**Supplementary Information**

# Synthesis and investigations of $In_2S_3:Ho^{3+}$ quantum dots on doping induce changes

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## Experimental section

### sample preparation and growth mechanism

Figure S1 presents the synthetic facility of $In_2S_3$:$Ho^{3+}$ nanoparticles by an easily reproducible gas–liquid phase chemical deposition (this is an effective atomization doping method). The sufficiently stirring reactive solution is atomized to form the fine droplets with the average diameter of 2-4 μm by using an ultrasonic nebulizer (the upper left portion of Fig. S1). The fog droplets will react with the $H_2S$ gas taken by the flowing nitrogen in condensers with circulating water (25 °C). Finally, the reaction products were collected in a flat bottom flask placed in an ultrasonic water bath (the bottom left portion of Fig. S1). The waste gas was absorbed by the NaOH solution to avoid air pollution.

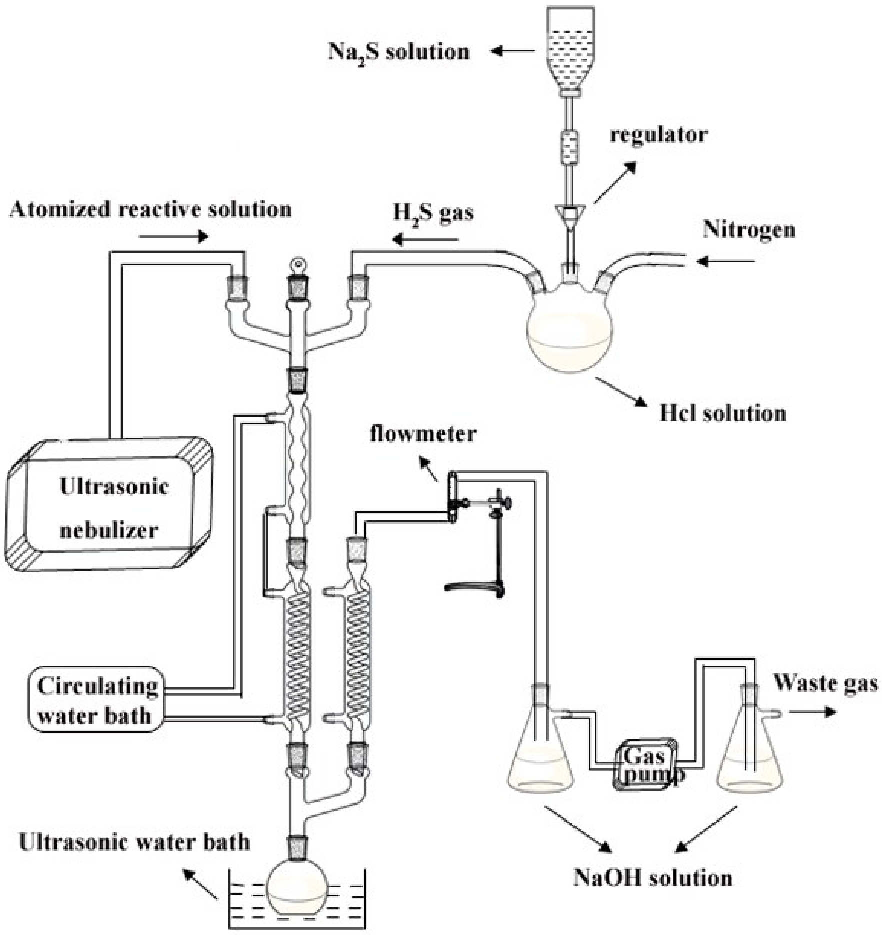


**Fig. S1** The synthetic facility of $In_2S_3$:$Ho^{3+}$ nanoparticles.

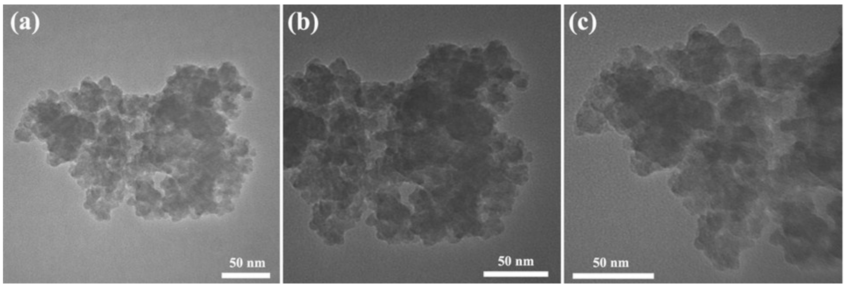


**Fig. S2** (a) A low-magnification TEM image, (b) enlarged TEM image, (c) high-magnification TEM image of $In_2S_3$:$Ho^{3+}$ nanoparticles (concentration of dopant 0.75 at. %).

