Supporting Information

Tuning the surface properties of alloyed CdS_xSe_{1-x} 2D nanosheets

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1. Experimental

Materials. Cadmium chloride ($CdCl_2$, 99.99%), selenium (200 mesh, 99.99%), sulfur, octylamine (OA) (99%), oleylamine (OLA) (70%) and trioctylphosphine (TOP, 90%), $NaBH_4$, 1-dodecanthiol (DDT) and triphenylphosphine (PPh_3) were purchased from Sigma-Aldrich and used without further purification.

Synthesis of CdS_xSe_{1-x} nanostructures. The 2D CdS_xSe_{1-x} nanosheets were synthesized by reacting $CdCl_2$ (OA, $OLA)_2$ complex and (S-Se) powder in a mixture of octylamine and oleylamine. $CdCl_2$ (OA, $OLA)_2$ complex solution was prepared by heating $CdCl_2$ (275 mg, 1.5 mmol) in 5 ml of octylamine and 5 ml of oleylamine at 120 °C for 2 hrs. After 2 hrs it was cooled down to room temperature. A reactive (S-Se) precursor was prepared with equimolar mixture of S and Se (total amount of S + Se is 4.5 mmol) with $NaBH_4$ (2.75 mmol) mixed with 2.5 ml of octylamine and 2.5 ml of oleylamine, sonicated for 55 min at room temperature. This (S-Se) precursor was injected swiftly into the preformed $CdCl_2$ (OA, $OLA)_2$ complex at room temperature. After injection of the precusor, the reaction temperature was gradually increased to 65 °C-95 °C and maintained for 10 hrs. After 10 h, it was cooled to room temperature and washed with ethanol with small amount of TOP to remove unreacted precursors.

Functionalization of CdS_xSe_{1-x} nanostructures with Triphenylphosphine (PPh_3) and 1-Dodecanthiol (DDT). 20 mg of solid PPh_3 was directly added to the nanosheet samples in chloroform. Then the solution was stirred for 3 hrs at room temperature and optical properties were measured. On the other hand, measured amount of dodecanthiol was directly added to the chloroform solution of the nanosheets in the cuvette, shaken and measurements were carried out.

Preparation of TEM samples. CdS_xSe_{1-x} nanosheets in chloroform were precipitated with ethanol and re-dissolved in chloroform. Then, a drop of the dilute solution was placed on Cu TEM grids (Ultrathin carbon film on Lacy carbon 400 mesh, TED PELLA, INC) and left to evaporate.

TEM measurements. TEM images were acquired on a CM120 Super Twin TEM (Philips) operating at 120 kV.

Preparation of XRD samples. The concentrated CdS_xSe_{1-x} samples in chloroform were drop-casted onto a small cleaned Si wafer, and the solvent was evaporated on a heating plate under mild heating (~ 50 °C). Data were collected on Panalytical Empyrean Powder Diffractometer equipped with position sensitive (PSD) X'Celerator detector using Cu K_α radiation (λ=1.5405 Å) and operated at 40 kV and 30 mA. The usual Bragg-Brentano $\theta/2\theta$ and grazing incident beam geometry were employed. The grazing incident scan was performed at a constant incident beam angle of 2^o in a 2θ range of 20^o-80^o with a step of 0.05^o and 2 s per step.

Optical measurements. A small amount (~ 0.1 ml) of each sample was taken from the stock and diluted with chloroform to comparable optical density. UV absorption spectra were measured with a Shimadzu UV-3600 spectrophotometer. Photoluminescence (PL) emission spectra were measured with a Shimadzu spectrofluorophotometer RF-5301pc.

