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Einladung zum Vortrag

"In silico discovery of novel topological materials"

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Termin: **Mittwoch, 9. Oktober 2019, 13:30 Uhr,** **Lehrvortrag 10:00 Uhr**

Ort: **Victor-Franz-Hess-Hörsaal, Währinger Straße 17,**
1. Stock (Hoftrakt), Raum 112

Abstract:
In my talk, I will focus on our recent efforts directed towards the search of novel topological materials. A large number of diverse topological electronic phases that can be realized in materials have been predicted recently. We have developed a high-throughput computational screening methodology for identifying materials hosting various topological phases among known materials. The entire dataset of results obtained using this high-throughput search is now publicly available via the Materials Cloud platform [1]. Several predictions resulting from this search that have been successfully confirmed by experiments. A new Z_2 topological insulator was theoretically predicted and experimentally confirmed in the β-phase of quasi-one-dimensional bismuth iodide Bi_4I_4 [2]. The electronic structure of β-Bi_4I_4, characterized by Z_2 invariants (1;110), is in proximity of both the weak TI phase (0;001) and the trivial insulator phase (0;000). We further predicted robust type-II Weyl semimetal phase in transition metal diphosphides MoP_2 and WP_2 characterized by very large momentum-space separation between Weyl points of opposite chirality [3]. Recent experiments on WP_2 revealed record magnitudes of magnetoresistance combined with very high conductivity and residual resistivity ratio [4], and many other extraordinary properties. I will also give a broader prospective of the computational materials discovery research in my group that covers two-dimensional materials and heterostructures, skyrmion materials and spin systems.

[1] G. Autès, Q. S. Wu, N. Mounet, and O. V. Yazyev, "TopoMat: a database of high-throughput first-principles calculations of topological materials", https://www.materialscloud.org/discover/topomat
[2] G. Autès et al., Nature Mater. 15, 154 (2016).
[3] G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov and O. V. Yazyev, Phys. Rev. Lett. 117, 066402 (2016).
[4] N. Kumar et al., Nature Commun. 8, 1642 (2017).

Im Rahmen des Vortrages findet eine Lehrprobe zum Thema „The quantum harmonic oscillator" statt.