Topological crystalline insulator: from symmetry indicators to material discovery

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Topological crystalline insulators (TCI) are insulating electronic phases of matter with nontrivial topology originating from crystalline symmetries. In the past decade, many materials have been demonstrated to be the topological insulators or the topological semimetals, however the exotic TCI states have remained elusive. Building upon recent theoretical works, we develop a feasible method to uniquely determine the novel rotational symmetry topological invariants based on first-principles calculations. In this talk, I will show how we predict new TCI materials and display their unusual electronic structures that entirely distinct from traditional topological materials.