Computational material design: from a simple chemical concept to 3D topological materials

A talk by Xing-Qiu Chen

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Within recent years, topological materials, including topological insulators, topological crystalline insulators, topological (Dirac) semimetals, topological Weyl semimetals and topological nodal line semimetals and even beyond, have attracted extensive interests in both condensed matter physics and materials sciences due to their potential applications and exotic properties. One of the current challenges is to see new topological materials with interesting properties. In this talk, we have proposed a simple chemical consideration to design three-dimensional topological materials according to the electronegativity concept in combination with first-principles calculations. Utilizing this method, I will represent four cases that were first proposed in our research group at the IMR. In addition, a special case where the Dirac cones or Weyl nodes forming a closed or continuous line in momentum space is also introduced, called as nodal line semimetals. I will introduce our prediction of realistic materials to realize them and some recent progress in revealing quasiparticle of massless new fermions are also discussed. Their corresponding experimental verifications will be emphasized.