Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$

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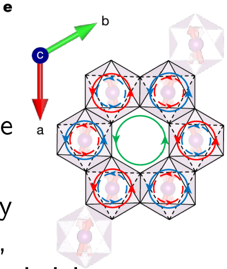
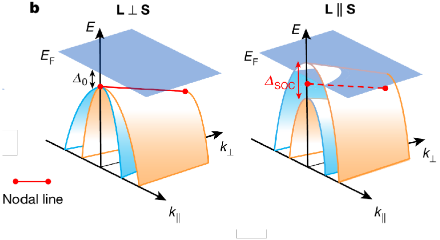
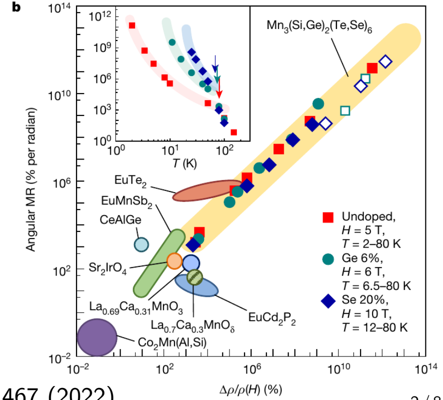
Properties of $Mn_3Si_2Te_6$

- Ferrimagnetic semiconductor with nodal-line degeneracy of bands close to the Fermi level
- Colossal magnetoresistance normally from field-induced spin polarization, which reduces spin scattering and resistivity
- $Mn_3Si_2Te_6$ is an exception, chiral orbital currents along edges of $MnTe_6$ octahedra [see Zhang *et al.*, Nature **611**, 467 (2022)]
- Nodal degeneracy is lifted depending on spin orientation, insulator to metal transition while staying in same ferrimagnet phase
- Avoided full magnetic polarization reduces ab plane resistivity



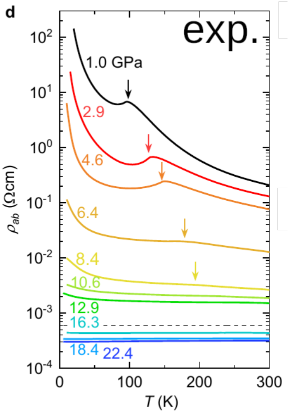


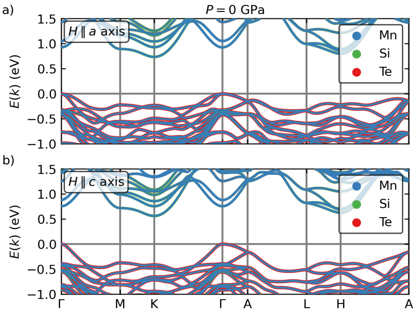


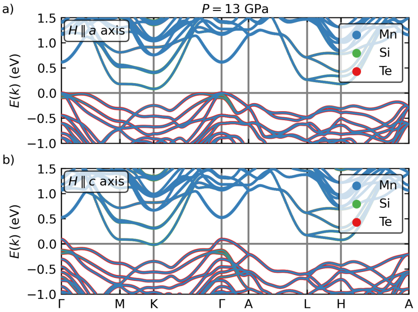
Figures: Seo *et al.*, Nature **599**, 476 (2021); Zhang *et al.*, Nature **611**, 467 (2022)

Electronic structure of $Mn_3Si_2Te_6$

- Strong reduction of resistivity as a function of pressure
- Experimental crystal structures under pressure available
- DFT calculations using FPLO in ferri state with SOC
- Pressure increases bandwidth, reduces gap
- ab easy plane, alignment along c leads to metallization under sufficient pressure
- $Mn_3Si_2Te_6$ becomes semimetal at phase transition from $P\bar{3}1c$ to $C2/c$, at $P_c = 15.4$ GPa



