$CrSbSe_3$: A pseudo-1D FM semiconductor

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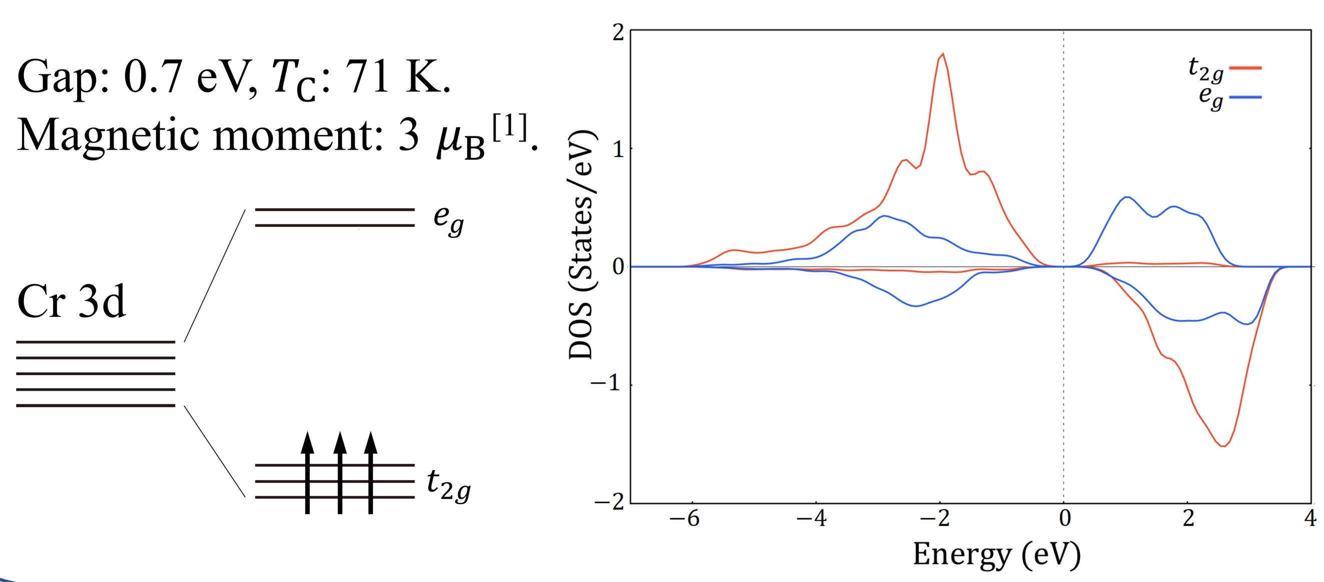
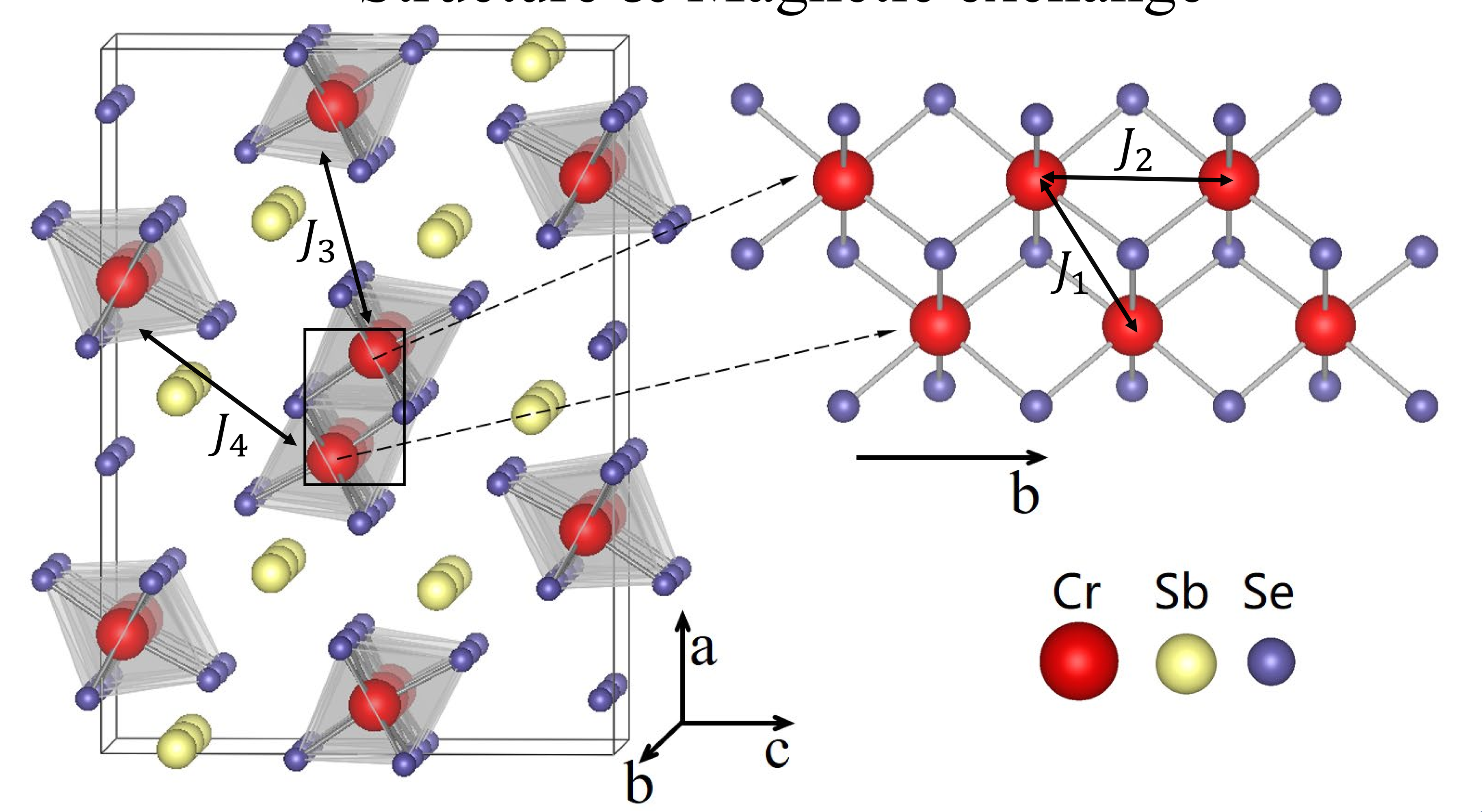
Introduction

