



Novel properties of 5d transition metal oxides

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Abstract

In 5d transition metal oxides such as the iridates and osmates, novel properties arise from the interplay of electron correlations and spin-orbit interactions. We investigate the electronic structure of the pyrochlore iridates, Spinel and Perovskite osmates using density functional theory, LDA+U method, and effective low energy models. We propose that pyrochlore iridates can be a Weyl semimetal, with vanishing density of states at the Fermi energy. It also exhibits topological properties - manifested by special surface states in the form of Fermi arcs, that connect the bulk Weyl points. We propose that hypothetical spinel osmates compounds such as CaOs_2O_4 and SrOs_2O_4 show some exotic electronic and magnetic properties in a reasonable range of on-site Coulomb correlation U such as ferromagnetism and orbital magnetoelectric effect characteristic to Axion electrodynamics. We also confirm NaOsO_3 is a Slater insulator.

About the Speaker

万贤纲, 男, 2000年毕业于南京大学物理系, 获博士学位。2003-2005年在日本国立材料研究所做博士后研究, 2005--2007在加州大学Davis分校访问。2009年起任南京的物理学系教授。主要研究方向是基于第一性原理的电子结构方法的发展, 程序化, 和在实际材料中的应用。