

Topological Quantum chemistry and its applications in materials search

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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 - 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.