Low-dimensional magnetic materials have attracted much attention due to their novel properties and high potential for spintronic applications. In this work, we systematically investigate the electronic structure and magnetic properties of the pseudo-one-dimensional (1D) CrSbSe3, using density functional calculations, superexchange model analyses, and Monte Carlo simulations.

Gap: 0.7 eV, T_C: 71 K.
Magnetic moment: 3 μ_B[1].



Structure & Magnetic exchange



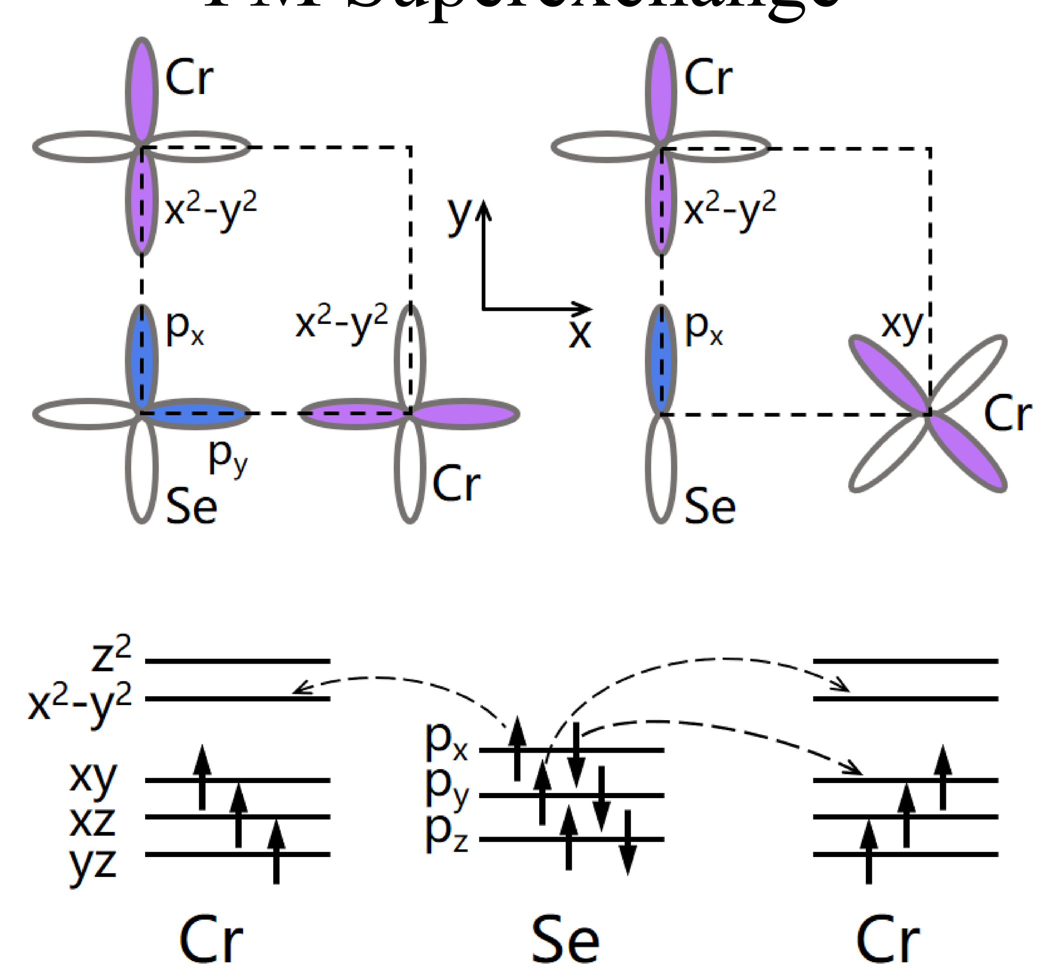
Magnetic exchange parameters

$$H = \sum_k \sum_{i,j} \frac{J_k}{2} \vec{S_i} \cdot \vec{S_j} + D \sum_i (S_i^z)^2 + E_n \sum_i \{(S_i^x)^2 - (S_i^y)^2\}$$

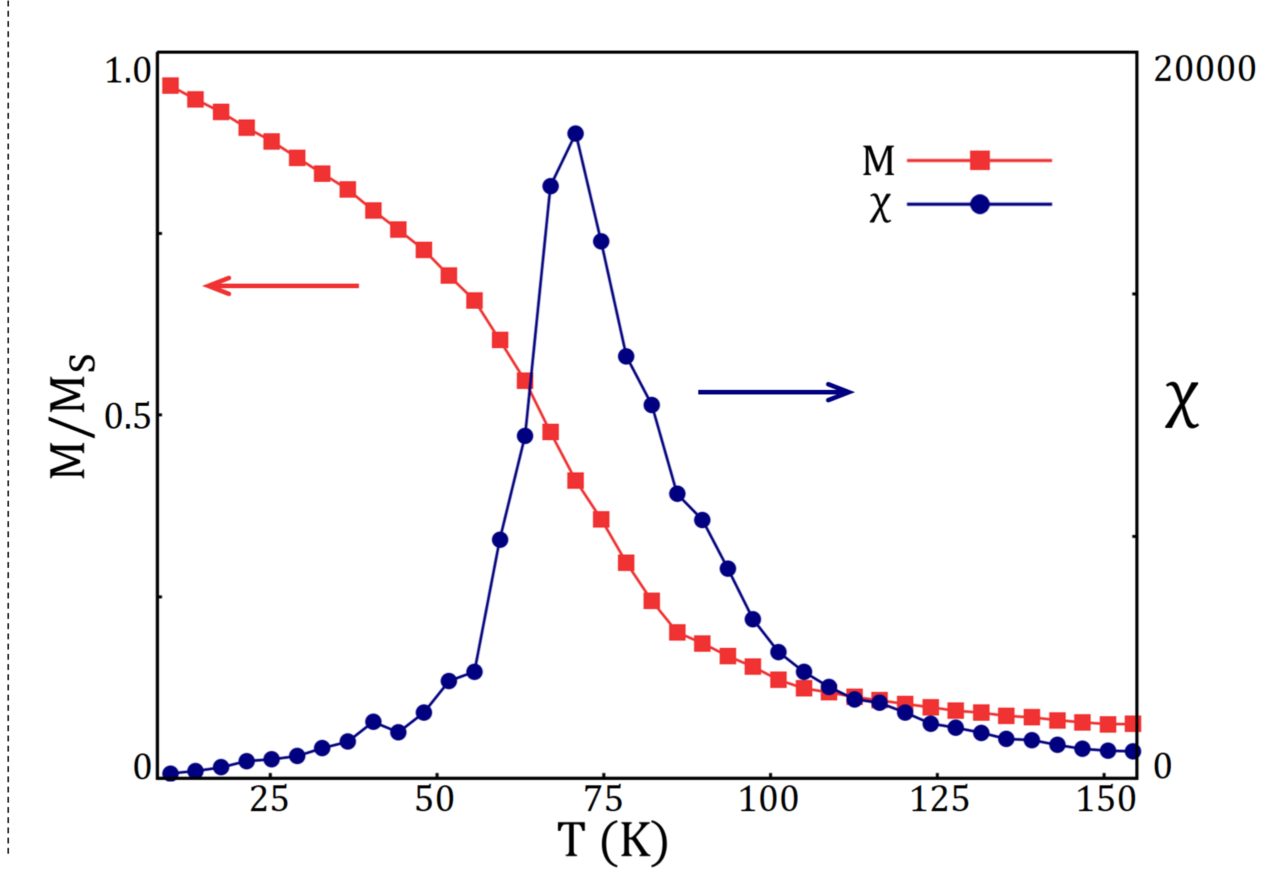
J_k (meV)	J_1	J_2	J_3	J_4
LSDA+U+SOC	−5.68	−4.94	0.24	-0.50

