

Supporting Information

Synthesis of stable γ -phase $\text{MnS}_{1-x}\text{Se}_x$ nanoflakes with inversion symmetry breaking

Bo Zheng^{1#}, Jun Fu^{2#}, Yuanmin Zhu^{3,6#}, Jing Liang^{4#}, Yongzhi She⁵, Junxiang Xiang¹,
Xiang Ma¹, Ying Zhang¹, Shasha Wang¹, Guojing Hu¹, Yuehui Zhou¹, Yan Feng¹,
Zhengping Fu¹, Nan Pan⁵, Yalin Lu^{1*}, Hualing Zeng², Meng Gu⁶, Kaihui Liu⁴, Bin
Xiang^{1*}

Note S1: Similar to the reported work, the SHG intensity increase with the increase of incident laser power, showing a parabola-like shape ($I \propto P^\theta$, $\theta = 2.04 \pm 0.02$), because SHG is a second-order nonlinear optical process, which should be quadratic proportional to the incident laser intensity. The electric dipole theory forecasts that under the first-order perturbation $I_{\text{SHG}} = |E(2\omega)|^2 \propto |P(\omega)|^2$, where I_{SHG} is the SHG intensity, $E(2\omega)$ is SHG electric field vector, and $P(\omega)$ is excitation power¹.

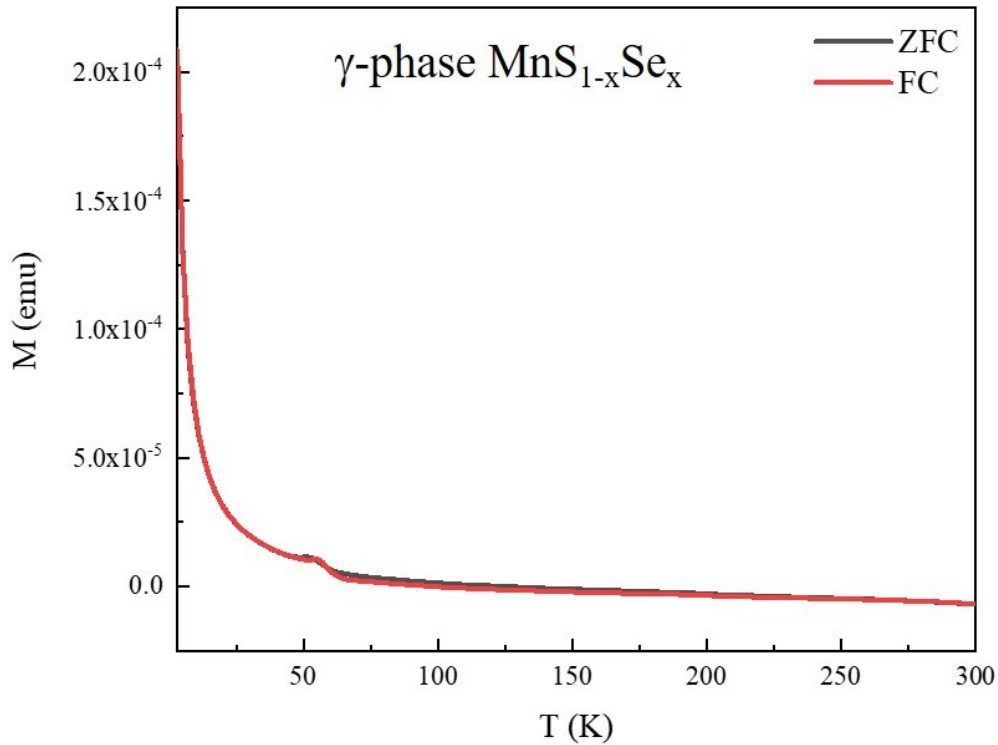


Figure S1. ZFC and FC magnetization curves of γ -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.09$) nanoflakes measured with the external magnetic field $H = 9$ T applied along the c axis.

