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Electronic Supporting Information

Bipolar magnetism in two-dimensional NbS_2 semiconductor with high Curie temperature

Yingjie Sun,[a,b] Zhiwen Zhuo,[b] and Xiaojun Wu[b,*]

a School of Science, Hebei University of Science and Technology, Shijiazhuang, Hebei 050018, China.

b Hefei National Laboratory of Physical Sciences at the Microscale, Synergetic Innovation of Quantum Information & Quantum Technology, School of Chemistry and Materials Sciences, and CAS Key Laboratory of Materials for Energy Conversion, University of Science and Technology of China, Hefei, Anhui 230026, China.

xjwu@ustc.edu.cn (X.J. Wu)

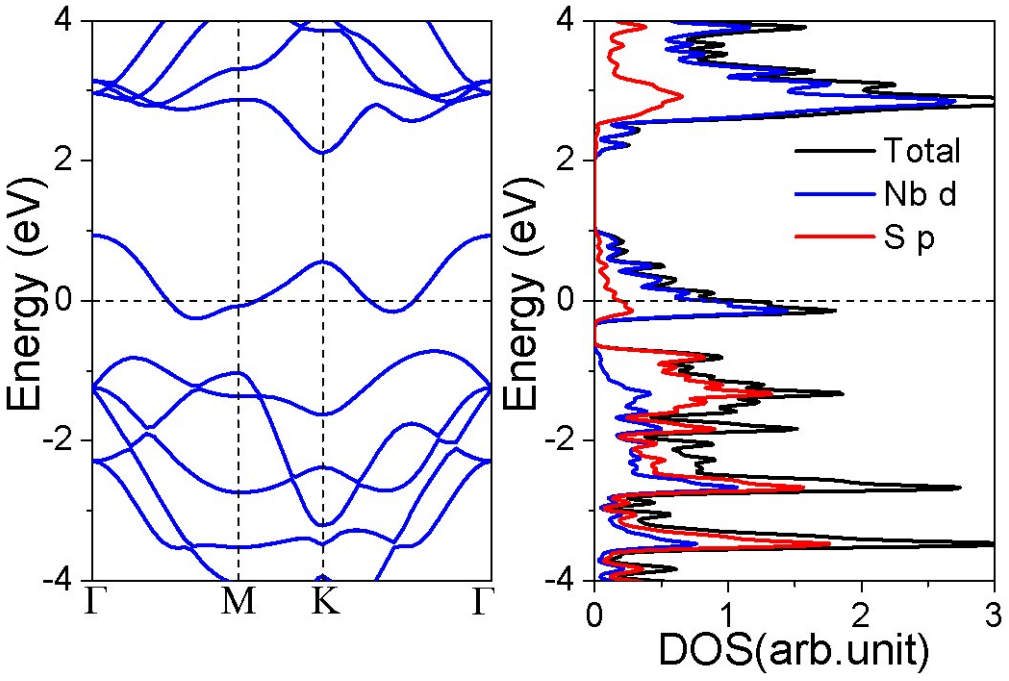

Fig. S1 Electronic structure calculated for NbS_2 monolayer at the PBE level.

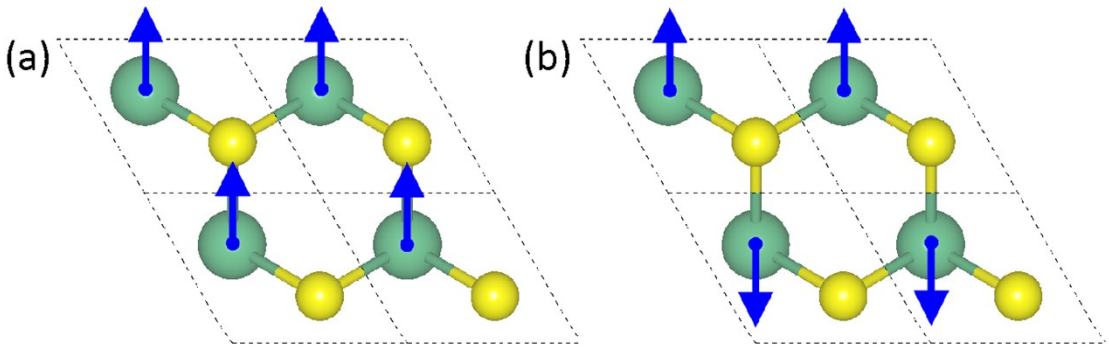

Fig. S2 Magnetic orders in NbS_2 monolayer (a) Ferromagnetic (FM). (b) antiferromagnetic (AFM)

