Introducing Topological Quantum Chemistry and Topological Materials Data Base

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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, ``high-quality'' materials in the world. We develop several code which can compute all characters of all symmetries at all high-symmetry points in the Brillouin Zone (BZ). Using TQC we then develop codes to check which materials are topological. Out of 26938 stoichiometric materials in our filtered ICSD database, we find around 7300 topological materials. For the majority of the ``high-quality'' topological materials, we compute: the topological class, the symmetry(ies) that protects the topological class, the representations at high symmetry points and the direct gap (for insulators), and the topological index. For topological semimetals we then compute whether the system becomes a topological insulator (whose index/class we compute) upon breaking symmetries - useful for experiments. Our exhaustive results show that a large proportion of all materials in nature are topological. I will also explain an open-source code and end-user button on the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cgi-bin/cryst/programs/topological.pl) which checks the topology of any material and a new materials data base (https://www.topologicalquantumchemistry.com/).

References

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Figures

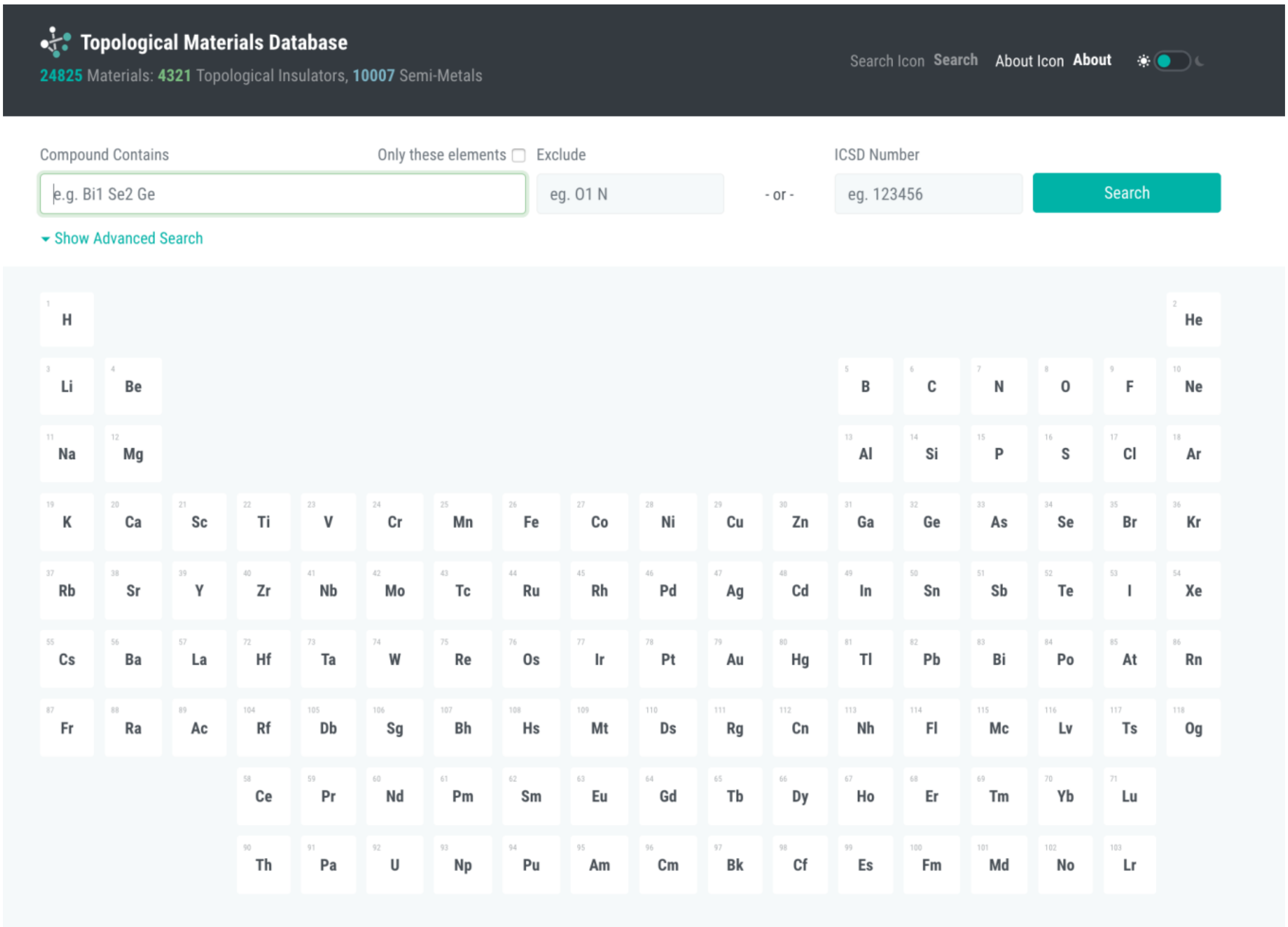

Figure 1. www.topologicalquantumchemistry.com, website for topological materials.