Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Effect of Ho dopant on ferromagnetic characteristics of MoS_2 nanocrystals

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From the EDS results (Table S1-S4), it can be concluded that the Ho doping concentration of the samples are 1.25, 1.54, 1.88 and 2.24 at.%.

Table S1.The composition of each elements of MoS_2:Ho^{3+} nanocrystals (1.25 at.%).

Element	Weight (%)	Atom (%)
S	38.77	66.04
Mo	57.46	32.71
Dy	3.77	1.25
Total	100	100

Table S2.The composition of each elements of MoS_2:Ho^{3+} nanocrystals (1.54 at.%).

Element	Weight (%)	Atom (%)
S	37.72	65.15
Mo	57.69	33.3
Dy	4.6	1.54
Total	100	100

Table S3.The composition of each elements of MoS_2:Ho^{3+} nanocrystals (1.88 at.%).

Element	Weight (%)	Atom (%)
S	39.44	66.98
Mo	54.86	31.14
Dy	5.7	1.88
Total	100	100

Table S4.The composition of each elements of MoS_2:Ho^{3+} nanocrystals (2.24 at.%).

Element	Weight (%)	Atom (%)
S	38.28	66.03
Mo	55.03	31.73
Dy	6.69	2.24
Total	100	100

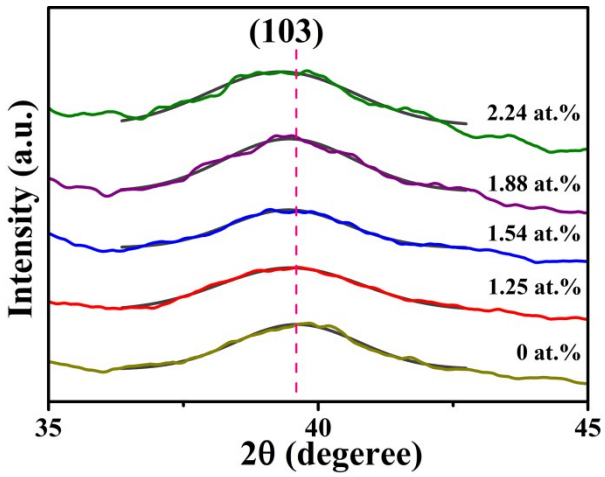

Figure S1 The variation of the (103) peak with Ho doping concentration obtained by Gaussian fitting.

Figure S2 shows the UV-Vis. Absorbance spectrum of pure and Ho-doped MoS_2 nanocrystals. The inset is plots of $(\alpha h\nu)^2$ vs $(h\nu)$ for the undoped and Ho-doped MoS_2 nanocrystals. From the pictures, it can be observed that the band gap values of are 2.19 eV, 2.27 eV, 2.32 eV, 2.34 eV and 2.37 eV for undoped, 1.25 at.%, 1..54 at.%, 1.88 at.% and 2.24 at.% MoS_2:Ho nanocrystals, which can be well in accordance with the reported results.[1] The increased band gap values as the increased Ho doping concentration indicate that the Ho ions are successfully incorporated into the MoS_2 host lattice.

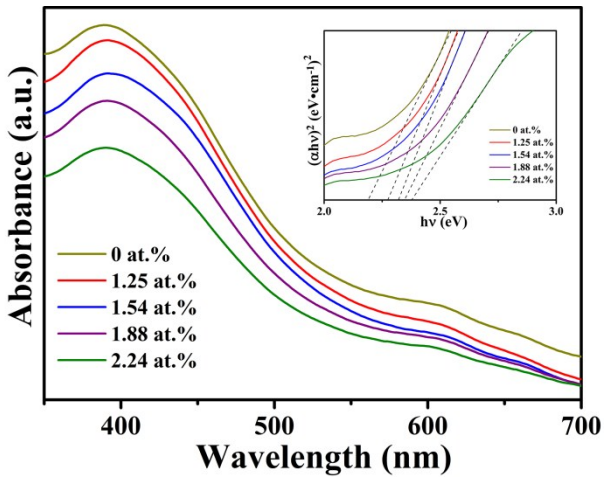

Figure S2 UV-Vis. absorbance spectrum of pure and Ho-doped MoS_2 nanocrystals. The inset is Plots of $(\alpha h\nu)^2$ vs $(h\nu)$ for the undoped and Ho-doped MoS_2 nanocrystals.

