Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Size-dependent d^0 room temperature ferromagnetism in undoped In_2S_3 nanoparticles

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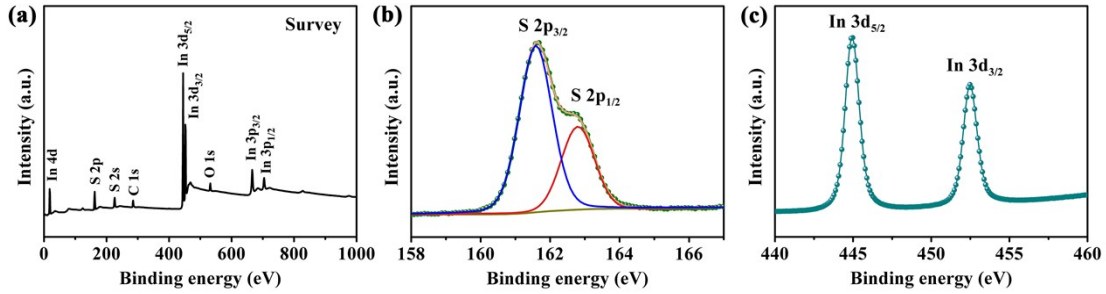

Fig. S1 XPS spectra of the sample S2: (a) survey scan, (b) high-resolution spectrum for S 2p, (c) high-resolution spectrum for In 3d.

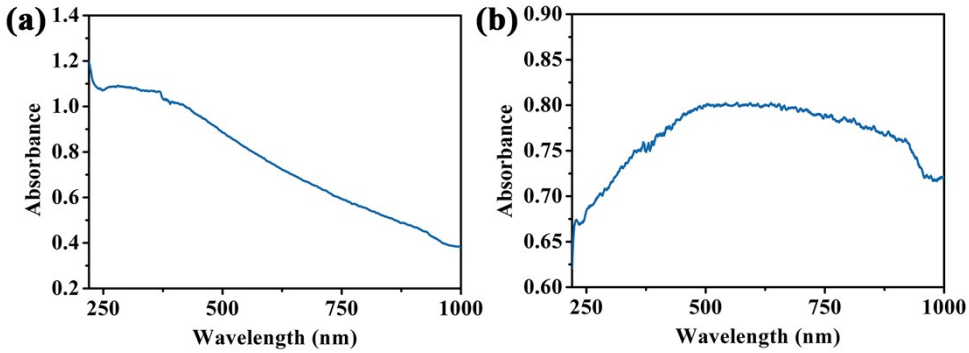

Fig. S2 The absorption spectra of samples (a) S1 and (b) S2.

The absorption spectrum of the sample S1 shows a step-like shape, which is attributed to the valence-to-conduction band transition and is consistent with the previously published studies.[1, 2] There is a significant blue shifted compared with bulk In_2S_3 (λ_{max}=601 nm, E_g=2.07 eV), which can be ascertained the quantum confinement effect.[3] The sample S2 displays weaker light absorption ability than the sample S1.

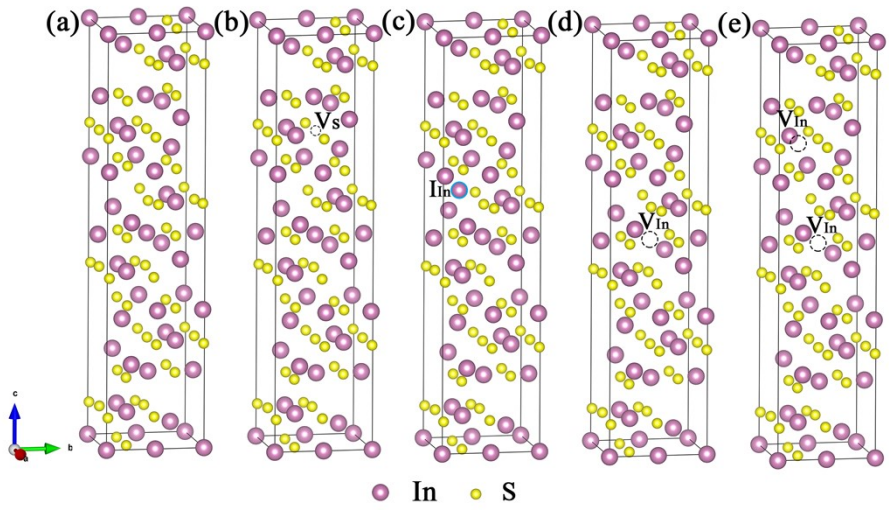

Fig. S3 Five calculation configurations: (a) an ideal system with no defects ($In_{32}S_{48}$), (b) a system with one S vacancy ($In_{32}S_{47}$), (c) a system with one In interstitial ($In_{33}S_{48}$), (d) a system with one In vacancy ($In_{31}S_{48}$), (e) a system with two In vacancies ($In_{30}S_{48}$).