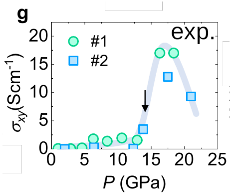


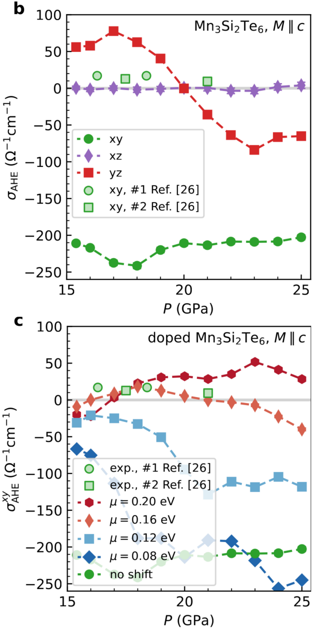


Figures: Susilo *et al.*, Nat. Commun. **15**, 3998 (2024); Venkatasubramanian *et al.*, arXiv:2509.18238

Anomalous Hall conductivity of $Mn_3Si_2Te_6$

- Insulator to metal transition at pressure of $P_c = 15.4$ GPa
- Dome-like Anomalous Hall conductivity under pressure in Susilo *et al.* [Nat. Commun. **15**, 3998 (2024)]
- AHC calculation based on FPLO Wannier functions and adaptive Monte Carlo integration
- No agreement between σ_{xy} from experiment and calculation
- AHC in $Mn_3Si_2Te_6$ is very sensitive to shifts of the Fermi level
- A shift of $\mu = 0.16$ eV produces reasonable agreement with experiment
- Electron doping is plausible, e.g. due to Te deficiency





Figures: Susilo *et al.*, Nat. Commun. **15**, 3998 (2024); Venkatasubramanian *et al.*, arXiv:2509.18238

Spin Hamiltonian of $Mn_3Si_2Te_6$: isotropic exchange from DFT

- Alternating honeycomb and triangular lattices of Mn
- Spin 5/2
- Ferrimagnetic Mn trimers
- AFM couplings in P$\bar{3}$1c phase largely unfrustrated
- Metallic phase C2/c very complex

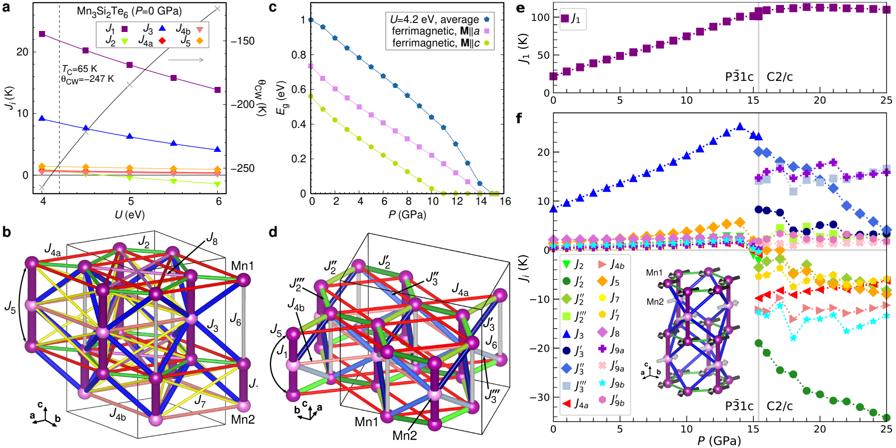
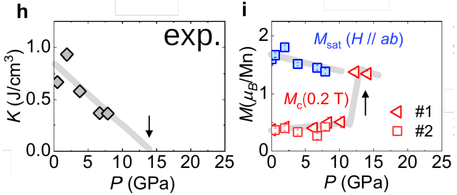
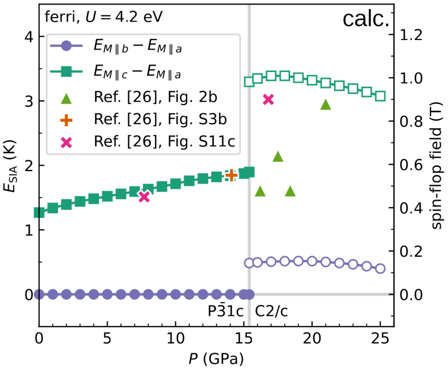


