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Designing Magnetic Topological Materials from First Principles

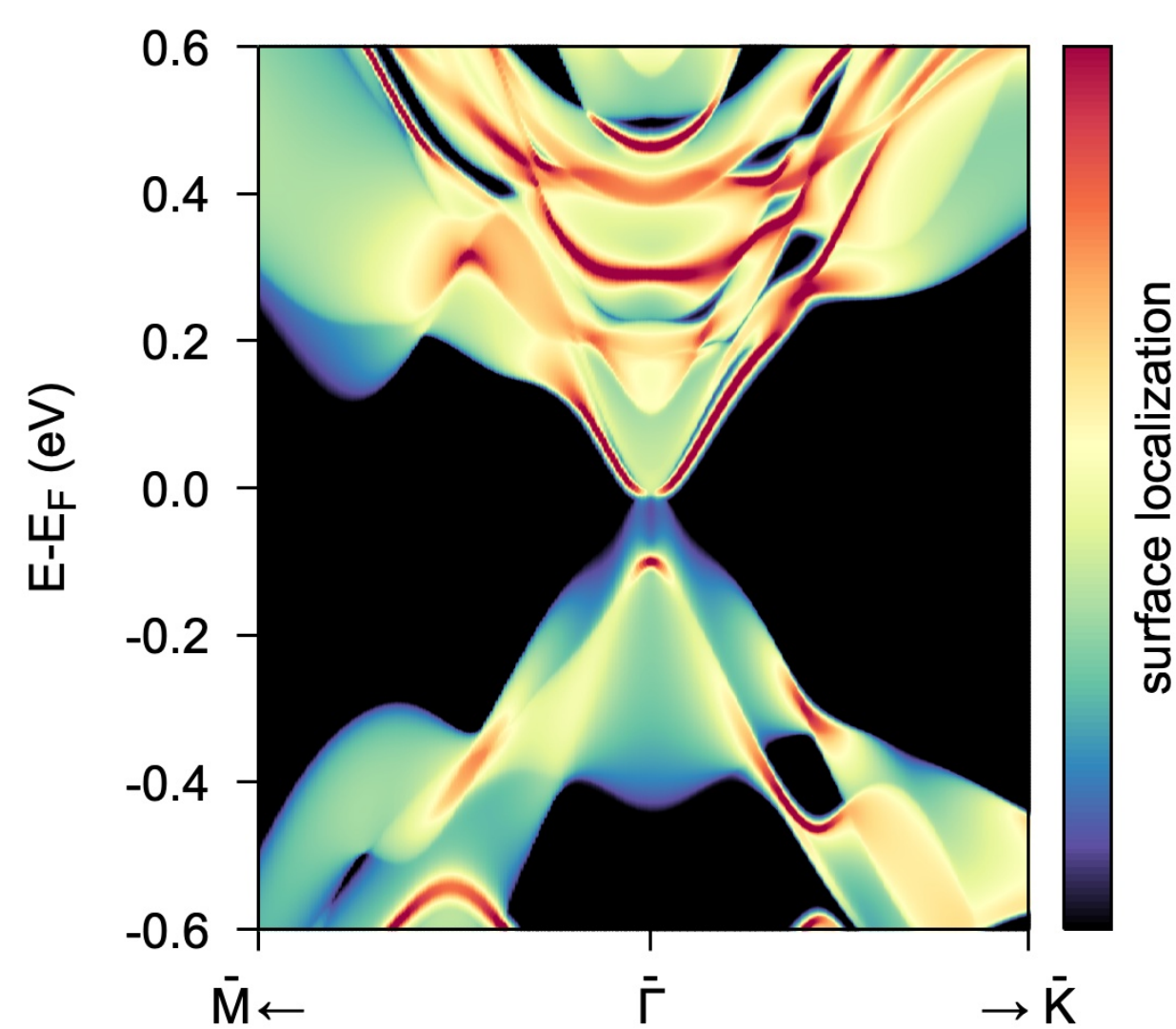
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Ort: H34

Since their experimental discovery in 2013, magnetic topological insulators have created a new platform in quantum materials research, where topology and magnetism intertwine to generate exotic quantum phenomena.

One of their most striking manifestations is the quantum anomalous Hall effect: a state with dissipationless edge conduction without an external magnetic field. Realizing this effect at higher temperatures can have potential applications in spintronics and quantum information technologies. However, this remains a major challenge, requiring materials that are simultaneously ferromagnetic, topological, and insulating.

In this talk, I will discuss MnSb_2Te_4 , a layered magnetic topological material that illustrates both the promise and the difficulty of this search. Using first-principles electronic-structure calculations, including density functional theory and GW corrections, we examine whether MnSb_2Te_4 satisfies the three key ingredients for observing the quantum anomalous Hall effect: ferromagnetic order, non-trivial band topology, and an insulating bulk electronic state. I will review the intricate electronic structure of this compound and our current efforts to boost its Curie temperature while retaining its topological nature.



Electronic structure of MnSb_2Te_4 , with red being surface states, yellow surface resonances, and green and blue bulk states (Figure credit: Tardieux, Tanzim, Grytsiuk, Isaeva, and Aguilera. Materials Today Quantum 10, 100069 (2026))