Supplementary Information

# Room Temperature Ferromagnetism Properties of $In_2S_3$ Nanoparticles Regulated by Doping with Gd ions

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Table S1. Various particle sizes of pristine $In_2S_3$ and $In_2S_3$: $Gd^{3+}$ samples.

| Sample | $\beta_{hkl}$ (FWHM) | D (nm) |
|---|---|---|
| pristine $In_2S_3$ | 2.78 | 3.27 |
| Gd doped $In_2S_3$ (0.39 at.%) | 3.01 | 3.02 |
| Gd doped $In_2S_3$ (1.20 at.%) | 2.37 | 3.83 |
| Gd doped $In_2S_3$ (1.68 at.%) | 2.34 | 3.89 |
| Gd doped $In_2S_3$ (2.17 at.%) | 1.98 | 4.58 |

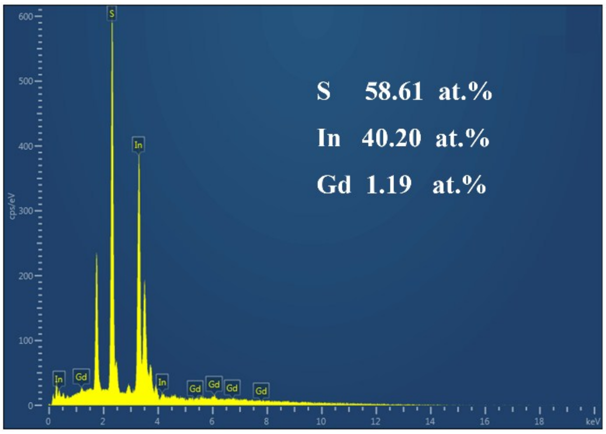


Figure S1. EDS pattern of the $In_2S_3$: $Gd^{3+}$ (1.20 at.%) nanoparticles.

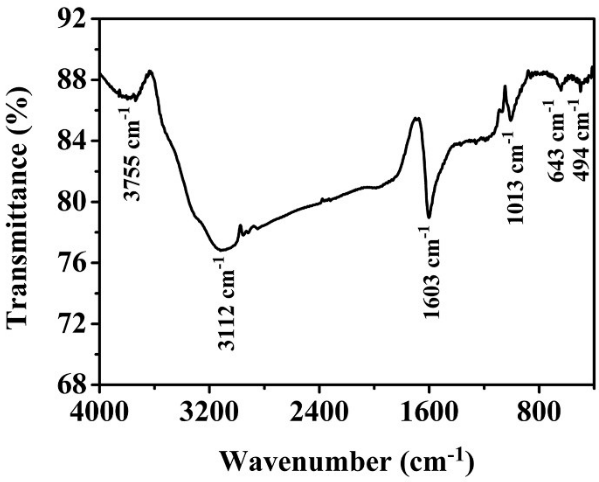


Figure S2. IR spectrum of the $In_2S_3$: $Gd^{3+}$ (1.20 at.%) nanoparticles.

The IR spectrum of the $In_2S_3$: $Gd^{3+}$ (1.20 at.%) nanoparticles is shown in Figure. S2, which is consistent with the reported results.[1, 2] The peaks at 494 $cm^{-1}$ and 643 $cm^{-1}$ may be caused by the mercaptoethanol absorbed on the surface of the $In_2S_3$: $Gd^{3+}$

nanoparticles.[3] The peak at 1013 $cm^{-1}$ is ascribed to the C-O stretching vibration. The peak at 1603 $cm^{-1}$ can be attributed to $CO_2$ absorbed on the surface of the $In_2S_3$: $Gd^{3+}$ nanoparticles. The peak centered at 3112 $cm^{-1}$ corresponding to O-H stretching vibration which may be due to absorbed water molecules in the sample. The peak at 3755 $cm^{-1}$ is associated with the interaction of $In^{3+}$, $S^{2-}$ and $Gd^{3+}$. The results of IR spectrum further indicate that the dangling bonds on the surface can bond with some ions like $(O\text{-}H)^-$, $H^+$ and $(HOCH_2CH_2S)^-$, and these non-magnetic ions had no effect on the magnetism of the sample.

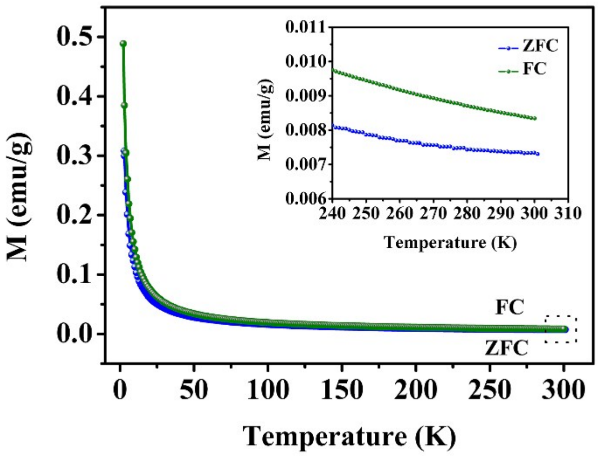


Figure S3. Temperature-dependent magnetization curves for the $In_2S_3$: $Gd^{3+}$ (1.20 at.%) nanoparticles in ZFC and FC modes at a magnetic field of 500 Oe. The inset shows the high-magnification of the curves between 240 and 300 K.