Triaxial MA: $E_n = -0.044$ meV
$D = -0.036$ meV

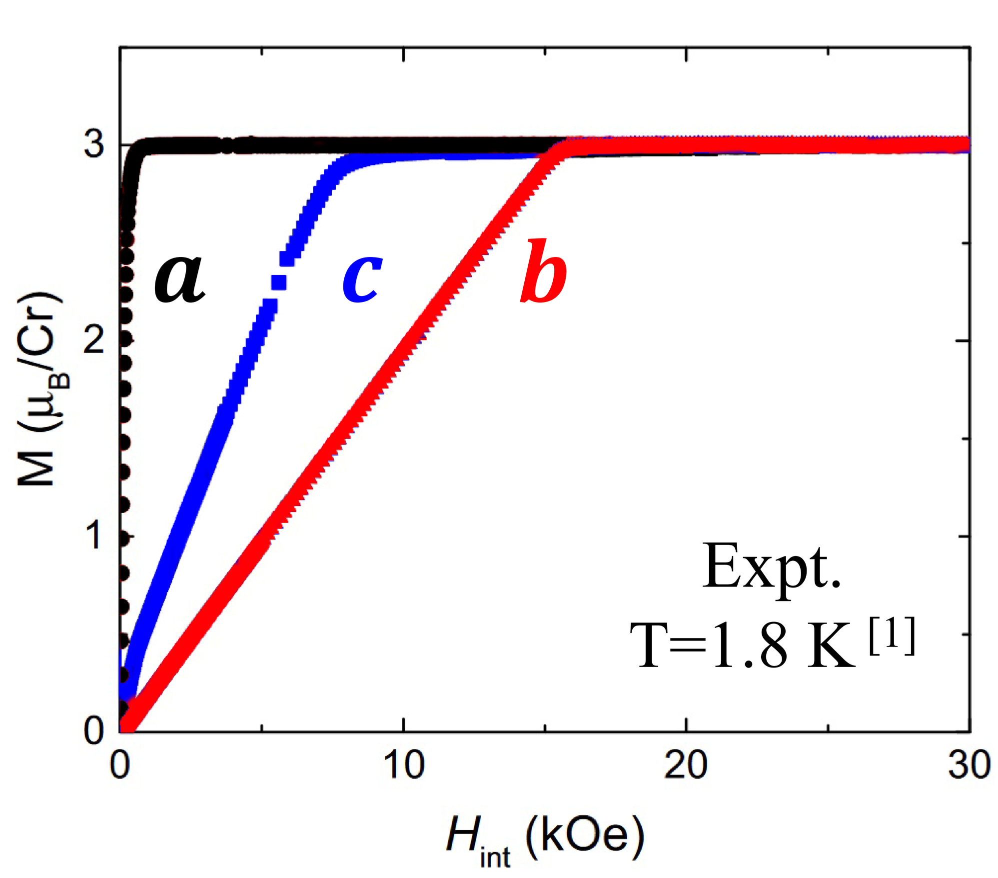
FM Superexchange

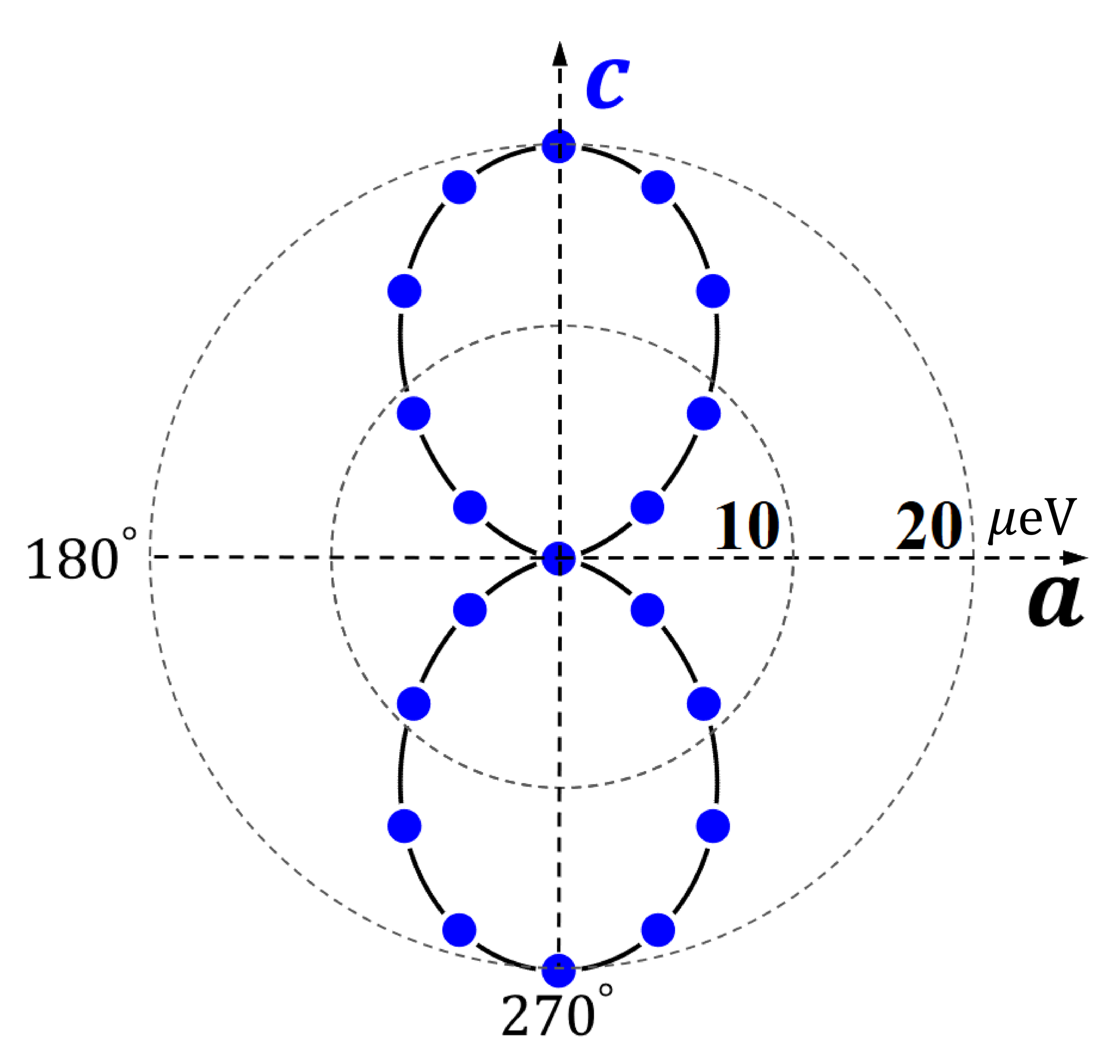


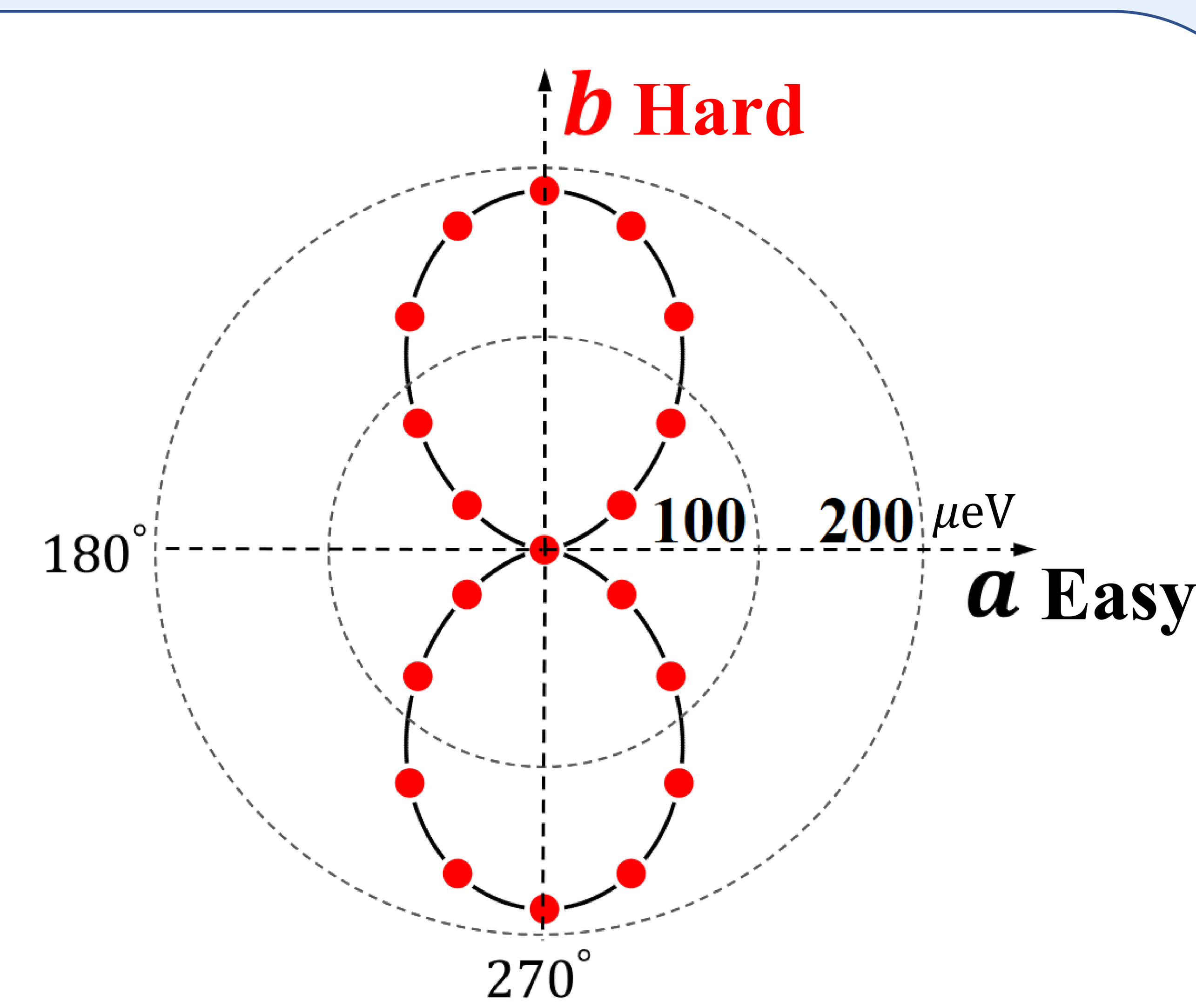
Monte Carlo simulations