Figure: Venkatasubramanian *et al.*, arXiv:2509.18238

Spin Hamiltonian of $Mn_3Si_2Te_6$: single-ion anisotropy

- At structural phase transition ($P_c = 15.4$ GPa) Susilo *et al.* [Nat. Commun. **15**, 3998 (2024)] claim reorientation of spins from ab plane to c axis
- Experimental data interpreted to show decreasing anisotropy energy K and jump of c axis magnetization M_c in low field
- Experimental magnetization and AHC however show saturation between 0.5 T and 0.9 T
- Unclear how this would be the case with c easy axis
- We calculate SIA energy from DFT, good agreement if we associate theoretical spin-flop field with experimental saturation field





Figures: Susilo *et al.*, Nat. Commun. **15**, 3998 (2024); Venkatasubramanian *et al.*, arXiv:2509.18238

Classical Monte Carlo simulation of $Mn_3Si_2Te_6$

- Heisenberg exchange couplings derived from DFT calculations for supercells with 100 different spin configurations for each pressure
- Classical Monte Carlo simulation using Metropolis algorithm
- $8 \times 8 \times 8$ supercell, 3072 Mn sites, spin 5/2
- $\sim 10^{11}$ MC steps for each temperature
- Negligible finite size effect
- Curie temperature determined from specific heat
- Very good agreement with experimental data, also in metallic phase

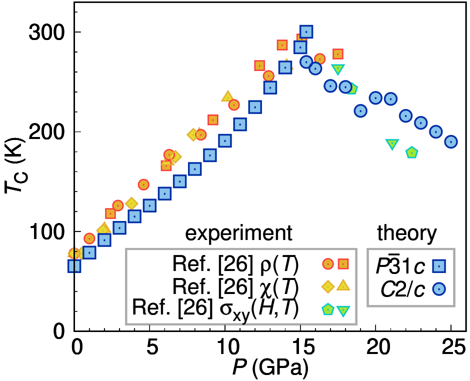
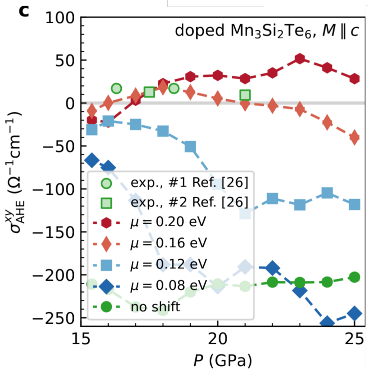
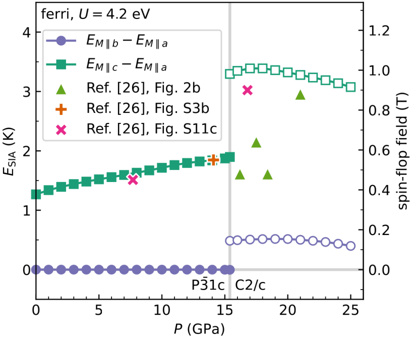


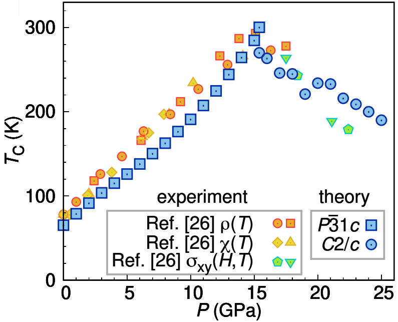
Figure: Venkatasubramanian *et al.*, arXiv:2509.18238

Summary

- Magnetism of $Mn_3Si_2Te_6$ described well by DFT
- Classical Monte Carlo agrees well with experimental T_C
- Hamiltonian tabulated in our manuscript
- No hint of c easy axis claimed by Susilo *et al.* [Nat. Commun. **15**, 3998 (2024)]
- Anomalous Hall effect very sensitive to electron doping, e.g. Te deficiency
- **Preprint arXiv:2509.18238** (to be published in Commun. Mater.)