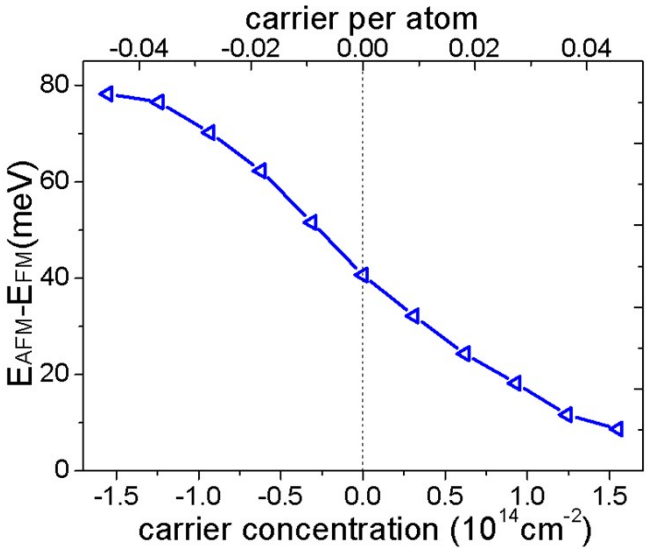

Fig. S3 Relative energy of AFM and FM states under the variation of carrier concentration for 2D NbS_2 nanosheet. The positive and negative values are for electron and hole doping, respectively.

Table S1 The optimized lattice constant (a in unit of Å), S-S bond length ($d_{s\text{-}s}$ in unit of Å) and Nb-S bond length ($d_{Nb\text{-}S}$ in unit of Å), local magnetic moment on per Nb atom (M, in unit of μB), and energy difference between FM and AFM states (ΔE, in unit of meV) are summarized.

Strain (%)	-9	-5	0	5	10
a (Å)	3.041	3.175	3.342	3.509	3.676
$d_{S\text{-}S}$ (Å)	3.32	3.23	3.12	3.04	2.96
$d_{Nb\text{-}S}$ (Å)	2.42	2.44	2.48	2.53	2.59
M (μB)	0.72	0.76	0.80	0.84	0.88
ΔE (meV)	13.1	32.0	40.7	51.8	78.5

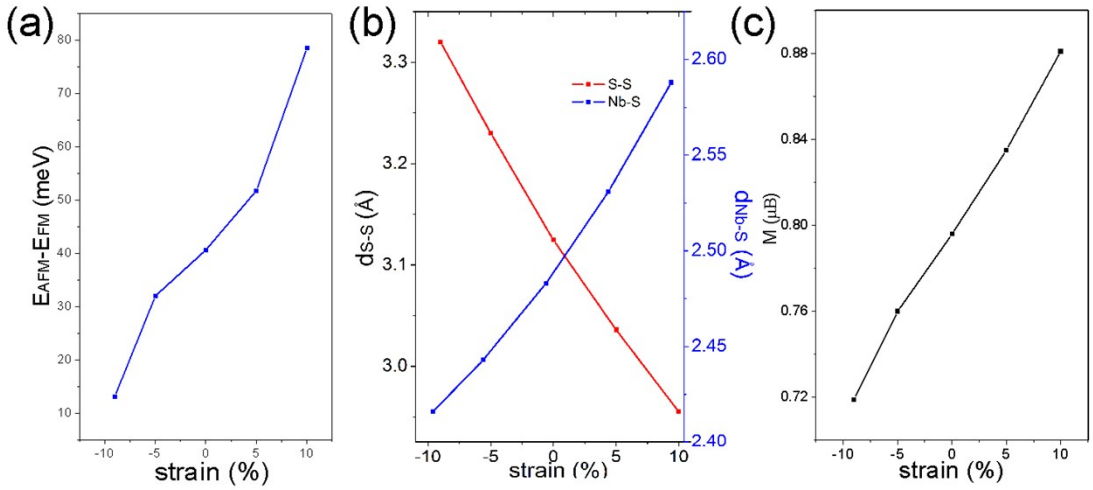

Fig. S4 Biaxial strain dependence of (a)relative energy of AFM and FM states in the 2D NbS_2 crystal. (b) S-S bond length and Nb-S bond length, and (c) magnetic moment on per Nb atoms.