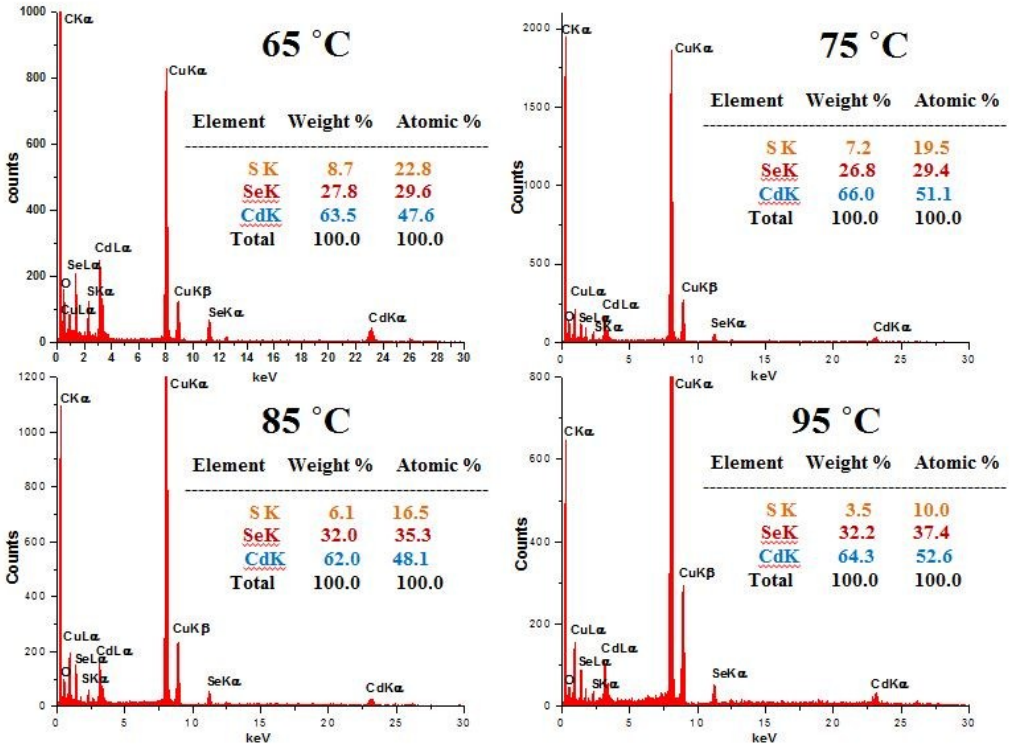

Figure S1: EDAX spectra (a-d) and corresponding elemental analysis of the as synthesized 2D CdS_xSe_{1-x} nanosheets.

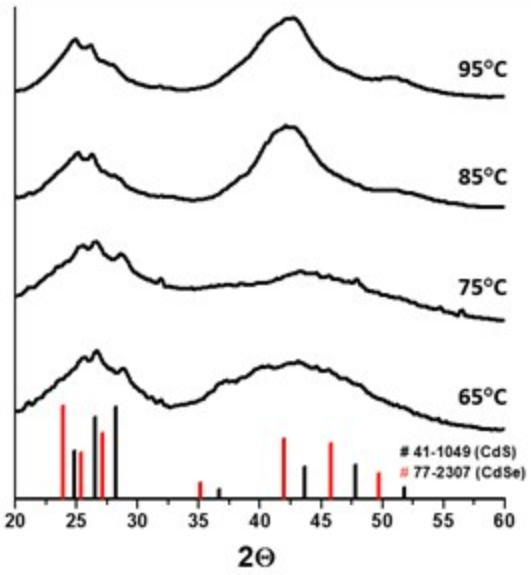

Figure S2: Wide-angle XRD spectra of the 2D CdS_xSe_{1-x} nanosheets deposited on Si-wafer. The standard XRD pattern for bulk wurtzite CdS#41-1049 (black) and CdSe#77-2307 (red) are included for comparison.

