北京大学物理学院凝聚态物理与材料物理所

凝聚态物理–北京大学论坛

2019年第 16期（No.466 since 2001）

Topological Quantum Chemistry and its applications in materials search

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简介：2014年在中国科学院物理研究所获博士学位。2014年-2018年在美国普林斯顿大学做博士后研究，合作导师为B. Andrei Bernevig教授。2018年通过中组部“青年千人”计划引进回国，现在为中科院物理所特聘研究员，博士生导师。主要研究方向是凝聚态物理与材料计算，关注材料中的新型拓扑电子态等。目前共发表SCI论文50余篇，共被引用7000余次，H 因子28。

报告摘要： Here we propose a complete electronic band theory, which builds on the conventional band theory of electrons, highlighting the link between the topology and local chemical bonding. For all 230 crystal symmetry groups, we classify the possible band structures that arise from local atomic orbitals, and show which are topologically non-trivial. Our electronic band theory sheds new light on known topological insulators, and can be used to predict many more. In addition, an open-source code -CheckTopologicalMat- is released at www.cryst.ehu.es/cryst/checktopologicalmat, which can be used to check the topology of any material by yourself. Finally, we perform a high-throughput search of ‘high-quality’ materials (for which the atomic positions and structure have been measured very accurately) in the Inorganic Crystal Structure Database in order to identify new topological phases. Among them, we present some topological materials to demonstrate the new topology in crystals.

时间：9月12日（星期四）15:00—16:40

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Photograph by Xiaodong Hu