PHYSICS SEMINAR SERIES:

In silico discovery of novel topological materials

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Date:
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Time:
10:30AM – 11:50PM

Location:
GRAN 135

About The Speaker:

Prof. Oleg Yazyev was born in Simferopol, Crimean peninsula. He obtained his degree in chemistry from Moscow State University in 2003 and then joined Ecole Polytechnique Fédérale de Lausanne (EPFL) completing his Ph.D. thesis in 2007. He spent the next two years as a postdoctoral fellow at the Institute of Theoretical Physics (ITP) and the Institute for Numerical Research in the Physics of Materials (IRRMA) of the same institution. In 2009-2011 he was a postdoctoral fellow at the Department of Physics of the University of California, Berkeley, and the Lawrence Berkeley National Laboratory. In September 2011 he started an independent research group supported by the Swiss National Science Foundation professorship grant. In 2012 he was awarded an ERC Starting grant. His current research focuses on the theoretical and computational physics of two-dimensional and topological materials with a strong emphasis on their prospective technological applications.

Source: https://www.epfl.ch/labs/c3mp/index-html/yazyev/

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 Z2 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 Z2 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 discuss in detail the physical mechanism underlying magnetotransport in WP_2 as well as in other trivial and topological semimetals [5].

[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).

[5] S. N. Zhang, Q. S. Wu, Y. Liu and O. V. Yazyev, Phys. Rev. B **99**, 035142 (2019).

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