



## Magnetic Anisotropy in Magnetic van der Waals FePS<sub>3</sub>

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### Introduction

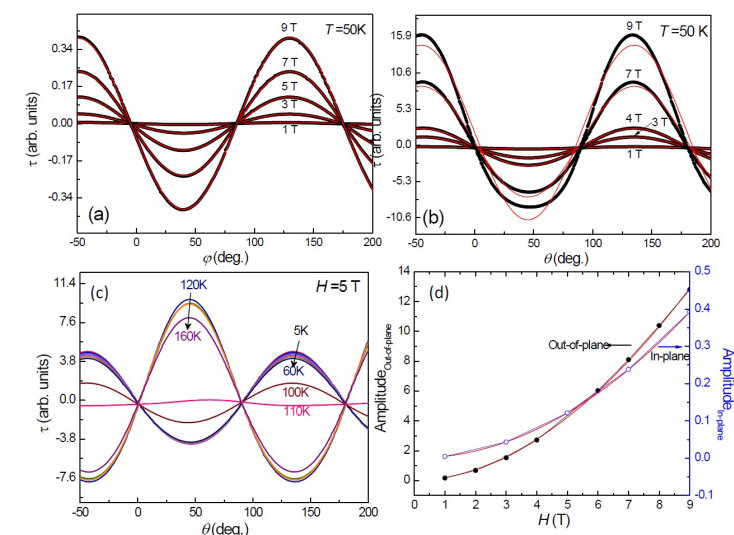
Layered transition metal tri-chalcogenides (TMPS<sub>3</sub>, TM = Fe, Co, Mn, and Ni) represents one of the known layered systems in which both magnetic and crystallographic lattices are 2D. The layers are separated by a vdW gap and represent an antiferromagnetic (AFM) order with a transition temperature in the range of 80–150 K [1, 2]. FePS<sub>3</sub> has a monoclinic honeycomb crystal structure with *C2/m* structural space group and performs an Ising-type AFM alignment along the *c*-axis below  $T_N = 118$  K. Magnetic anisotropy plays an important role in the understanding of magnetic vdW materials, which exhibit magnetocrystalline anisotropy owing to the layered structure, and a reduced symmetry. We investigated magnetic properties and magnetic anisotropy for both in-plane and out-of-plane directions using torque magnetic measurements on FePS<sub>3</sub> single crystals.

### Experimental

FePS<sub>3</sub> single crystal was mounted on a piezoelectric resistance cantilever. We measured the angle-dependent torque  $\tau(\theta)$  and magnetic field dependent torque  $\tau(H)$ . We used 18/20 T superconducting magnet (SCM-2). The angular position of the sample was controlled via a rotator, with respect to the applied magnetic field.

### Results and Discussion

The in-plane angle dependence of torque,  $\tau(\phi)$ , at different applied magnetic fields at  $T = 50$  K as shown in Fig. 1(a), indicates a perfect  $\sin 2\phi$  pattern (red lines) that represents the isotropic behavior of FePS<sub>3</sub> along the *a-b* plane. Fig. 1(b) shows the out-of-plane angle dependent torque measurement  $\tau(\theta)$ . This curve shows a perfect  $\sin 2\theta$  pattern at low magnetic field, but at 4 T or higher it deviates from  $\sin 2\theta$ , the positive torque becomes sharper, and the negative torque becomes flatter. The amplitudes, as a function of the applied magnetic field, obtained from simple sinusoidal fitting of the  $\tau(\phi)$  and  $\tau(\theta)$  curves are shown in Fig. 1(d). Larger amplitudes in out-of-plane demonstrate the larger anisotropy of FePS<sub>3</sub>.



The amplitudes are evaluated using the power-law method  $A \propto H^\alpha$  where  $\alpha = 1.99$  for the in-plane and  $\alpha = 1.89$  for the out-of-plane configurations. As shown in Fig. 1(c), out-of-plane  $\tau(\theta)$  curves at different temperatures at 5 T show consistent behavior from 5 K to 100 K. The amplitude slightly decreases with increasing temperature. However, the amplitude sharply decreases at 110 K, and the phase is reversed at 120 K above  $T_N$  and the amplitude again increases. It is noted that a sign change in the  $\tau(\theta)$  curves with increasing temperature is caused by the magnetic transition from the antiferromagnetic to paramagnetic state.

**Fig. 1** (a) In-plane and (b) out-of-plane angle dependent torque measurements of FePS<sub>3</sub>, (c) angle dependent torque at different temperatures, (d) Amplitudes of torque vs. magnetic fields for in-plane and out-of-plane rotations.

### Conclusions

A pronounced and explicit difference between out-of-plane and in-plane torque signal was observed that pertains to large anisotropy along these two directions. All the results suggest an imperfect AFM ordering along the *c*-axis with difference in net magnetization along +*c* and -*c* direction. A mixture of Zeeman energy, spin-orbit coupling and single ion anisotropy due to trigonal distortion of FeS<sub>6</sub> octahedra contribute to the overall anisotropy of FePS<sub>3</sub>.

### Acknowledgements

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### References

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- [2] Kim, S. Y. *et al.*, Physical review letters, 120, 136402 (2018).