**Electronic Supporting Information**

# Compositional Engineered Cd-Mo-Se Alloyed QDs toward Photocatalytic $H_2O_2$ Production and Cr (VI) Reduction with Detailed Mechanism and Influencing Parameters

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**Characterization:**

**Physical characterizations:**

To investigate the crystallographic structure and phase purity of the synthesized sample X-ray diffraction (XRD) pattern was collected on a Rigaku Miniflex Ultima IV with Cu Kα radiation (power rating: 100mA, 40kV, and λ=1.54Aº). The morphological analysis of the as-synthesized photocatalysts was carried out by using HR-TEM 300 kV of model Tecnai G2, F30 for the HRTEM study. UV-Vis diffuse reflectance spectroscopy was obtained using a JASCO-V-750 UV-visible spectrophotometer. Photoluminescence (PL) spectroscopy was used to investigate the recombination rate and separation efficiency of quantum dots at ambient temperature using a JASCO FP-8300 spectrofluorometer with an excitation wavelength of 380 nm. The surface chemistry and elemental composition of the photocatalysts are examined by XPS using a Kartos axis ultra-x-ray photoelectron spectrometer, which is equipped with a monochromatized X-ray source (Al Kα). Photoelectrochemical measurements, using an IVIUMSTAT multichannel workstation were performed where a conventional three-electrode Pyrex cell with Pt and Ag/AgCl respectively as counter and reference electrodes. An electrophoretic deposition (EPD) method was employed to prepare a working electrode, in which photocatalysts were deposited on Fluorine doped tin oxide (FTO). Typically, in a beaker, 20 mg of photocatalyst with 20 mL of acetone and iodine were taken and then the solution was dispersed by sonication for 10 min. In the above well-dispersed solution two parallel FTOs (separated by 10-15 mm) were dipped, and under controlled potentiostatic condition, 60 V bias was subjected (5 min) to coat the FTO surface by the photocatalyst as a thin film in 1 $cm^2$ area. The photocatalyst was deposited on FTOs and kept in the oven for 6 h to remove impurities from the FTO surface. Linear sweep voltammetry (LSV) was executed at a scan rate of 25 mV/s applying a potential of 0 to -0.8 V. Electrochemical impedance spectroscopy was also performed at zero biased potential at frequencies $10^{-1}$ to $10^5$ Hz. In dark conditions, the Mott-Schottky analysis was also carried out. All the above electrochemical analyses were carried out using 0.1 M $Na_2SO_4$ solution.

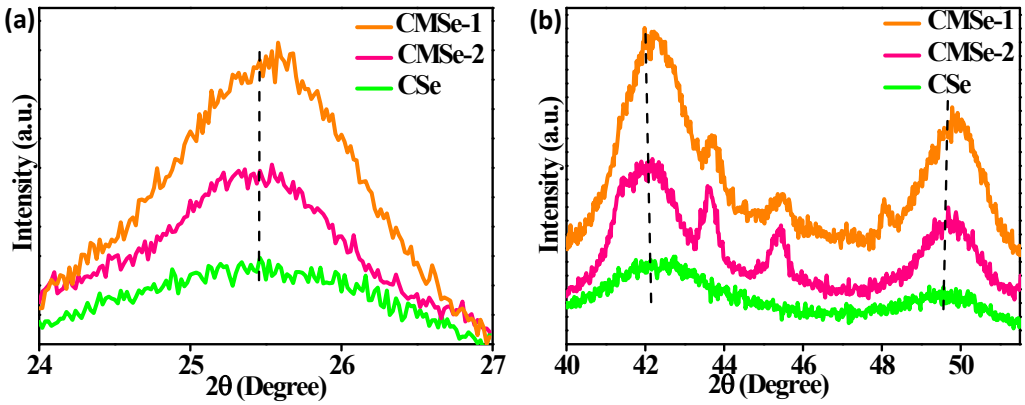


**Figure S1**. Enlarged view of XRD of CMSe-1 and CMSe-2 concerning binary CdSe QD to show shifting (a) at 25.5º and (b) at around 42 º and 49º.