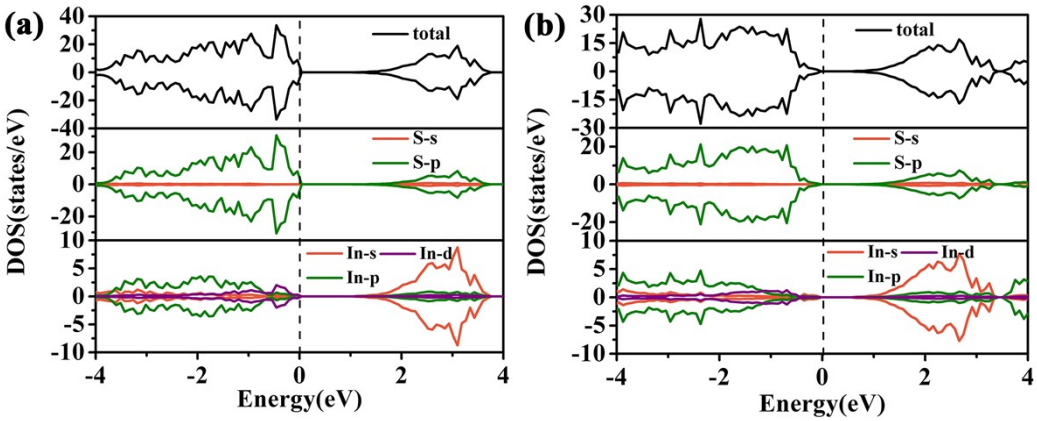

Fig. S4 TDOS and PDOS of (a) $In_{32}S_{48}$ and (b) $In_{32}S_{47}$ configurations. The Fermi energy levels are indicated by black dashed lines.

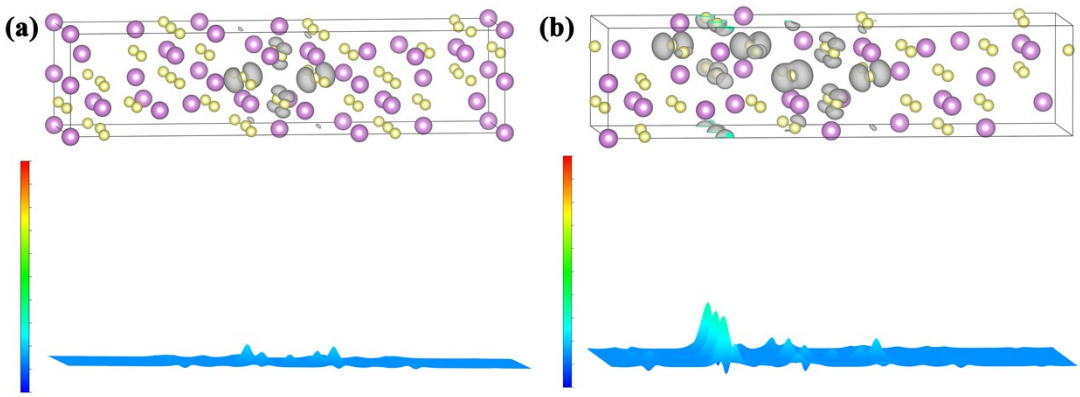

Fig. S5 Spin-density distribution and spin-density map of (a) $In_{31}S_{48}$ and (b) $In_{30}S_{48}$ models.

References

1. K. H. Park, K. Jang and S. U. Son, *Angew. Chem.*, 2006, **118**, 4724-4728.
2. W. Du, J. Zhu, S. Li and X. Qian, *Cryst. Growth Des.*, 2008, **8**, 2130-2136.
3. S. K. Batabyal, S. E. Lu and J. J. Vittal, *Cryst. Growth Des.*, 2016, **16**, 2231-2238.