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Topological Quantum Chemistry

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The past decade has seen tremendous success in predicting and experimentally discovering distinct classes of topological insulators (TIs) and semimetals. We review the field and we propose an electronic band theory that highlights the link between topology and local chemical bonding, and combines this with the conventional band theory of electrons. Topological Quantum Chemistry is a description of the universal global properties of all possible band structures and materials, comprised of a graph theoretical description of momentum space and a dual group theoretical description in real space. We classify the possible band structures for all 230 crystal symmetry groups that arise from local atomic orbitals, and show which are topologically nontrivial. We show how our topological band theory sheds new light on known TIs, and demonstrate the power of our method to predict a plethora of new TIs.

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