Magnetic Anisotropy





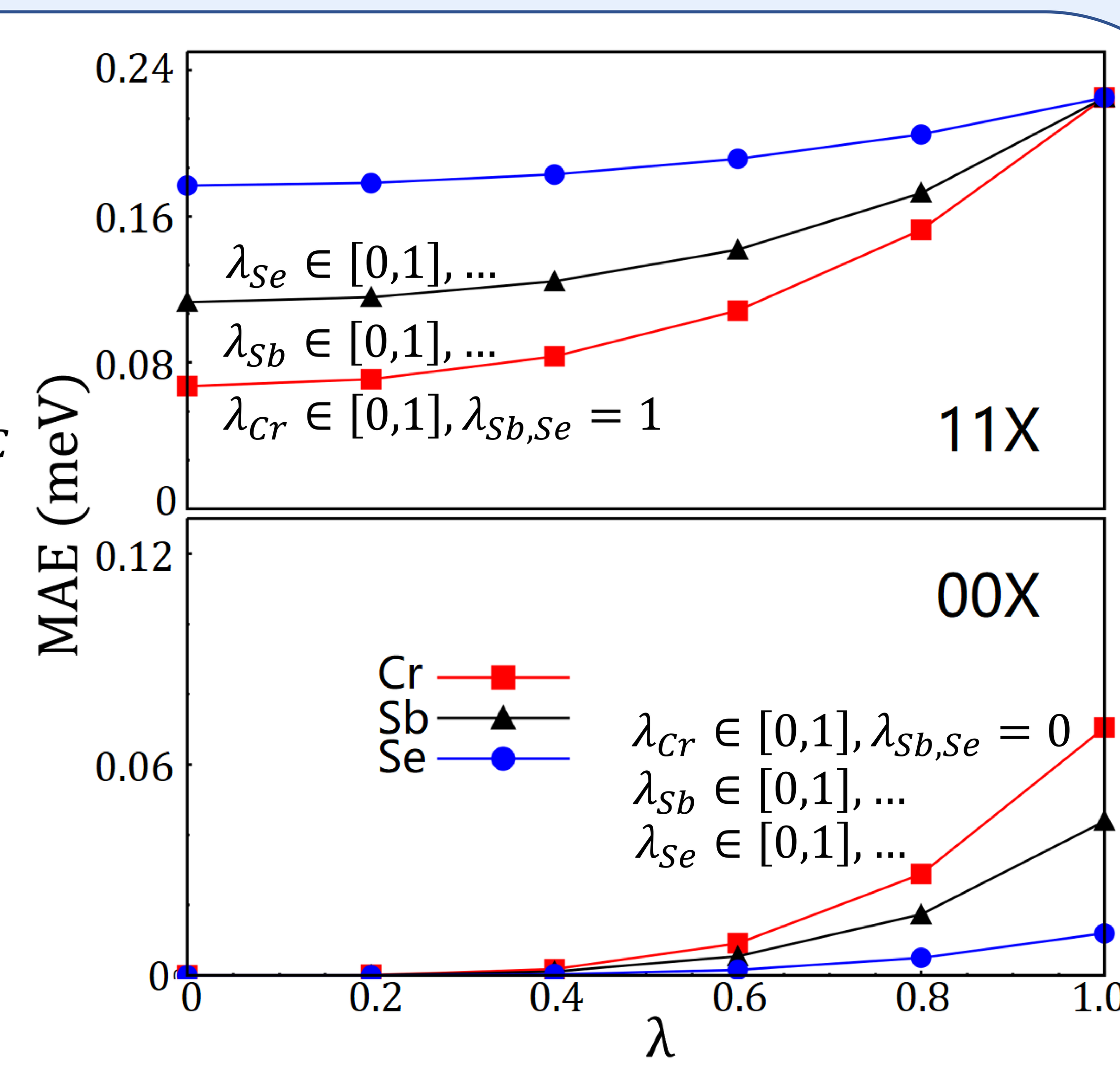


MAE vs scaling SOC

$$H_{tot} = H_0 + \lambda_{Cr} H_{Cr}^{SOC} + \lambda_{Se} H_{Se}^{SOC} + \lambda_{Sb} H_{Sb}^{SOC}$$

MAE from Cr: Single ion anisotropy.

MAE from Se\Sb: Exchange anisotropy.



Conclusion

1. We identified two major FM channels along the zigzag chain.
2. We confirmed triaxial magnetic anisotropy with the easiest x-axis, where single ion anisotropy and exchange anisotropy have comparably moderate contributions.
3. Our MC well reproduces experimental T_C.

References

1. Tai Kong *et. al.*, Phys. Rev. Mater. 2, 014410 (2018).
2. Guangyu Wang, Ke Yang, Lu Liu, Hua Wu*. submitted