

Chapter 1 Research Activities and Future Plans

Theory of Solid State Physics

Prof. **Sadamichi Maekawa** (1997.4~)

【Staff Members】

Prof. Sadamichi Maekawa, Assoc. Prof. Takami Tohyama, Res. Assoc. Tomio Koyama,
Res. Assoc. Saburo Takahashi, Res. Assoc. Wataru Koshibae (Researcher : 4 / Supporting Staff : 3)

【Research Activities】

In this group, the electronic states in transition metal oxides are theoretically studied. Transition metal oxides exhibit novel properties such as high temperature superconductivity and metal-insulator transition based on strong electron correlation and, thus, are important targets in condensed matter physics. They also attract attention as future electronic materials.

In 2004, the electronic states of Mott insulating states and doped ones in Cu-oxide (**Ref. 1, 2, 3**), Co-oxides (**Ref. 4**) and Mn-oxides (**Ref. 5**) were theoretically studied:

- (1) The nature of the spin-charge separation in one-dimensional correlated electrons was clarified, and was shown to be the key for the giant non-linear opto-electronic responses. The idea for the development of the non-linear opto-electronic materials was proposed.
- (2) The interaction among the internal degrees of freedom of electrons (spin, charge, orbital) in strongly correlated electrons, the competition of their orders, the elementary excitations and the observation methods were studied. In particular, the methods that may be used in the synchrotron radiation facilities were proposed.
- (3) Cobaltates with triangular lattice structure attract attentions as thermo-electric materials and novel superconductors. It was shown that in the cobaltates, the electronic lattice is different from that of the crystal and is the Kagome. This is because the orbital degeneracy causes the different symmetry to the electrons from the crystal.
- (4) The textbook entitled "Physics of Transition Metal Oxides" was prepared for several years and has finally been published from Springer (Germany) in June 2004 (**Ref. 1**).

1. Maekawa S., Tohyama T., Barnes S.E., Ishihara S., Koshibae W., Khaliullin G.
Physics of Transition Metal Oxides
Springer Series in Solid-State Sciences, Vol. 144 (2004), ISBN: 3-540-21293-0
2. Mori M., Tohyama T., Maekawa S., Riera J. A.
Friedel oscillations in a two-band Hubbard model for CuO chains.
Phys. Rev. B 69 (2004), 014513
3. Onodera H., Tohyama T., Maekawa S.
Temperature and dimensionality dependencies of optical absorption spectra in Mott

insulators.

Phys. Rev. B 69 (2004), 245117

4. Khaliullin G., Koshibae W., Maekawa S.

Low Energy Electronic States and Triplet Pairing in Layered Cobaltate.

Phys. Rev. Lett. 93 (2004), 176401

5. Ishii K., Inami T., Ohwada K., Kuzushita K., Mizuki, J., Murakami Y., Ishihara S., Endoh Y., Maekawa S., Hirota K., Moritomo Y.

Resonant inelastic x-ray scattering study of the hole-doped manganites $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($x = 0.2, 0.4$).

Phys. Rev. B 70 (2004), 224437

【Plan】

Most of transition metal oxides are the so-called strongly correlated electron systems, since the Coulomb interaction between electrons is strong. In the oxides, electrons stay in the ionic cores for long time and, thus, the internal degrees of freedom of electrons (spin, charge, orbital) behave almost independently. The degrees exhibit the ordered states that compete with each other. As a result, a variety of quantum phenomena occur. The same physics is applied to organic molecular materials and bio-materials as well. Because of the competition among the degrees, a small change of spin (magnetism) and/ or orbital (spatial behavior of electron cloud) causes a giant response of charge (electrical transport). The reverse response occurs as well. Since these quantum phenomena are due to the many-body effects of electrons, the band calculation based on the local density approximation and the mean-field approximation calculation do not always catch the fundamental physics of the phenomena.

On the other hand, numerical simulation based on the microscopic model works well to solve the physics. Our research group has been developing the numerical simulation methods for the strongly correlated electron systems. The methods are applied to a variety of novel quantum phenomena in the correlated electron systems. The group reveals the physics of the phenomena and proposes the idea of developing materials for the future electronics.