Metallic antiferromagnetism and enhanced Dzyaloshinskii–Moriya interactions in the MnTeI Janus monolayer

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Spin-orbit coupling effects in two-dimensional (2D) materials enable the existence of long-range magnetic order at finite temperatures. This has triggered research in van der Waals magnets in the last decade, as experimentally feasible candidates to obtain truly bidimensional magnets with tunable features. The vast variety of possible materials confers relevance to preliminary explorations based on accurate ab initio models aimed to identify the most promising candidates. In particular, the recent experimental realization of Janus transition-metal dichalcogenide monolayers [1] has sparked strong interest in Janus engineering as a unique tool in the search of new 2D magnets with critical temperatures approaching room temperature, yet a challenge in this field. The intrinsic inversion-symmetry breaking of Janus materials provides a suitable platform for spin–orbit-driven phenomena, and Janus dichalcogenides have already shown promising magnetic properties [2].
To further enhance these features, a natural possibility is to replace one of the chalcogen atoms with a halogen, constructing Janus chalcohalide systems. Here, we investigate monolayer MnTeI using first-principles calculations combined with atomistic spin dynamics. Mn-based chalcohalides still remain scarcely explored, and we will prove that MnTeI offers singular features in this family. It is a metallic antiferromagnet with large magnetic critical temperature, and a magnetically driven structural distortion linked to inequivalent exchange pathways. Such distorted lattice hosts a collinear in-plane antiferromagnetic ground state, in contrast to the out of plane ferromagnetic ordering reported in related MnXY systems [3]. The broken inversion symmetry further gives rise to a sizable Dzyaloshinskii–Moriya interaction and a pronounced magnetic anisotropy that locks the spins to the distortion direction, providing favorable conditions for the stabilization of chiral magnetic textures. Altogether, the unusual coexistence of antiferromagnetism, metallicity, and enhanced chiral interactions places MnTeI among a small class of two-dimensional materials with strong potential for high-frequency antiferromagnetic spintronics.

References:

[1] A.-Y. Lu, H. Zhu et al. Nat. Nanotechnol. 12 (2017) 744
[2] J. Liang, W. Wang, et al. Phys. Rev. B 101 (2020) 184401
[3] X.-F. Huang, K.-J. Li, et al. Appl. Phys. Lett. 124 (2024) 252402

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