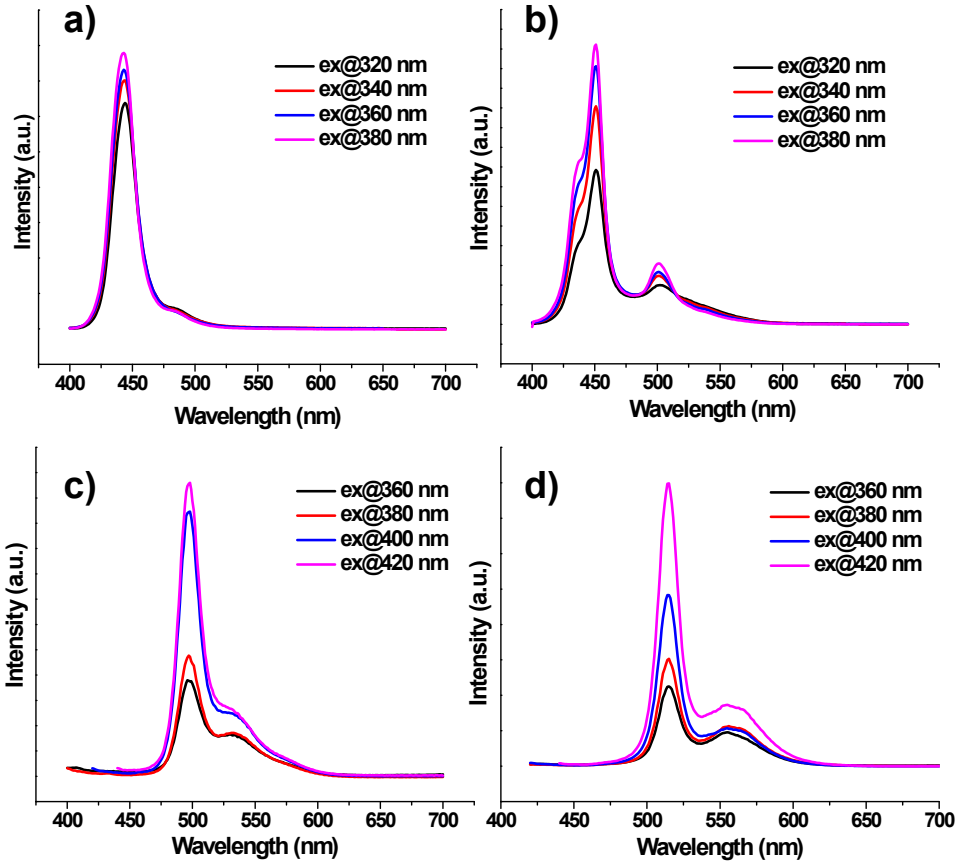

Figure S3: Photoluminescence spectra (a-d) of the as synthesized CdS_xSe_{1-x} nanosheets at (a) 65 °C, (b) 75 °C, (c) 85 °C and (d) 95 °C with different excitation wavelength.

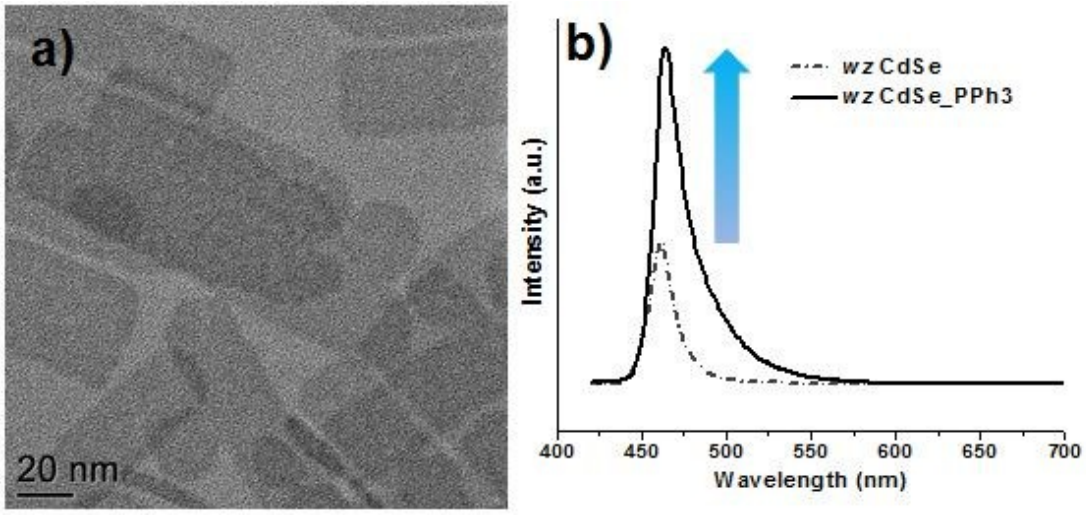

Figure S4: TEM image (a) and corresponding emission (b) spectra of *w*-CdSe nanosheets before and after modification with tripheylphosphine (TPP).