Figure. S3 shows temperature-dependent magnetization curves for the $In_2S_3$: $Gd^{3+}$ (1.20 at.%) nanoparticles in zero-field cooling (ZFC) and field cooling (FC) modes at a magnetic field of 500 Oe. Note that the ZFC-FC curves measured in the temperature range of 2-300K do not exhibit magnetic transition. The sharp increase of magnetization both in the ZFC-FC curves below 30 K and the presence of hysteresis at higher temperatures can be considered as ferromagnetic behavior. The small disparity between ZFC and FC curves indicates the existence of antiferromagnetic.[4]

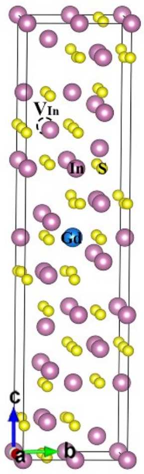


Figure S4. one In vacancy in a Gd doped $In_2S_3$ system ($In_{30}GdS_{48}$).

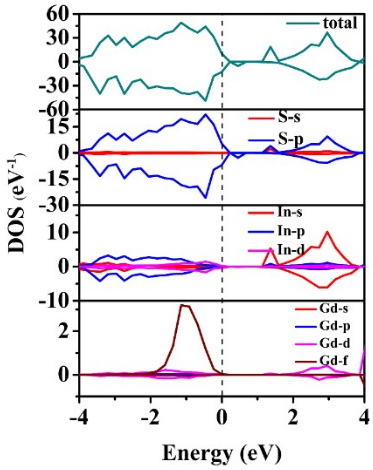


Figure S5. Spin-polarized total and partial DOS of one dopant Gd plus one vacancy defect ($In_{30}GdS_{48}$).

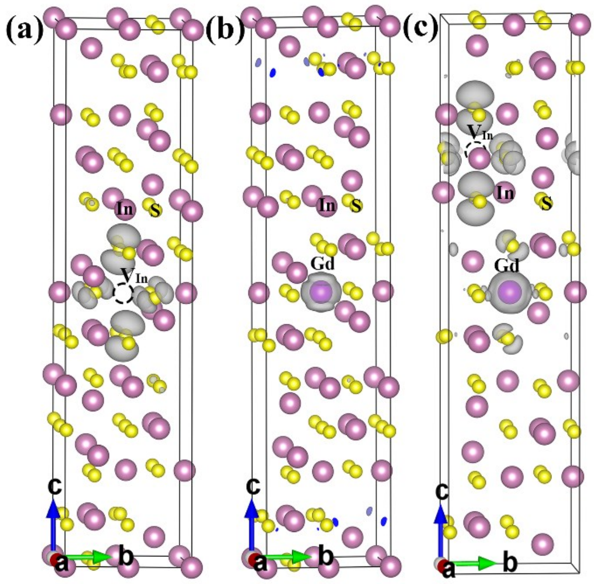


Figure S6. Spatial distribution of the spin density for (a) $In_{31}S_{48}$ ($V_{In}$), (b) $In_{31}Gd_1S_{48}$ ($Gd_{In}$) system, (c) $In_{31}Gd_1S_{48}$ ($Gd_{In}$+$V_{In}$) system. The black circle is the site of the removable In atom, the purple solid ball is the site of substituted Gd atom.

Table S2. The defect formation energies of $In_{31}S_{48}$ and $In_{30}GdS_{48}$ system under In-rich and S-rich conditions.

| $E_f$ | In-rich | S-rich |
|---|---|---|
| $In_{31}S_{48}$ | 4.992 eV | 2.514 eV |
| $In_{30}GdS_{48}$ | 0.752 eV | -4.204 eV |

References


1. S. H. Yu, L. Shu, Y. S. Wu and J. Yang, *J. Am. Ceram. Soc.*, 1999, **82**, 457-460.
2. B. Vigneashwari, A. K. Tyagi, S. Dash, P. Shankar, I. Manna and S. A. Suthanthiraraj, *J. Nanosci. Nanotec*, 2009, **9**, 5183-5187.
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4. R. N. Aljawfi and S. Mollah, *J. Magn. Magn. Mater.*, 2011, **323**, 3126-3132.