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 Bi₄I₄ [2]. The electronic structure of β-Bi₄I₄, 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 MoP₂ and WP₂ characterized by very large momentum-space separation between Weyl points of opposite chirality [3]. Recent experiments on WP₂ 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 WP₂ as well as in other trivial and topological semimetals [5].