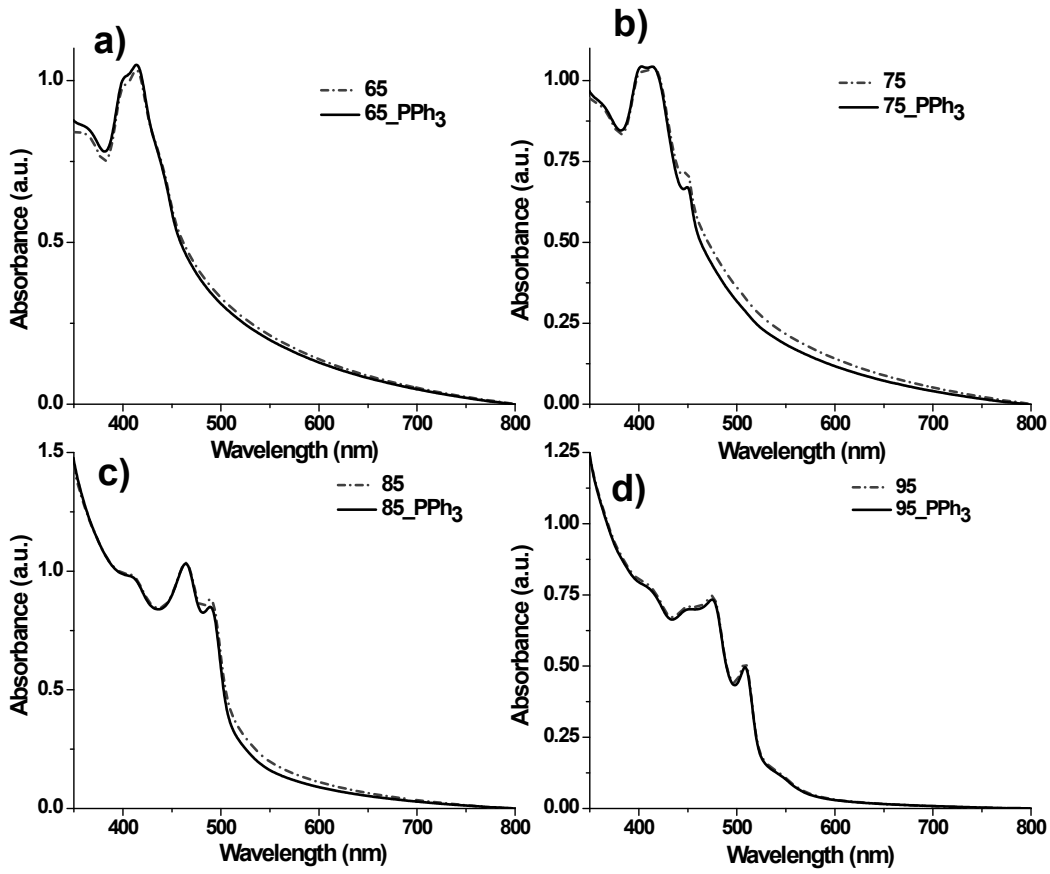

Figure S5: Absorbance spectra (a-d) of 2D CdS_xSe_{1-x} nanosheets before (black) and after (red) functionalization with triphenylphosphine (TPP) as recorded at room temperature.