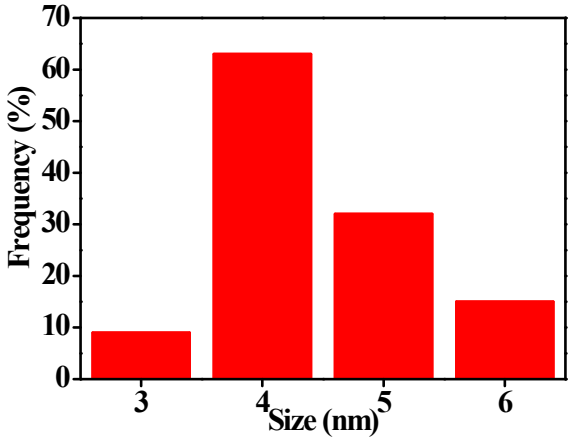


**Figure S2.** Particle size distribution of CMSe-1 QDs.

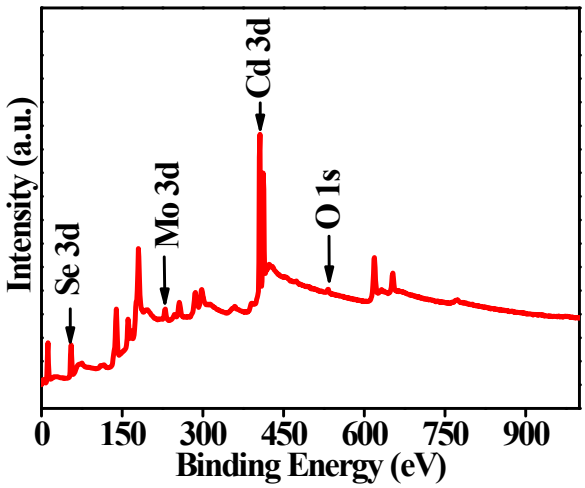


**Figure S3.** XPS survey of CMSe-1.

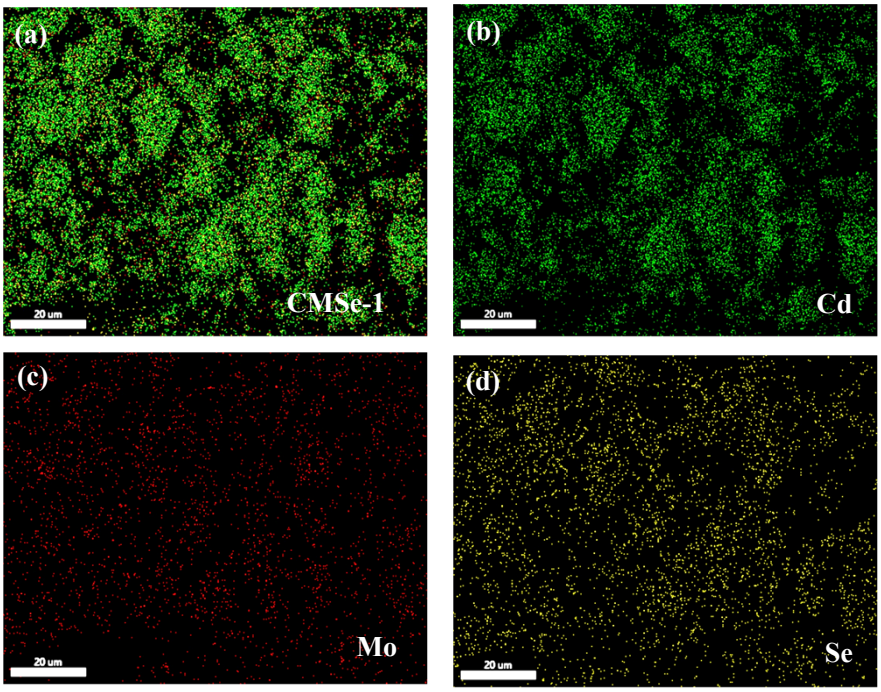


**Figure S4.** Elemental colour mapping image of (a) CMSe-1, (b) Cd, (c) Mo, and (d) Se elements.

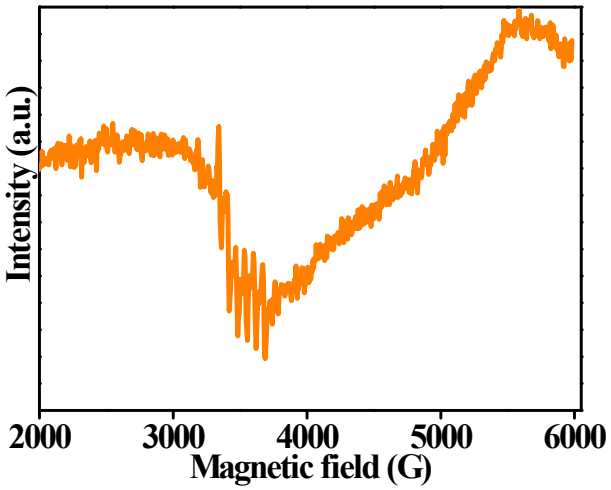


**Figure S5.** EPR spectra of CMSe-1

**Table S1.** Biexponential-Curve-Fitted TRPL parameters of CMSe-1 and CMSe-2 QD.

| Photocatalyst | $\alpha_1$ | $\tau_1$ (ns) | $\alpha_2$ | $\tau_2$ (ns) | $\tau_{avg}$ (ns) |
|---|---|---|---|---|---|
| CMSe-1 | -205.6427 | 1 | 230.8681 | 1.1 | 1.53 |
| CMSe-2 | -81.4482 | 1 | 91.8009 | 1.1 | 1.51 |

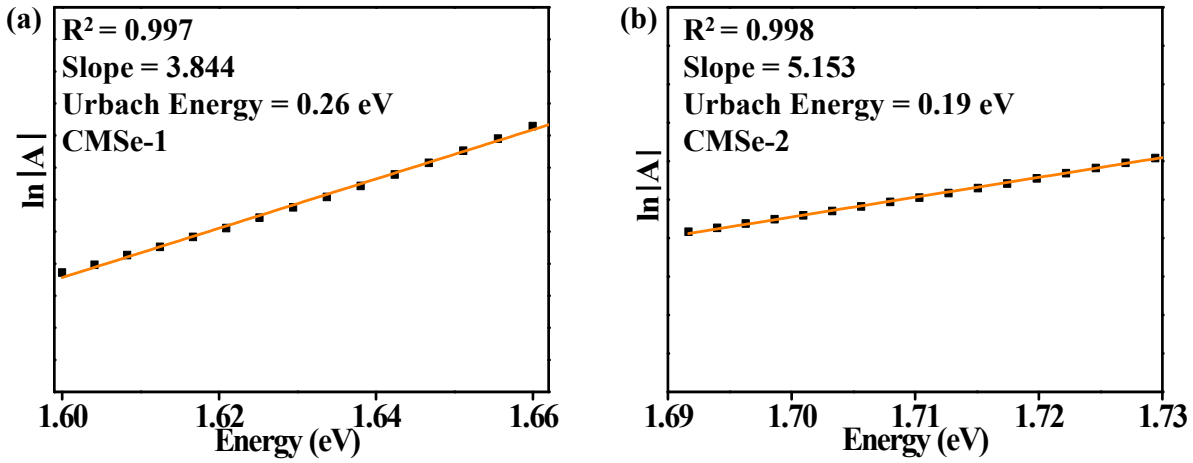


**Figure S6.** Urbach energy of (a) CMSe-1, and (b) CMSe-2 QD.

**Calculation of solar to chemical conversion efficiency (SCC %)**

SCC % of CMSe-1 QDs towards $H_2O_2$ production under 250 W Hg-lamp can be calculated by following the equation below:

$$SCC = \frac{\Delta G^{\circ}\ for\ H_2O_2\ Production\ \times\ H_2O_2\ produced\ (mol)}{Input\ energy\ (W) \times reaction\ time\ (sec)} \times 100 \quad \text{S1}$$

Furthermore, $\Delta G^0$ for $H_2O_2$ evolution is 117 kJ.mol$^{-1}$. The irradiance of 250 W Hg-lamp is 1.33 W.cm$^{-2}$ and 127.2 cm$^2$ irradiated area. In a 1 h of reaction time, the amount of $H_2O_2$ produced is 28.06 µmol.

$$Input\ energy\ (W) = irradiance\ (Wcm^{-2}) \times irradiated\ area\ (cm^2)$$

$$= 1.33 \times 127.2$$

$$= 169.14$$

According to equation (1), the SCC efficiency is determined to be 0.27%.

