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A possible family of Ni-based high temperature superconductors

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We suggest that a family of Ni-based compounds, which contain $[Ni_2M_2O]^{2-}$(M=chalcogen) layers with an antiperovskite structure constructed by mixed-anion Ni complexes, NiM_4O_2, can be potential high temperature superconductors upon doping or applying pressure. The layer structures have been formed in many other transitional metal compounds such as $La_2B_2Se_2O_3$(B=Mn, Fe,Co). For the Ni-based compounds, we predict that the parental compounds host collinear antiferromagnetic states similar to those in iron-based high temperature superconductors. The electronic physics near Fermi energy is controlled by two e_g d-orbitals with completely independent in-plane kinematics. We predict that the superconductivity in this family is characterized by strong competition between extended s-wave and d-wave pairing symmetries.

Keywords: Iron-based superconductors, Cuprates, Nickel chalcogenides, $s(d)$-wave pairing symmetry

INTRODUCTION

Since the discovery of cuprates [1], the Cu-based high temperature superconductors, more than thirty years ago, there have been intensive efforts to find Ni-based counterparts [2–5] as Ni is the nearest neighbor element to Cu among the 3d transition metal elements in the Period Table. However, although numerous discovered Ni-based compounds share similar physics in a variety of aspects to cuprates, none of the known Ni-based materials exhibits high T_c superconductivity.

Recently, we have suggested that there is a direct roadmap to design possible high T_c materials [6, 7]. In order to achieve unconventional high T_c, it is necessary to have an electronic structure in which those d-orbitals of transition metal atoms with the strongest in-plane coupling to the p-orbitals of anions are isolated near Fermi energy. In such an electronic structure, the superexchange antiferromagnetic interactions can be maximized to provide superconducting pairing. Both cuprates and the recently discovered iron-based superconductors [8] are shown to satisfy this condition. Specifically, in the perovskite-type of structure such as cuprates, the $d_{x^2-y^2}$ e_g orbital can only be isolated near the d^9 filling configuration of Cu^{2+}, and in iron-based superconductors, the d^6 configuration of Fe^{2+} is an unique configuration to isolate the t_{2g} orbitals near Fermi energy [6, 7]. More importantly, we have pointed out that such an electronic environment exists rarely in nature because of symmetry and chemistry constrains. Thus, the condition can be considered as the gene of unconventional high T_c superconductors to serve as a guide to search for or design high T_c materials. Following this understanding, we have predicted that there are two specific cases in which the condition can be satisfied with a d^7 filling configuration, namely, Co^{2+}-based compounds [6, 9, 10].

The d-orbital filling configuration of Ni^{+2} is d^8. In the d^8 configuration, it is difficult to design a structure to meet the above condition. The reasons are as follows. With an even filling configuration, similar to iron-based superconductors, it is necessary to isolate two near-degenerated orbitals at Fermi energy and both of them should strongly couple to in-plane p-orbitals. The isolation requires a large energy separation between the selected two orbitals and the rest. The octahedra complex is the only complex structure to achieve large energy separation in which the two e_g orbitals have much higher energy than the three t_{2g} orbitals. Unfortunately, in the conventional perovskite-type structure, the two e_g orbitals have completely different in-plane kinematics because the d_{z^2} orbital has little in-plane coupling to p-orbitals. These facts can explain why it is difficult for Ni-based materials to achieve high T_c superconductivity.

In this letter, we show that it is possible to make both e_g orbitals to strongly participate in-plane kinematics in a structure with mixed anion Ni-octahedra complexes, NiM_4O_2 as shown in Fig. 1a. The idea is to rotate the complex and connect them so that the apical oxygens can form a square lattice as shown in Fig. 1c. In this case, the layered sheets of $[B_2M_2O]^{2-}$ compose of face-sharing tilted Ni_2M_2O octahedra where the Ni atom is surrounded by two axial oxygen atoms and four M atoms. The two d_{z^2} and $d_{x^2-y^2}$ e_g orbitals before the rotation are labeled as $d_{x^2-y^2}$ and $d_{xz/yz}$ orbitals in the new axis coordination as shown in Fig. 1a. The new $d_{x^2-y^2}$ gains in-plane kinematics through oxygens and the new $d_{xz/yz}$