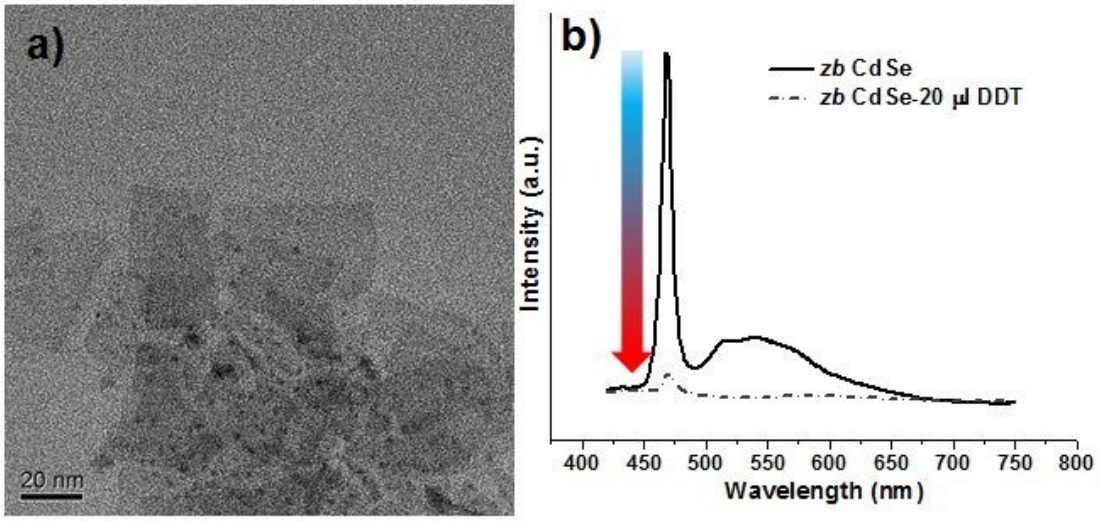

Figure S6: TEM images (a) and corresponding emission spectra (b) of *zb*-CdSe nanosheets before and after addition of 1-dodecanthiol (DDT) as recorded at room temperature.

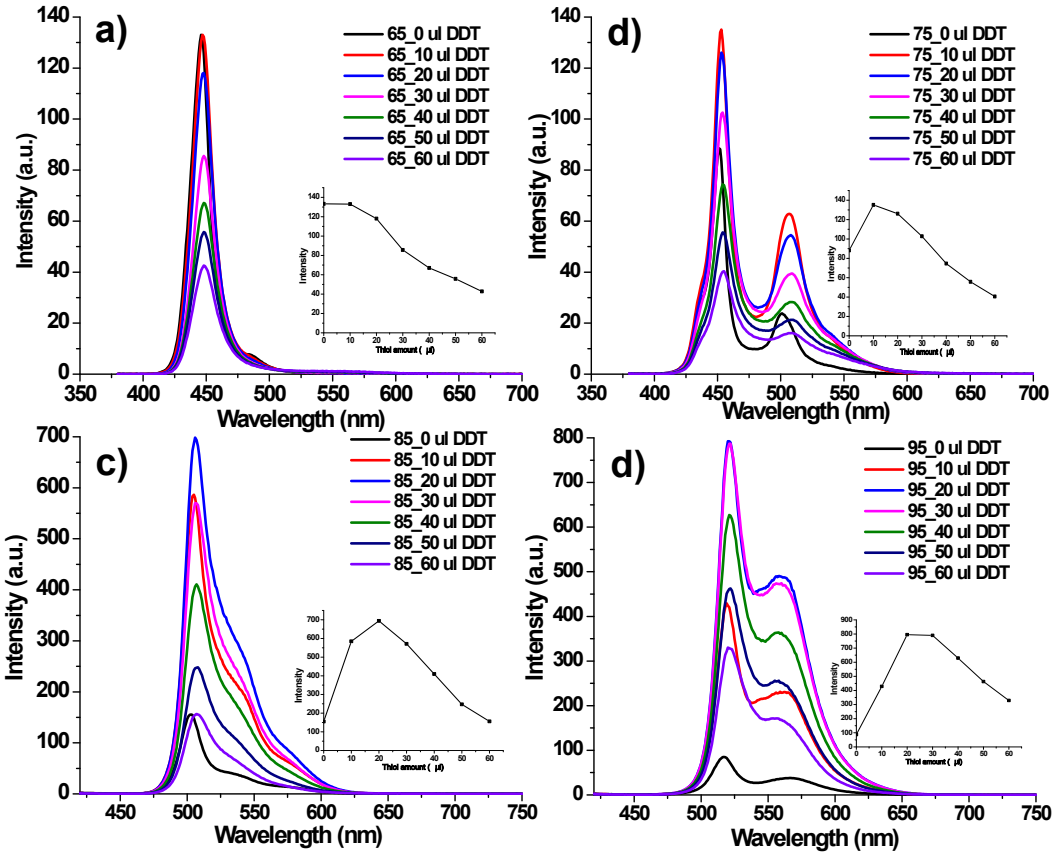

Figure S7: Emission spectra (a-d) of 2D CdS_xSe_{1-x} nanosheets before and after addition of 1-dodecanthiol (DDT) as recorded at room temperature.