Chemical design principles for magnetic topological materials

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Abstract: The search for magnetic topological insulators and semimetals has often relied on experimental serendipity (as in the case of $MnBi_2Te_4$) and computational high-throughput screening amongst known materials. Establishing a chemical principle for realizing stable magnetic topological materials would provide a means to systematically and rationally design them. Such principles are yet lacking. Here we propose two general strategies based on orbital interactions, one for realizing ideal type-II Weyl semimetals, and one for realizing magnetic topological insulators. For type-II Weyl semimetals, we focus on the prototypical material $MnBi_2Te_4$ in its ferromagnetic phase, and discuss how its type-II Weyl point is related to zone folding of p_z orbital dispersions. For magnetic topological insulators, we discuss how Peierls instability manifest in existing and predicted magnetic topological insulators.