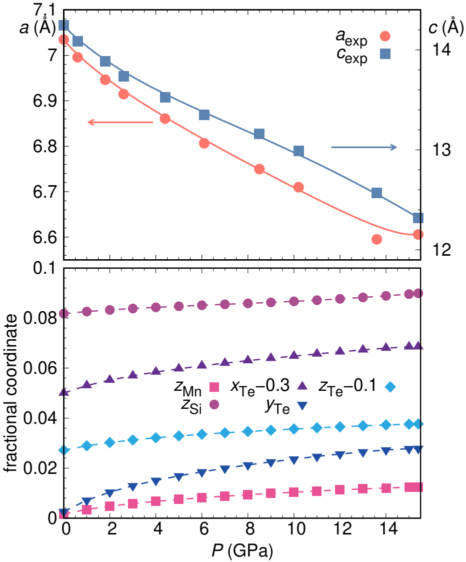






Figures: Venkatasubramanian *et al.*, arXiv:2509.18238

Appendix: Interpolation of experimental crystal structures



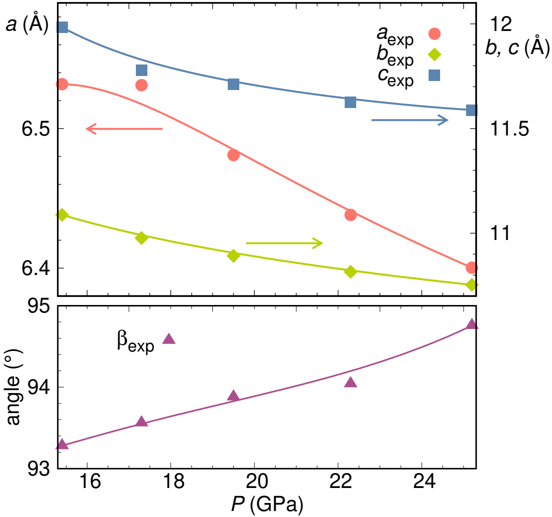


Figure: Venkatasubramanian *et al.*, arXiv:2509.18238

Appendix: Berry curvature and Anomalous Hall conductivity

- Intrinsic AHE from Berry curvature $\Omega_n(\underline{k}) = \underline{\nabla} \times \underline{A}_n(\underline{k})$ with $\underline{A}_n(\underline{k}) = i \langle u_{n\underline{k}} | \underline{\nabla}_{\underline{k}} | u_{n\underline{k}} \rangle$
- z-Component of Berry curvature tensor:

$$\Omega_{n,z}(\underline{k}) = -2\,\mathrm{Im} \left\langle \frac{\partial u_{n\underline{k}}}{\partial k_z} \middle| \frac{\partial u_{n\underline{k}}}{\partial k_z} \right\rangle$$

- Total Berry curvature $\Omega_z(\underline{k})$ is defined as the sum over all bands n of the band-resolved Berry curvature $\Omega_{n,z}(\underline{k})$ weighted by the respective occupation number $f_n(\underline{k})$:

$$\Omega_z(\underline{k}) = \sum_n f_n(\underline{k})\, \Omega_{n,z}(\underline{k})$$

- Anomalous Hall conductivity is the integral of the total Berry curvature $\Omega_z(\underline{k})$ over the entire Brillouin zone (PRB **74**, 195118 (2007)):

$$\sigma_{xy} = -\frac{e^2}{\hbar} \int_{BZ} \frac{d\underline{k}}{(2\pi)^3}\, \Omega_z(\underline{k})$$

- Total Berry curvature from FPLO Wannier interpolation
- BZ integration with adaptive Monte Carlo method

Appendix: Isotropic exchange terms from DFT energy mapping

- DFT calculations in FPLO for 100 supercell spin configurations
- Mn atoms carry spin 5/2
- Fit energy landscape with classical Heisenberg Hamiltonian with ordinary least squares
- Metallic phase requires some regularization due to large number of possible exchange paths