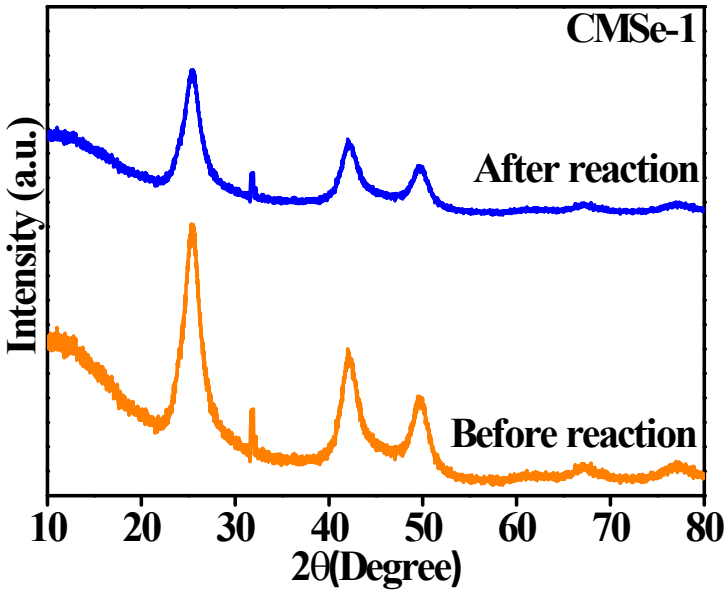


**Figure S7.** Powder XRD of CMSe-1 after performing photocatalytic activity.

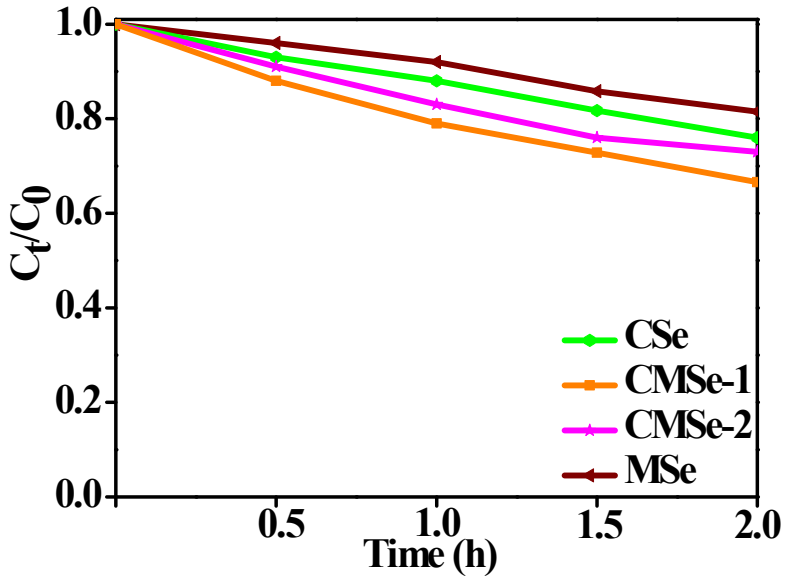


**Figure S8.** Photocatalytic decomposition of $H_2O_2$ by CMSe-1, CMSe-2, CSe, and MSe under visible light irradiation**.**