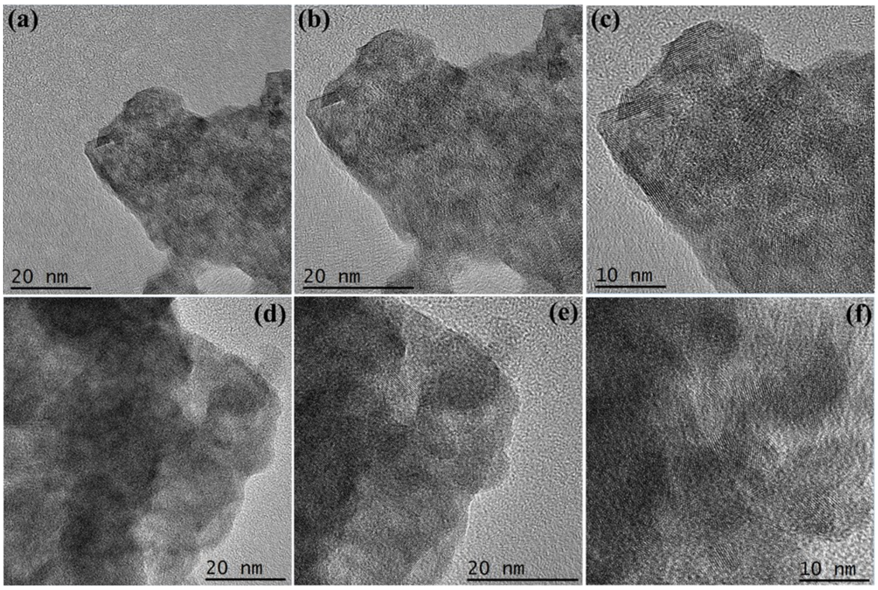


**Fig. S3** HRTEM images with different magnification. (a), (b) and (c) for $In_2S_3$:$Ho^{3+}$ nanoparticles (concentration of dopant 0.75 at. %); (d), (e) and (f) for pure $In_2S_3$ nanoparticles.

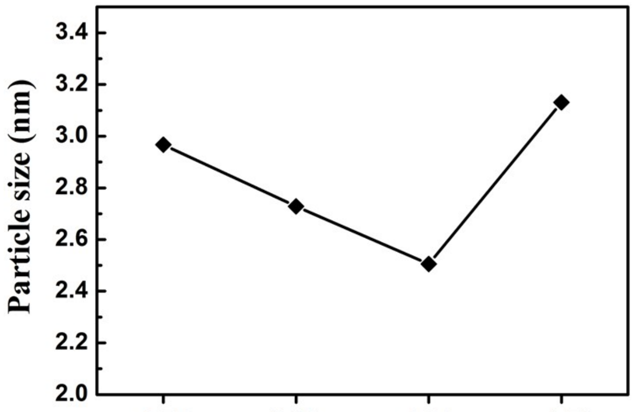


**Fig. S4** The effect of $Ho^{3+}$ concentration on the particle sizes of $In_2S_3$:$Ho^{3+}$ nanoparticles.

**First-principles calculations**

As shown in Figure S5, two conventional cell models have been built. Figure S5a is corresponding to the ideal system of pure $In_2S_3$ ($In_{16}S_{24}$) with the optimized lattice constants (a = 10.774 Å), which agree well with the experimental values. Figures S5b is corresponding to $In_{15}Ho_1S_{24}$.

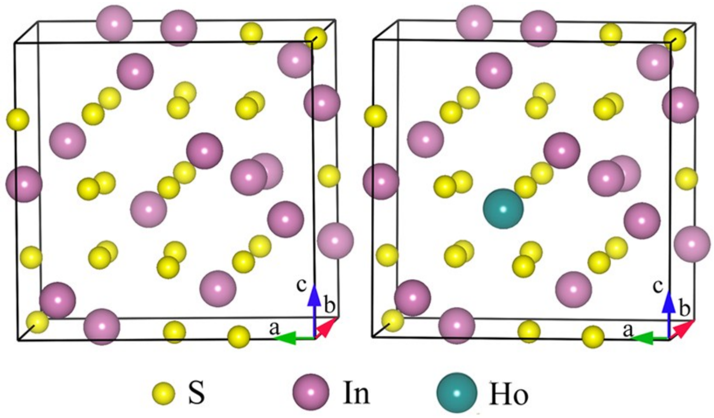


**Fig. S5** Two calculation models: (a) the ideal system with no defect and doping ($In_{16}S_{24}$); (b) one In atom replaced by one Ho atom ($Ho_{In}$) ($In_{15}Ho_1S_{24}$).

| **Sample (the molar concentration ratios of $Ho^{3+}$ and $In^{3+}$)** | **ICP** | | | **EDX** | | |
|---|---|---|---|---|---|---|
| | In (ppm) | Ho (ppm) | Ho/In (Mass ratio) | In (wt %) | Ho (wt %) | Ho/In (Mass ratio) |
| **0.02** | 29.25 | 0.825 | 0.0282 | 68.26 | 1.91 | 0.0279 |
| **0.04** | 26.14 | 0.923 | 0.0353 | 68.65 | 2.38 | 0.0346 |
| **0.06** | 25.02 | 1.180 | 0.0472 | 68.28 | 3.24 | 0.0474 |
| **0.08** | 26.19 | 1.370 | 0.0523 | 73.80 | 3.89 | 0.0527 |

**Table S1.** Comparison of different doping concentrations In $In_2S_3$:$Ho^{3+}$ nanoparticles by the ICP and EDX methods.