Atomic altermagnetism

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Altermagnetism has recently been verified experimentally by photoemission mapping of the spin order in MnTe and CrSb [1], which feature two anisotropic sublattices with antiparallel magnetic dipole moments. In this talk , I will introduce the concept of atomic altermagnetism[2]—a form of ferroic higher-order partial waves of the atomic spin density. Using spin-symmetry analysis and partial-wave decomposition of first-principles spin densities, we explicitly demonstrate such non-dipolar spin order in MnTe, KV_2Se_2O, and Ba_2CaOsO_6. In MnTe we identify a ferroically ordered g-wave form factor around the Mn site. In KV_2Se_2O (and related Lieb-lattice compounds), we show a ferroically ordered d-wave spin density coexisting with antiferroic dipoles on V sites, while O sites display a pure d-wave spin density without any dipole. In the Mott insulator Ba_2CaOsO_6, we uncover a striking case of pure atomic altermagnetism, entirely absent of dipolar sublattice order. These results highlight that altermagnetic order can exist without a Néel vector of staggered dipole moments, thus distinguishing it fundamentally from conventional collinear antiferromagnetism. Finally, I will show that KV_2Se_2O and Ba_2CaOsO_6 are predicted to host giant spin-splitter angles of up to 42° and 26°, respectively—demonstrating that strong altermagnetic responses can emerge without requiring the staggered Néel order of local dipole moments.

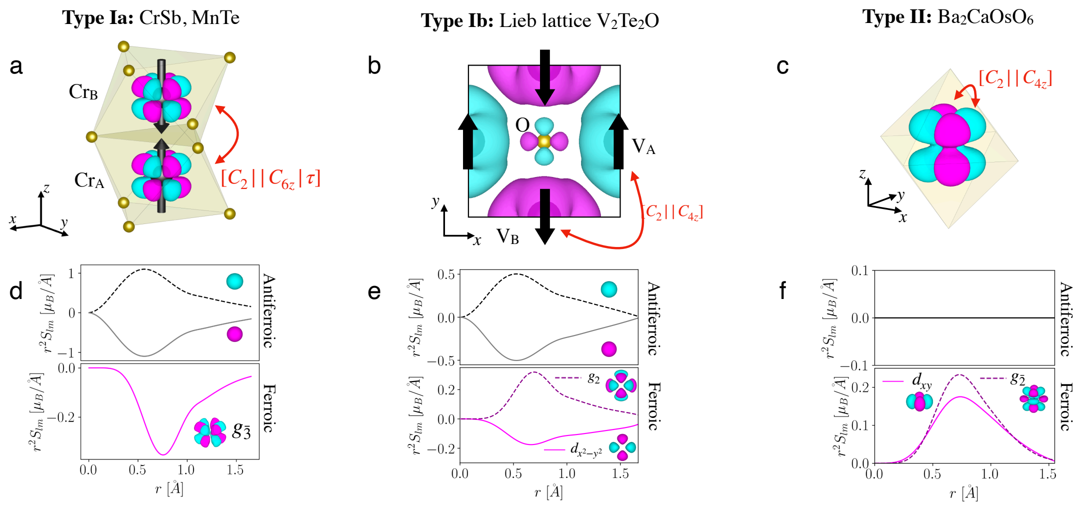

Figure 1. Partial-wave expansion of the spin density from non-relativistic DFT for CrSb, V_2Te_2O, and Ba_2CaOsO_6.

References

[1] L. Šmejkal, J. Sinova, and T. Jungwirth, "Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry," *Physical Review X*, vol. 12, p. 031042, sep 2022.

[2] R. Jaeschke-Ubiergo, V.-K. Bharadwaj, W. Campos, R. Zarzuela, N. Biniskos, R. M. Fernandes, T. Jungwirth, J. Sinova, and L. Šmejkal, "Atomic altermagnetism," *arXiv preprint arXiv:2503.10797*, 2025.