The PL spectra of the undoped MoS_2 nanocrystals and Ho-doped MoS_2 nanocrystals are shown in Figure S3. It can be observed a broad emission peak located at 650 nm which is similar to the reported results.[2, 3] The PL spectrum of 1.54 at.% MoS_2:Ho shows the weak emission peak at 630 nm which is associated with excitonic transition [3, 4].

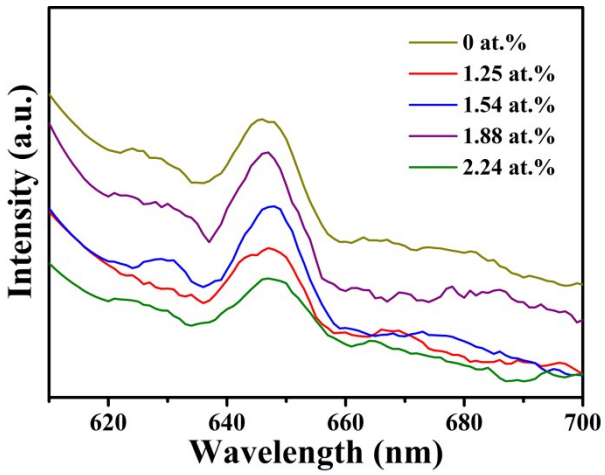

Figure S3 PL spectra of the undoped MoS_2 nanocrystals and the Ho-doped MoS_2 nanocrystals upon excitation by 475 nm at room-temperature.

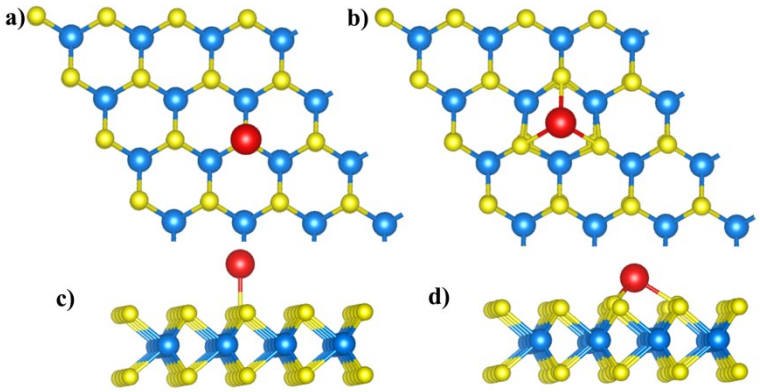

Figure S4 The atomic structures of 4 × 4 × 1 MoS_2 supercells from top view of a) S-top (a Ho atom above the top of S atom) and b) HC (a Ho atom above the center of the S-Mo-S hexagonal ring). c) and d) The side view of the two structures.

In this work, a 4 × 4 doping slab model was built to study the magnetic properties of the Ho-doped MoS_2, including 48 atoms (32 S atoms, 15 Mo atoms and 1 Ho atom). The 15 Mo atoms contain 6 nearest neighboring Mo_1 atoms, 5 the next nearest neighboring Mo_2 atoms and 4 Mo atoms on other positions. Based on the new results, the magnetic moments of Mo_1 atoms are 0.976 μB, 0.968 μB, 0.964 μB, 0.966 μB, 0.966 μB and 0.975 μB. The magnetic moments of Mo_2 atoms are -1.823 μB, 0.566 μB, 0.554 μB, -1.824 μB and -1.823 μB. The magnetic moments of Mo atoms on other positions are 1.09 μB, 1.092 μB, 1.092 μB and 0.551 μB. The overall magnetic moment of all the Mo atoms is 4.848 μB. The overall magnetic moment of all the S atoms is -1.103 μB. The magnetic moment of Ho atom is -2.348 μB. Hence, the overall magnetic moment is 1.839 μB.

References

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