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RESEARCH HIGHLIGHTS

PHYSICS

Special Topic: Topological Insulators

Predicting organic topological materials

Feng Liu[1,*] and Jian Wu[2]

Topological insulators (TIs) are a recently discovered class of materials with insulating bulk electronic states, but conducting boundary states inside the bulk band gap distinguished by nontrivial topology. The concept of topological order in condensed matter physics provides a new perspective for understanding the origin of different quantum phases and has generated intense recent interest in searching for nontrivial topological materials. The boundary states of a TI have a topological origin and bulk correspondence, giving rise to a quantized surface (for 3D TI) or edge (for 2D TI) conductance. They are also so-called helical Dirac states, characterized by a spin-momentum-locking property. These unique properties make the spin-polarized electron transport of topological materials protected from elastic backscattering and localization, lending them great potential for applications in spintronics and quantum computation devices.

To date, several generations of 2D and 3D TIs have been predicted theoretically and confirmed experimentally. However, all the previously known TIs are based on inorganic materials. Conversely, many conventional inorganic materials and devices have later found their organic counterparts, such as organic semiconductors and superconductors. In general, organic counterparts of inorganic materials have the added advantages of low cost, easy fabrication and mechanical flexibility. To this end, the work of Professor Feng Liu's group at University of Utah, leading to the prediction of the existence of organic topological materials in a series of publications [1–4], is an exciting development.

Designed by assembling molecular building blocks of triphenyl-metal compounds with strong spin–orbit coupling (SOC) into a hexagonal lattice, they first proposed 2D organic TIs (OTIs) [1], i.e. spin Hall insulators, in organometallic lattices made of triphenyl-Pb $[Pb(C_6H_5)_3]$ and triphenyl-Bi $[Bi(C_6H_5)_3]$ molecules. Using first-principles band structure and band-topology calculations complemented by tight-binding edge-state calculations and model analyses, this new class of OTIs exhibits nontrivial topological edge states that are robust against significant lattice strain [1]. Next, by replacing Pb or Bi with a transition metal element, Mn, they designed a magnetic OTI, i.e. a Chern insulator, made of triphenyl-Mn $[Mn(C_6H_5)_3]$ molecules, for realizing the anomalous quantum Hall effect [2]. Chern number and edge-state calculations confirm that the 2D $[Mn(C_6H_5)_3]$ lattices have nontrivial topological Dirac-gap states, originating from the intrinsic SOC and strong magnetization provided by Mn atoms [2]. Furthermore, by using yet another different metal element, In, they designed a topological flat-band material, i.e. a fractional Chern insulator, in the 2D triphenyl-In lattice [3], which potentially spawns high-temperature fractional quantum Hall states. A nearly flat Chern band is shown to arise right around the Fermi level from the combined lattice geometry, SOC and ferromagnetism. Finally, they identify a recently experimentally made 2D organometallic Kagome lattice, consisting of π-conjugated nickel-Bisdithiolene with a chemical formula $Ni_3C_{12}S_{12}$ [5] that exhibits nontrivial topological states in both a Dirac band and a flat band [4].

It is envisioned that more organic topological materials will be discovered in the future, which will greatly broaden the scientific scope and technological impact of topological materials. These pioneering studies introduce organometallic frameworks as an ideal 2D platform for material's realization of the lattice Hamiltonian of strongly correlated topological states, with a high degree of tenability and versatility by implementing a wide variety of metal ions, organic ligands and lattice symmetries.

Feng Liu and Jian Wu
[1]Department of Materials Science and Engineering, University of Utah, USA
[2]Department of Physics, Tsinghua University, China
***Corresponding author.**
E-mail: fliu@eng.utah.edu

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