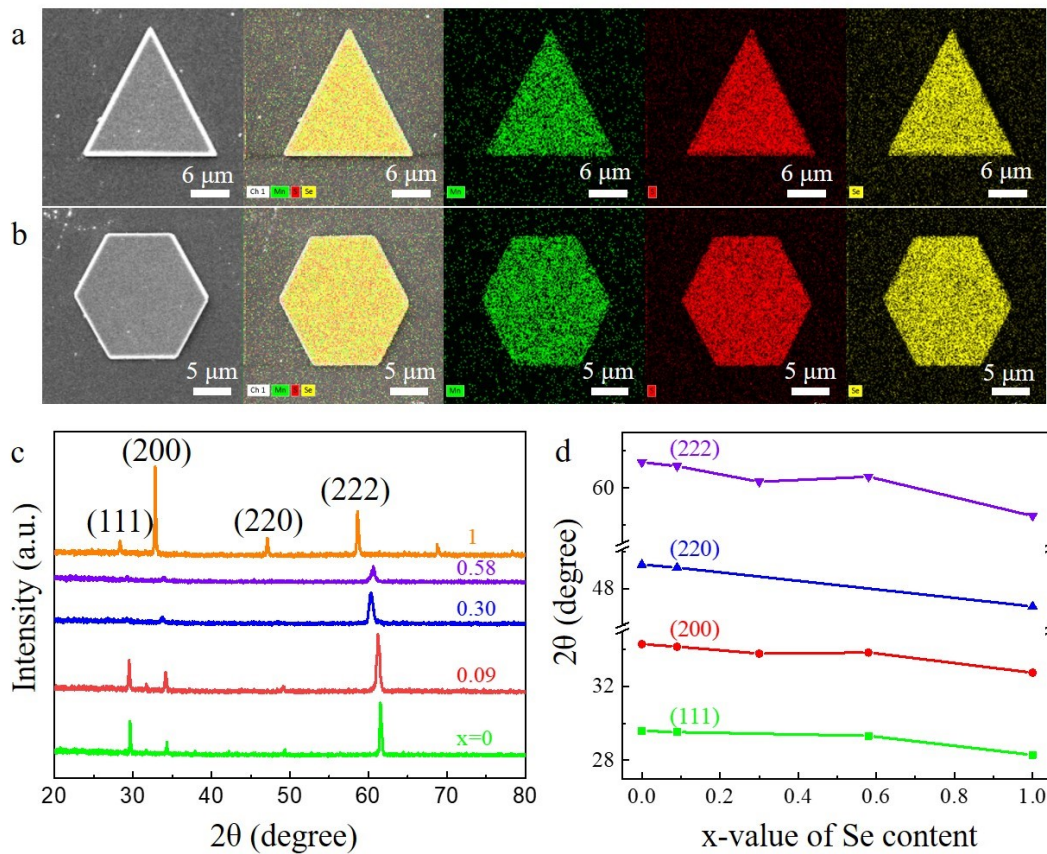


Figure S2. EDS elemental mapping images of Mn, S and Se in a typical MnS_{1-x}Se_x (x=0.30) nanosheet with the shape of a triangle (a) and hexagon (b). (c) XRD patterns of as-synthesized α-phase MnS_{1-x}Se_x nanosheets with x values of 0, 0.09, 0.3, 0.58 and 1. (d) Plots of XRD diffraction peaks determined from (c) as a function of the Se composition x.

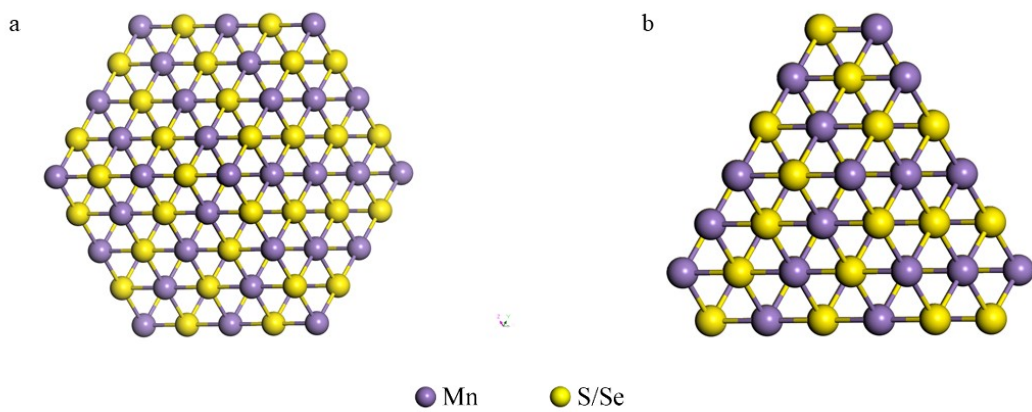


Figure S3. The ball-and-stick models of the α -phase $\text{MnS}_{1-x}\text{Se}_x$ crystal with the shape of hexagon (a) and triangle (b).

