

Supplementary Information

Defect-induced room temperature ferromagnetism in Cu-doped In_2S_3

QDs

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Table S1 Summary of some structural parameters of 2-theta, lattice parameter (a), FWHM, average crystallite size, dislocation density and micro strain for Cu-doped In_2S_3 QDs with different doping concentrations.

Sample	$(2\theta)_{22\ 12}$	c(nm)	FWHM $_{(22\ 12)}$	D(nm) $_{22\ 12}$	$\delta (\times 10^{-3})$	$\epsilon (\times 10^{-3})$
pristine In_2S_3	48.20	3.202	3.21	2.68	373	31.31
0.5% Cu	48.22	3.201	3.15	2.73	366	30.71
1.5% Cu	48.25	3.199	3.04	2.83	353	29.62
2% Cu	48.27	3.198	3.09	2.79	358	30.09

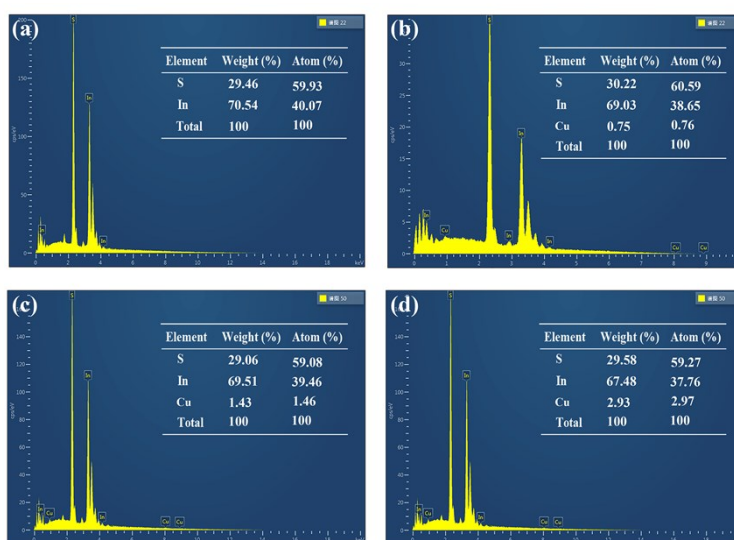


Fig. S1 EDX patterns of pristine In_2S_3 (a) and Cu-doped In_2S_3 QDs with dopant concentration of 0.5% (b), 1.5% (c), 2% (d).

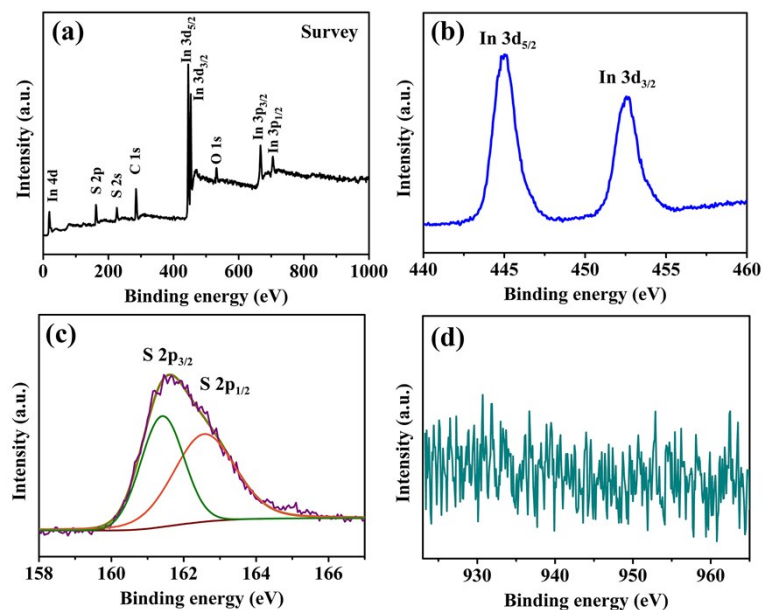


Fig. S2 (a) XPS survey spectrum and high resolution XPS spectra of the pristine In_2S_3 QDs corresponding to (b) In 3d, (c) S 2p, (d) Cu 2p regions.

