# Progress Report:

In recent years, my research works are mainly concentrated on investigating the interesting phenomena in transition metal oxides such as metal-insulator transition (Verwey transition), entropy change, and charge-orbital ordering in magnetite Fe3O4, orbital ordering and Jahn-Teller distortion in perovskite ruthenate SrRuO3, and carrier properties in electron doped perovskite La0.7Ce0.3MnO3. In addition, part of my research work is devoted to surface systems such as charge transfer and interface reconstruction of C60 monolayer on Cu(111) as well as the electronic structures of W(111) single atom tip. The results of the above mentioned systems are discussed below.

Magnetite Fe3O4:

Fe3O4 has attracted much attention in recent years because of the interesting half-metallic properties as well as the industrial applications. In a half-metal, one spin channel is conductive while the other is insulating. The unusual transport property of 100% spin polarization at the Fermi level makes these half-metallic materials fairly potential for future spintronics. On the other hand, there have been many works debating on the existence of charge ordering in magnetite. Recently we found robust theoretical evidence of charge ordering accompanied with an orbital ordered ground state, which might be a breakthrough into this issue. There have been intensive investigations on the metal-insulator Verwey transition and charge ordering of Fe3O4 in the past 60 years, however questions about the existence of charge ordering and the fundamental mechanism of the Verwey transition remain unresolved [1]. Recently we performed detailed theoretical investigations on the electronic structure of magnetite in the high-temperature (T) cubic and low-T monoclinic phases using one of the most advanced method: local density approximation plus Hubbard U (LDA+U) method, which takes into consideration the strong electron correlation in the localized d orbitals. We found for the low-T phase an insulating charge ordered ground state whose configuration and charge separation are in good agreement with that inferred from recent powder diffraction measurements. More importantly, we also found that in the low-T phase, conduction electrons form a t2g orbital ordered state by occupying spin-down dyz, dxz, and dxy orbitals on different B Fe^{2+} sublattices (Fig. 1). This finding resolves several fundamental issues about the Verwey transition such as the nature of the low-T electronic state, the importance of on-site U as the driving force of the charge-orbital ordering and M-I transition, the long puzzle of the disagreement between the theoretical and experimental entropy change at the Verwey transition, and also the question why the Anderson criterion for the charge ordering breaks down. The results have been published in Physical Review B [2] and Physical Review Letters [3,4]. As for the high-T phase, we found a large unquenched orbital magnetic moment in B-site Fe, indicating that even in high-T phase that the Fe-3d electrons are relatively itinerant, the electron correlation plays an important role in the orbital polarization. The obtained results in combination with the large unquenched orbital magnetic moment observed in synchrotron radiation research center (SRRC) by Prof. D. J. Huang are published in Physical Review Letters [5].

Fig. 1: Charge-orbital ordering in low-T Fe3O4.
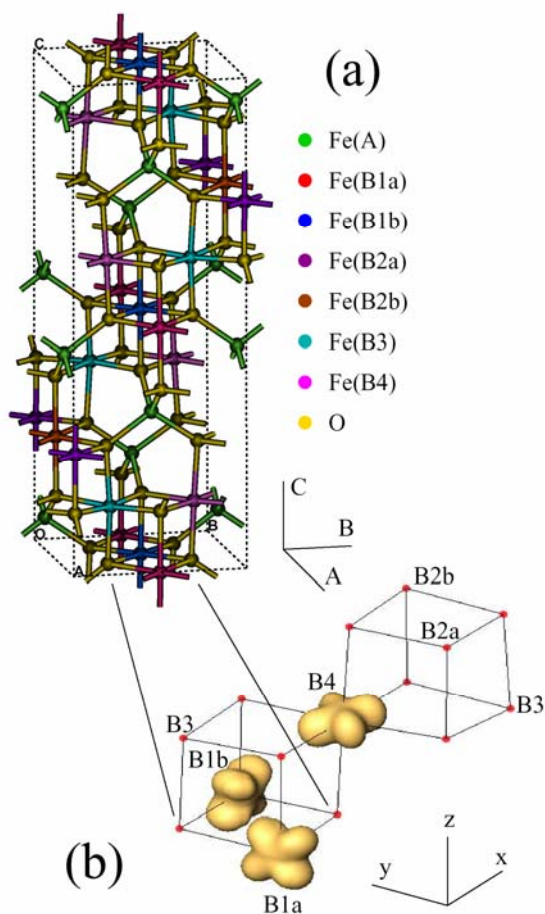
Perovskite Ruthenate SrRuO3:

Ruthenium-based oxides have attracted increasing attention in recent years because of the interesting electronic and magnetic properties and of the newly discovered unconventional superconductivity in layered ruthenate Sr2RuO4 at about 1 K [6]. It is generally believed that 4d electrons are relatively itinerant so that electron correlation is less important than that in 3d oxides [7]. Nevertheless, measurements on specific heat, infrared and optical reflectivity, and photoemission and x-ray absorption spectroscopy of SrRuO3 indicate the importance of electron correlation effects in Ru-4d orbitals, and suggest that the electron correlation should be taken into consideration [8]. Recently, we investigated electronic structures of SrRuO3 using LDA+U method to explore the importance of on-site U in relatively delocalized Ru-4d orbitals. Surprisingly we find not only a half-metallic ground state in consistent with the ionic model, but also an associated tilting 4d-t2g orbital ordering on the Ru sublattice closely related to the Jahn-Teller distortion (Fig. 2). Our finding resolves the nature of the orbital ordering, the close connection with the Jahn-Teller distortions, and the importance of the on-site correlation U in the relatively extended Ru-4d orbitals of SrRuO3. The results have been recently published in Physical Review Letters [9].

