Organic Dirac materials, data-driven modeling and materials prediction -- application of the Organic Materials DataBase (OMDB)

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Abstract: In the recent years an ongoing effort in implementing data science into physics can be observed. Among others, this tendency is connected to the exponential growth of computational power and the resulting accessibility of a vast amount of scientific data. We implement the organic materials database which is freely accessible via omdb.diracmaterials.org [1]. During the talk, the database and it's basic functionality is introduced and future developments for novel materials prediction are discussed. As an example, the combination of data mining and model development is examined for the search of organic Dirac materials. The study of Dirac materials, i.e. materials where the low-energy fermionic excitations behave as massless Dirac particles has been of ongoing interest for more than two decades [2]. Such massless Dirac fermions are characterized by a linear dispersion relation with respect to the particle momentum. A combined study using group theory and data mining within the Organic Materials Database leads to the discovery of stable Dirac-point nodes [3] and Dirac line-nodes [4] within the electronic band structure in the class of 3-dimensional organic crystals. The origin of the crossings will be discussed and the mechanism of topological protection is introduced.

[1] S. S. Borysov, R. M. Geilhufe, A. V. Balatsky, PloS one, 12:2, e0171501, 2017.
[2] T. O. Wehling, A. M. Black-Schaffer, A. V. Balatsky, Adv. Phys., 42, 1-76, 2014.
[3] R. M. Geilhufe, S. S. Borysov, A. Bouhon, A. V. Balatsky, arXiv:1611.04316, 2016.
[4] R. M. Geilhufe, A. Bouhon, S. S. Borysov, A. V. Balatsky, Phys. Rev. B, 95, 041103(R), 2017.

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