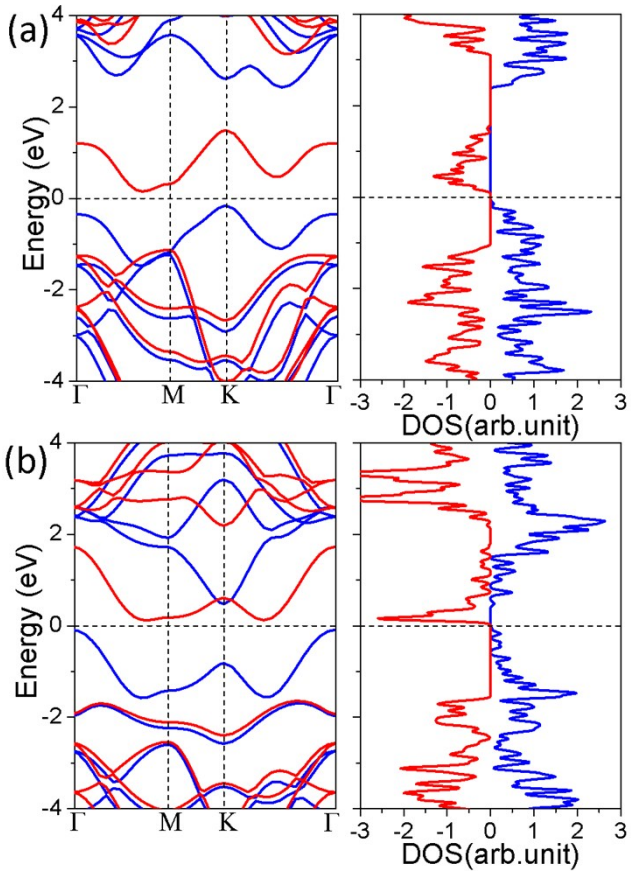

Fig. S5 Band structure, total and partial DOS for (a) -5% and (b) 5% 2D NbS_2. The Fermi levels are all set to zero.

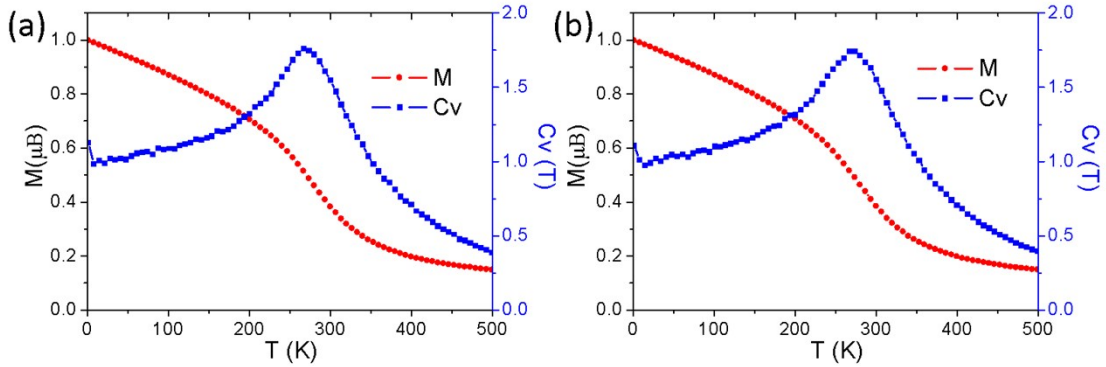

Fig. S6 The simulated magnetic moment (M) and specific heat (C_v) with respect to temperature for (a) hole doping with the carrier concentration of 1.55×10^{14} cm^{-2}, and (b) a tensile strain of 10%.