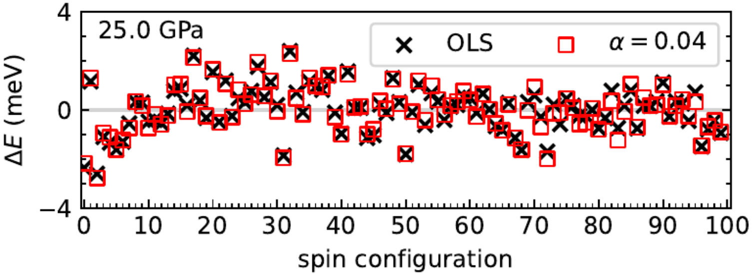


Figure: Venkatasubramanian *et al.*, arXiv:2509.18238

Appendix: Anisotropic terms in the spin Hamiltonian

- Exchange anisotropies J_1^{yy} and J_1^{zz}
- Single-ion anisotropy K^y and K^z
- ab easy plane in low-pressure phase
- a easy axis in high-pressure phase
- Non-monotonic pressure dependence from FM energies

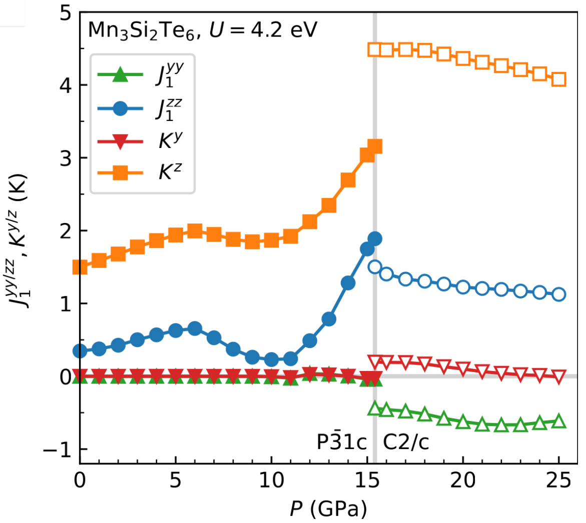
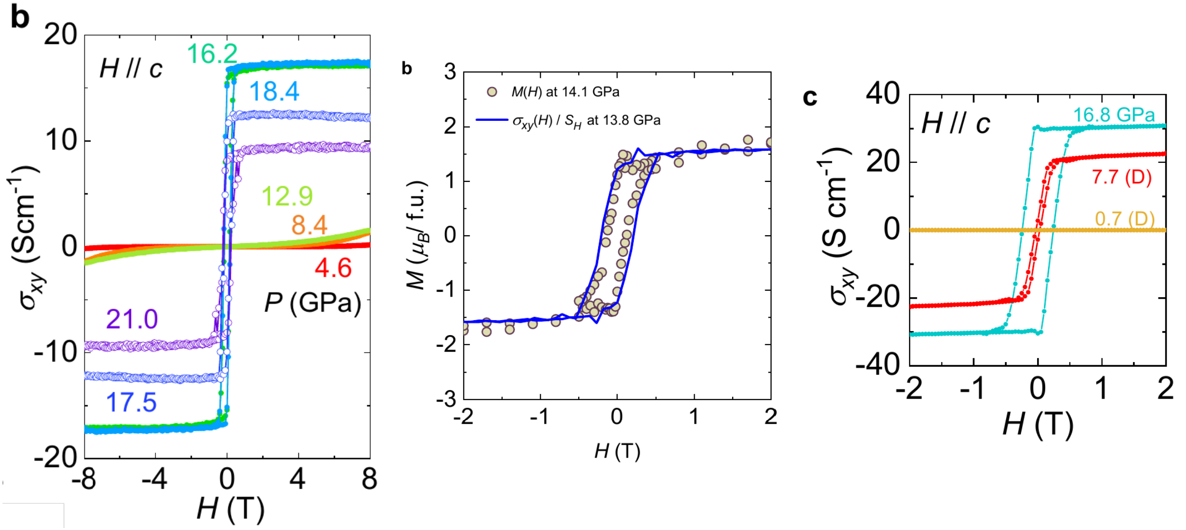


Figure: Venkatasubramanian *et al.*, arXiv:2509.18238

Appendix: Information on the anisotropy energy from Susilo *et al.*



Figures: Susilo *et al.*, Nat. Commun. **15**, 3998 (2024)