Fig. 2: Orbital ordering in SrRuO3.
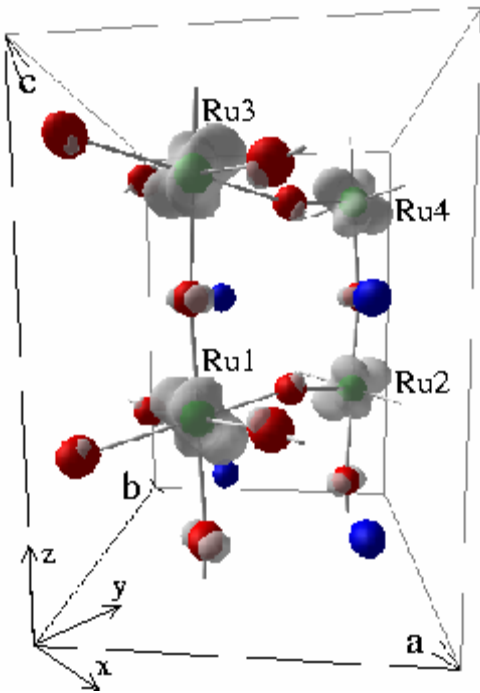
Electron Doped Perovskite La0.7Ce0.3MnO3:

Owing to the colossal magnetoresistance for the practical application potential in the so-called "spintronics" and the rich phase diagrams arising from competing order parameters, the hole-doped manganites, in the form of R1-xAxMnO3 (R, rare-earth ion; A, divalent cation), have been attracting a rapt attention over the last decade. On the other hand, it has been widely anticipated that electron-doped RMnO3 compounds obtainable by replacing the divalent dopants with tetravalent ones (e.g., cerium or tin) should also possess similar colossal magnetoresistance effects. As a result, many experimental and theoretical groups have devoted to realizing electron-doped RMnO3 compounds and on investigating the electronic structures of such systems [10]. Professor J. Y. Lin in National Chiao Tung University has done many measurements on the possible electron doped perovskite La0.7Ce0.3MnO3. However he found no evidence for electron doped feature in this system. Recently he has done Hall-effect measurement and confirm that the charge carriers in this system are actually holes rather than electrons. I also calculated the electronic structures of this system and obtained the same conclusion: in La0.7Ce0.3MnO3, Ce ions are not tetravalent so that the conduction Mn-eg band with hole character is not fully filled. This can be seen in Fig. 3 where the band structures of La0.7Ce0.3MnO3 is compared with those of a standard electron doped system La0.7Ca0.3MnO3. This new finding do not agree with the electron-doped property of La0.7Ce0.3MnO3 claimed in previous papers. The manuscript about this issue has been published in PRB [11].

Fig. 3: Band structures of La0.7Ca0.3MnO3 (upper panels) and La0.7Ce0.3MnO3 (lower panels).
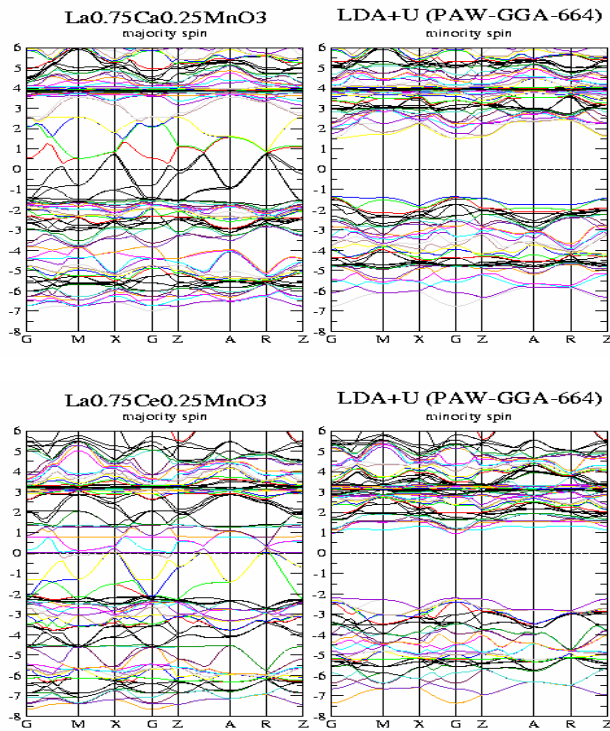
Reference:

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