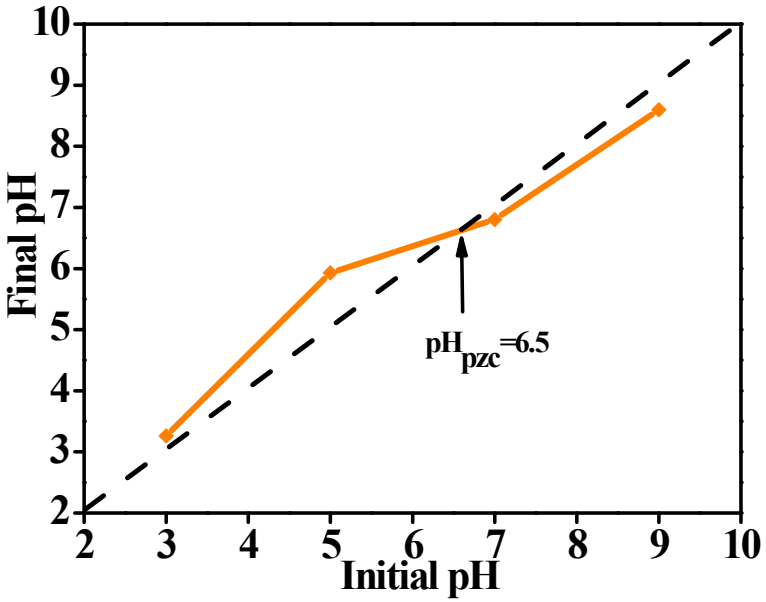


**Figure S9.** The $pH_{PZC}$ value of CMSe-1 QD.

**Figure S10.** NBT test for detection of superoxide radicals of CMSe-1 and CMSe-2 QDs.

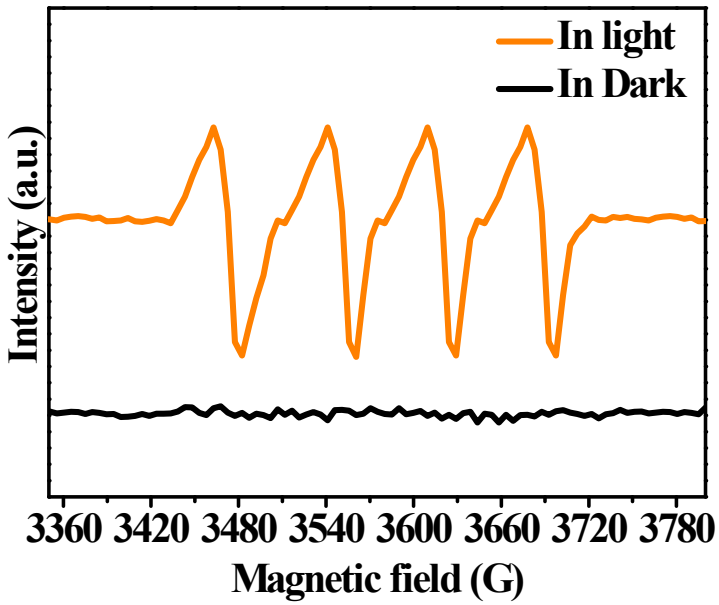


**Figure S11.** DMPO-ESR spin trapping spectra of CMSe-1 for detection of superoxide radical ($^{\bullet}O_2^-$)

**Table S2.** Comparison Study on $H_2O_2$ Production and Cr (VI) Reduction over other photocatalysts.

| **Photocatalyst** | **Rate Of $H_2O_2$ production** | **Efficiency of Cr (VI) reduction** | **Ref.** |
|---|---|---|---|
| $CdSe_{550}$/5CdS/2ZnS QD | 126 mmol$L^{-1}$ in 2 hours | - | 1 |
| CdSe QD/KPN-HCP | 900 µmol g−1 in 1hour | - | 2 |
| CdSe/Se/BiOBr | 4180 µmol $L^{-1}$ in 4h | - | 3 |
| CdS/$Ti_3C_2T_x$ | 401 µmol $L^{-1}$ within 1 h | | 4 |
| ZnS/ZnSe/$MoSe_2$ | - | 96 % for 1.5 h | 5 |
| $MoS_2$-PVP | - | 99.5 % for 3 h | 6 |
| CQD/$MoSe_2$ | - | 99% for 3 h | 7 |
| CdS/ $Bi_2MoO_6$ | - | 97% for 1 h | 8 |
| CMSe-1 | 1403.5 µmol$g^{-1}h^{-1}$ | 93.6% in 2 hours | This work |

**References:**


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