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Topology – in chemistry and materials science

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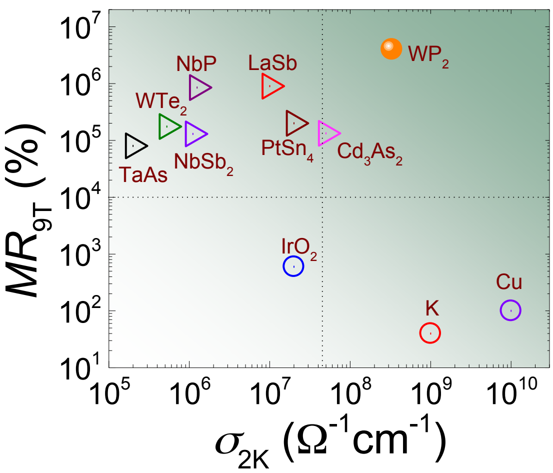
Topology a mathematical concept became recently a hot topic in condensed matter physics and materials science. However, the concept of topology plays also an important role in chemistry, examples are chiral molecules and Möbius annulenes.

The topology of the electronic structure determines the electronic, thermal and magnetic properties of solids. Classically, we know insulators, semimetals and metals, determined by their band gaps and electronic structure. However, all known materials can be reclassified through the lens of topology. Topological insulators, Weyl and Dirac Semimetals and topological metals are a new quantum state of matter, which have attracted interest of condensed matter science and materials science. Surprising new properties such as protected surface states in topological insulators, extremely low conductivities, giant charge career mobilties and magneto resistance effects were predicted and experimentally realized in many compounds. Tunable families of compounds such as Heusler compounds, binary phosphides and chalcogenides allows for a design of these new properties and their systematic study. One important criteria for the identification of the material is in the language of chemistry the *inert pair effect* of the s-electrons in heavy elements and the symmetry of the crystal structure. Many of the identifies materials are good thermoelectric materials and heterogenous catalysts. These observations raise the question whether the topology of the electronic structure can have impact on chemistry, too.

Binary phoshides are the ideal material class for a systematic study of Dirac and Weyl physics. Weyl points, a new class of topological phases was also predicted in NbP, NbAs. TaP, MoP and WP_2. [1-4]. Some of the Weyl semimetals were tested for catalysis [5], and have shown excellent performance. All this materials show exceptional properties such as high conductivity (higher than copper), high mobilties and a high magneto-resistance effect.



Graph of MR vs. conductivity of some well-known metals and semimetals plane at 2 K and 9 T for comparison. Semimetals are denoted by triangles, metals by hollow circles and WP_2 by a solid circle. Metals with high conductivity have smaller MR and semimetals with smaller conductivities have larger MR. WP_2 exhibits both very large conductivity as well as extremely high MR.

1. C. Shekhar, et al., Nature Physics 11 (2015) 645
2. Z. K. Liu, et al., Nature Mat. 15 (2016) 27
3. L. Yang, et al., Nature Physics 11 (2015) 728
4. C. Shekhar, et al. preprint arXiv:1703.03736
5. J Gooth et al., Nature accepted, arXiv:1703.03736
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7. B. Bradlyn, et al., Science 353 (2016) aaf5037