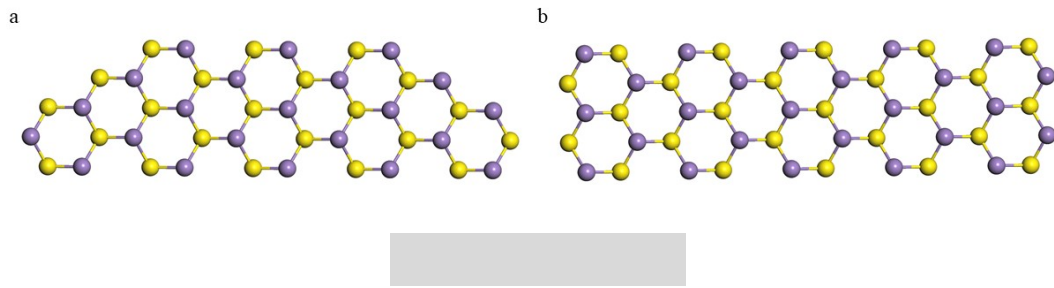


Figure S4. The ball-and-stick models of the γ -phase $\text{MnS}_{1-x}\text{Se}_x$ crystal with the shape of trapezoid (a) and rectangle (b).

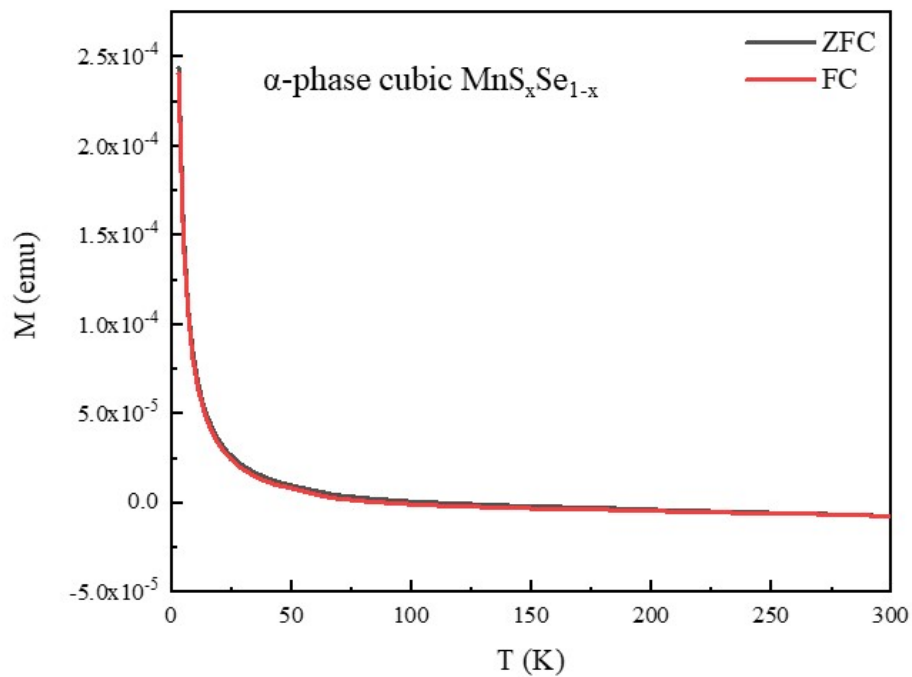


Figure S5. ZFC and FC magnetization curves of α -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.58$) measured with the external magnetic field $H = 9$ T applied along the c axis.

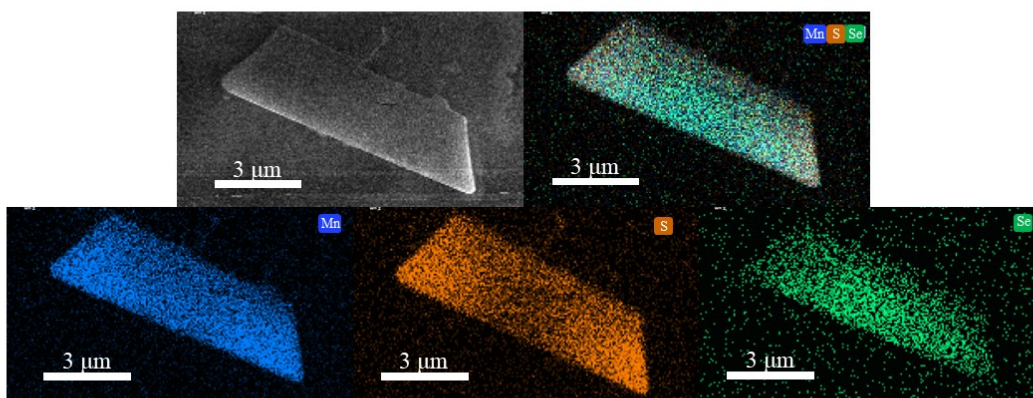


Figure S6. EDS elemental mapping images of Mn, S and Se in a typical γ -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.27$) nanosheet with the shape of a trapezoid.

