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Topological Insulators, Semi-Metals and Superconductors From First Principles Electronic Structure Calculations

SERGEY SAVRASOV, University of California Davis

Using first-principles electronic structure calculations we investigate novel phases that emerge from the interplay of electron correlations, strong spin-orbit coupling and electron-phonon interactions. We first [1] focus on describing the topological semimetal, a three-dimensional phase of a magnetic solid, and argue that it may be realized in a class of pyrochlore iridates (such as Y2Ir2O7) based on calculations using the LDA + U method. This state is a three-dimensional analog of graphene with linearly dispersing excitations and provides a condensed-matter realization of Weyl fermions that obeys a two-component Dirac equation. It also exhibits remarkable topological properties manifested by surface states in the form of Fermi arcs, which are impossible to realize in purely two-dimensional band structures. We second [2] predict that osmium compounds such as CaOs2O4 and SrOs2O4 can be stabilized in the geometrically frustrated spinel crystal structure. They show ferromagnetic order in a reasonable range of the on-site Coulomb correlation U and exotic electronic properties, in particular, a large magnetoelectric coupling characteristic of axion electrodynamics. Finally, the issue of topological superconductivity and the possibility of the odd pairing will be discussed in Cu doped Bi2Te3 materials where electron-phonon coupling constant is calculated for various pairing symmetries using density functional linear response approach [3].

[1] Xiangang Wan, Ari Turner, Ashvin Vishwanath, Sergey Y. Savrasov, *Phys. Rev.* B **83**, 205101 (2011);
[2] Xiangang Wan, Ashvin Vishwanath, and Sergey Y. Savrasov, *Phys. Rev Lett.* **108**, 146601 (2012);
[3] Xiangang Wan, and Sergey Y. Savrasov, arXiv:1308.5615.