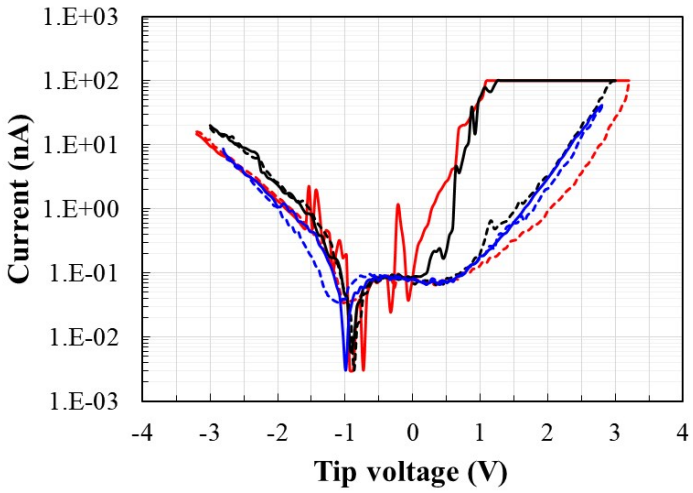

Fig. S9: Current-voltage (*I-V*) characteristics of the monolayer of 2% Mn^{2+} doped quantum dots devices with a STM tip for both sweep directions between $-V_{Max}$ and $+V_{Max}$ by varying V_{Max}= 2.8, 3.0, & 3.2 V.

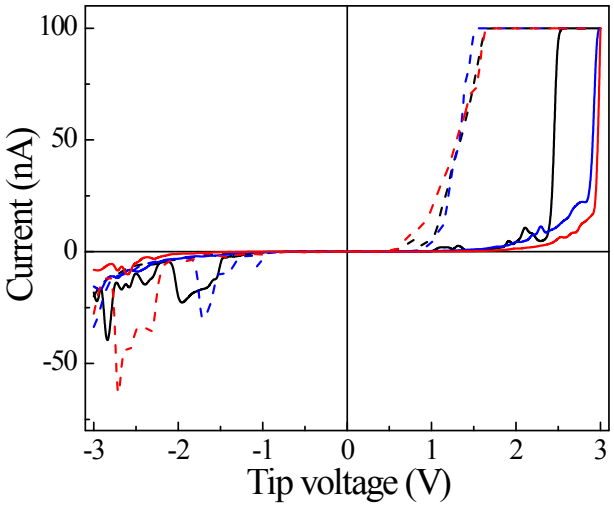

Fig. S10: Current-voltage (*I-V*) characteristics of the monolayer of 2% Mn^{2+} doped quantum dots device with a STM tip at different points on the film for both sweep directions between – V_{Max} and + V_{Max} with V_{Max}= 3.0 V. Different colour represent characteristics at different points on the film. Dashed and solid lines depicts forward and backword sweep direction respectively.