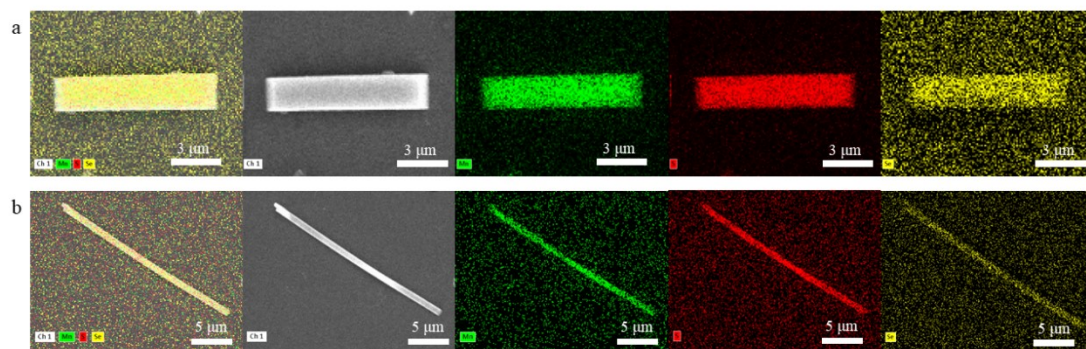


Figure S7. EDS elemental mapping images of Mn, S and Se in a typical rectangular (a) γ -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.09$) nanosheet and (b) γ -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.27$) nanowire.

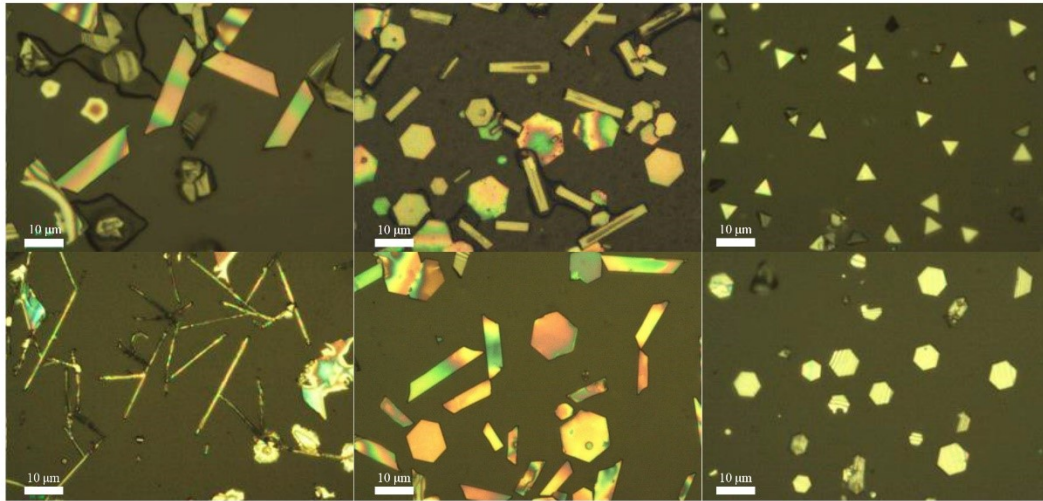


Figure S8. The different morphology of γ -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.09$) and α -phase $\text{MnS}_{1-x}\text{Se}_x$ ($x=0.30$).

	x value (calculated from precursor loading amount)	x value of γ -MnS _{1-x} Se _x (obtained from EDS)	x value of α -MnS _{1-x} Se _x (obtained from EDS)
1	0	0	0
2	0.25	0.02	0.09
3	0.5	0.09	0.30
4	0.75	0.27	0.58
5	1	0.45	1

Table S1. The x value of the as-grown γ -phase MnS_{1-x}Se_x and α -phase MnS_{1-x}Se_x.

REFERENCES

1. X. Zhou, J. Cheng, Y. Zhou, T. Cao, H. Hong, Z. Liao, S. Wu, H. Peng, K. Liu and D. Yu, *J. Am. Chem. Soc.*, 2015, **137**, 7994-7997.