

Theory Lunch Seminar

Computational discovery and design of novel materials

The field of topological phases of matter has seen spectacular growth during the past decade due to the discovery of novel materials realizing topologically non-trivial electronic structures. I will present our efforts towards discovering novel topological materials by means of high-throughput computational screening of the databases of known compounds. This search strategy allowed us to identify topological phases in a number of candidate materials, some of which has already received experimental confirmation. Two success stories will be covered - the discovery of quasi-1D topological insulator β -Bi₄I₄ and Weyl semimetals MoP₂ and WP₂. If time permits, I will also present some ideas of computational design of materials that were never synthesized previously.



Prof. Oleg Yazyev

Thursday April 19th 2018 at 12:30 pm

Auditoire II, room N°234, BSP (Cubotron), EPFL