Topological States Protected by Magnetic Space Groups and Spin Space Groups

Zhida Song1+, Benjamin J. Wieder2,3,4, Luis Elcoro5, Zhen-Yu Xiao1, Jian-Zhou Zhao6, Yuanfeng Xu2, Barry Bradlyn7, B. Andrei Bernevig2

1 International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China
2 Department of Physics, Princeton University, Princeton, NJ, USA
3 Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA
4 Department of Physics, Northeastern University, Boston, MA, USA
5 Department of Condensed Matter Physics, University of the Basque Country UPV/EHU, Bilbao, Spain
6 Co-Innovation Center for New Energetic Materials, Southwest University of Science and Technology, Mianyang 621010, China.
7 Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign, Urbana, IL, USA

songzd@pku.edu.cn

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The group-theoretic characterization of crystalline solids has provided the foundational language for diverse problems in physics and chemistry. However, the group theory of crystals with commensurate magnetic order has remained incomplete for the past 70 years, due to the complicated symmetries of magnetic crystals. In this work, we (i) complete the representation theory of the magnetic space group by deriving the small corepresentations, momentum stars, compatibility relations, and magnetic elementary band corepresentations of the 1,421 magnetic space groups (MSGs). We also (ii) extend Topological Quantum Chemistry to the MSGs to form a complete, real-space theory of band topology in magnetic and nonmagnetic crystalline solids – Magnetic Topological Quantum Chemistry (MTQC). Using a combination of real space layer construction and the MTQC method, we derive the complete set of symmetry-based indicators of electronic band topology, for which we identify symmetry-respecting bulk and anomalous surface and hinge states. In the end, we (iii) fully classify the spin space groups (SSGs) (more than 50 thousands) that characterize magnetic materials with negligible spin-orbit coupling and discuss exotic topological states protected by SSGs.

[3] Zhen-Yu Xiao, Jian-Zhou Zhao, and Zhida Song, Full Classification of Spin Space Groups, to appear