Topological Quantum Chemistry

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In this talk a new field that classifies all topological crystalline phases of all known materials will be introduced: Topological Quantum Chemistry (TQC). It links the chemical and symmetry structure of a given material with its topological properties. This field tabulates the data of the 10398 real-space atomic limits of materials, and solves the compatibility relations of electronic bands in momentum space. A material that is not an atomic limit or whose bands do not satisfy the compatibility relations, is a topological insulator/semimetal. We use TQC to find the topological stoichiometric non-magnetic, materials in the Inorganic Crystal Structure Database at any filling. Topologically nontrivial materials were once thought to be the exception rather than the rule. In this talk I will show you that, by means of high-throughput computations, many more materials are topological than was initially thought. We have made our results publicly accessible through the https://topologicalquantumchemistry.com/

References

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Figures

Figure 1: Topological Materials Database: https://topologicalquantumchemistry.com/