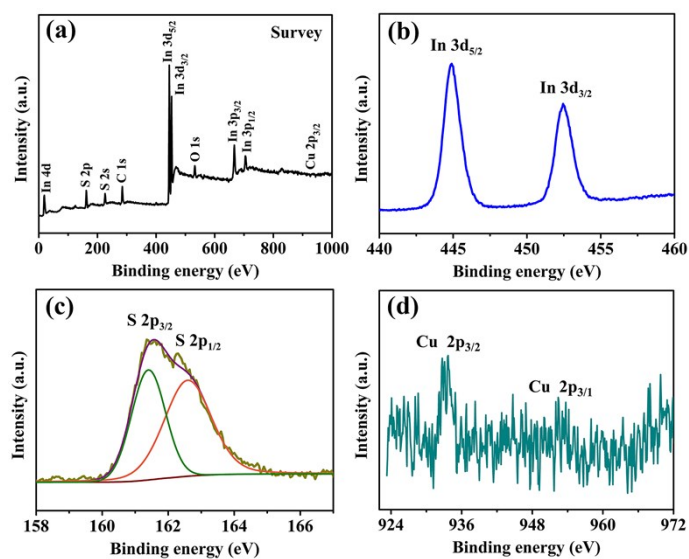


Fig. S3 (a) XPS survey spectrum and high resolution XPS spectra of Cu (0.5 %) doped In_2S_3 QDs corresponding to (b) In 3d, (c) S 2p, (d) Cu 2p regions.

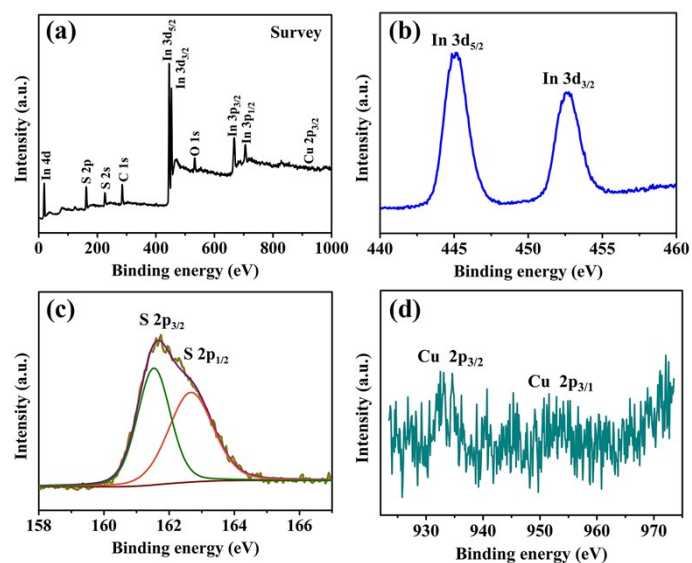


Fig. S4 (a) XPS survey spectrum and high resolution XPS spectra of Cu (1.5 %) doped In_2S_3 QDs corresponding to (b) In 3d, (c) S 2p, (d) Cu 2p regions.

