Abstract

Transition Metal Oxides (TMOs) show a wealth of intriguing properties which are governed by the interplay of charge, spin, and orbital degrees of freedom. Moreover, the comprehension of the features of strongly correlated TMOs with significant Spin Orbit Coupling (SOC) represents a challenging work and the interplay between large SOC and lattice geometry is undoubtedly a relevant ingredient in the exploration of such features. The most dramatic example of that occurs in iridates, where SOC deeply impacts the magnetic state, changing the character of the multiplet state within the t_{2g} manifold in the case of an octahedral arrangement of the ions. Corresponding effects in e_g manifold have rarely been considered, due to the conventional wisdom that e_g subshells ensure a perfectly quenched orbital momentum.
In the first part of the thesis, we study the influence of SOC on the magnetic state of a d^1 TM ion located in a tetrahedral environment, proving that its effect can be strongly enhanced in the case of distorted geometry. Under this condition, our theoretical research reveals that SOC can induce a substantial anisotropic unquenched orbital angular momentum and can affect the hierarchy of the lowest energy levels involved in the magnetic superexchange.
Since particular geometries can give rise to novel SOC effects, the structure

of the insulating compound $KOsO_4$, whose Os^{7+} ions are characterized by an e^1 configuration, seems to be particularly relevant for our study. $KOsO_4$ crystallizes in a scheelite-like structure, consisting in isolated and quite distorted tetrahedra; the isolated tetrahedra imply a reduction of the hopping connectivity and, as a consequence, the effects of the local energy scales are emphasized. Furthermore, the Os ions are covalently bonded to the oxygens in a tetrahedral configuration, which is distorted. The competition between strong electronic correlations, SOC and tetrahedral deformations has been analyzed through a study based on an exact diagonalization approach, which allows to completely characterize the local magnetic moment and the nature of the static spin/orbital correlations over finite clusters. Our study reveals that an entangled spin-orbital state emerges, marked by a strong anisotropy. Moreover, results show a link between the bond direction and the sign of the superexchange coupling per spin component, which reminds a Kitaev-like coupling.

The choice of a specific geometry may enhance the influence of SOC on the magnetic state of a system. However, there are also other strategies in order to emphasize the effects of the SOC; one of them is to lower the connectivity, thus enhancing the interplay between the local energy scales, which include SOC. In the second part of the thesis, we consider a trilayered structure composed by TM ions stacked in the z direction, where the hopping connectivity is highly damped. The tight-binding Hamiltonian model which describes the trilayer shows both time-reversal and inversion symmetries, which ensure the Kramer's degeneracy of its eigenstates, and a layer-interchange symmetry, related to the particular structure of the system. We analyze the evolution

and eventually the closing of the energy gaps of the trilayer, opening the possibility to find novel topological nodal semimetals, which are protected by the layer-interchange symmetry. We simulate different local environment by modifying the value of the parameters of the model, verifying that transitions between different topological configurations occur in the limit of weak and strong SOC regime.