Prediction of a Two-Dimensional Organic Topological Insulator

ZHENGFEI WANG, NINGHAI SU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Topological insulators (TI) are a class of materials exhibiting unique quantum transport properties with potential applications in spintronics and quantum computing. To date, all of the experimentally confirmed TIs are inorganic materials. Recent theories predicted the possible existence of organic TIs (OTI) in two-dimensional (2D) organometallic frameworks. However, those theoretically proposed structures do not naturally exist and remain to be made in experiments. Here, we identify a recently experimentally made 2D organometallic framework, consisting of π-conjugated nickel-bis-dithiolene with a chemical formula $\text{Ni}_3\text{C}_{12}\text{S}_{12}$, which exhibits nontrivial topological states in both a Dirac band and a flat band, therefore confirming the existence of OTI.

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