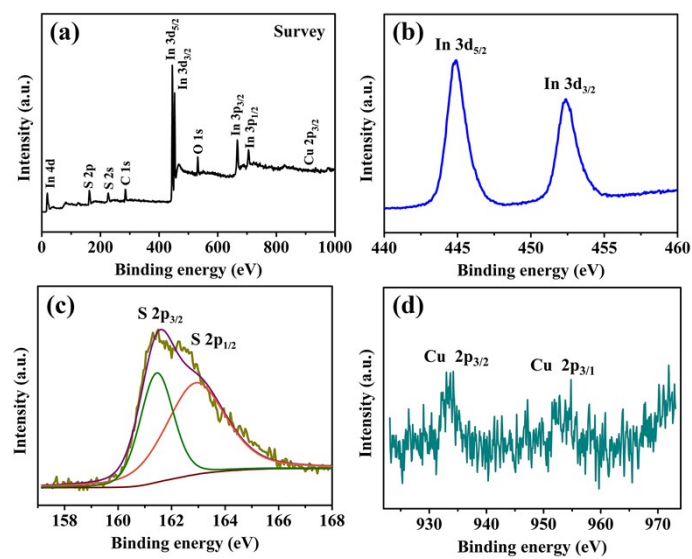


Fig. S5 (a) XPS survey spectrum and high resolution XPS spectra of Cu (2 %) doped In_2S_3 QDs corresponding to (b) In 3d, (c) S 2p, (d) Cu 2p regions.

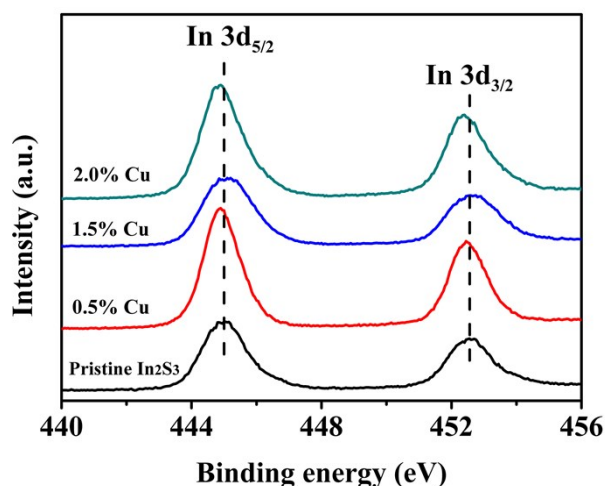


Fig. S6 In 3d core levels measured from the pristine In₂S₃ and Cu-doped In₂S₃ QDs. From the XPS survey spectrum of the all sample, the Cu-doped In₂S₃ spectrum consists of In, S, O and Cu elements except for the C 1s peak, and no impurities and magnetic contamination are detected, indicating the high purity of Cu-doped In₂S₃ QDs. The O 1s peak recorded on the sample may be due to absorbed O₂, H₂O and CO₂ on the surface of the material. The In 3d spectrum (Fig. S2b) shows two peaks at 444.9 eV and 452.7 eV, corresponding to the binding energy of In 3d_{5/2} and In 3d_{3/2} for In³⁺ ions, respectively. In the S 2p spectrum (Fig. S2c), two peaks with binding energies at 161.4 eV and 162.6 eV are assigned to S 2p_{3/2} and S 2p_{1/2}, respectively, indicating the existing of S²⁻ in In₂S₃.

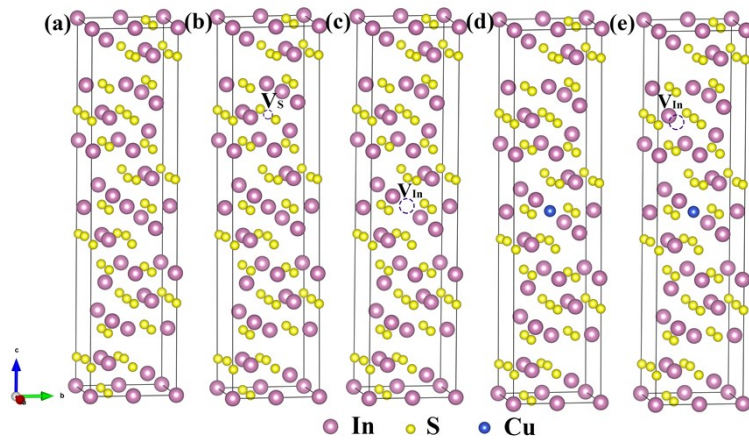


Fig. S7 Five calculation models: (a) the ideal system with no defects or dopants ($\text{In}_{32}\text{S}_{48}$), (b) one S vacancy system (V_S), (c) one In vacancy system (V_{In}), (d) one Cu atom doped system (Cu_{In}), (e) one In vacancy and one Cu atom doped system ($\text{Cu}_{In}+V_{In}$).