**Role of inter-site Coulomb interaction on charge and stripe order of $La_{2-x}Sr_xNiO_4$**

Susumu Yamamoto[1] and Takeo Fujiwara[1, 2]
[1]*Core Research for Evolutional Science and Technology, Japan Science and Technology Corporation (CREST-JST), Japan*
[2]*Center for Research and Development of Higher Education, University of Tokyo, Tokyo 113-8656, Japan*
yanagen@coral.t.u-tokyo.ac.jp

$La_{2-x}Sr_xNiO_4$ (LSNO) shows novel charge and spin stripe order whose period depends on the value of $x$ and is insulator throughout in the range of $0 \leq x < 0.9$ at low temperatures. [1] There are two candidates for the origin of the stripe order. One is Jahn-Teller mechanism and the other is long ranged Coulomb interaction.

Recently we have studied these systems with $x$=0, 1/3, 1/2, 1 by using LSDA+U method. [2] The results of mother material LSNO ($x$=0) and low-doped LSNO ($x$=1/3) show good agreement with observed width of energy gap and localized spin moment. LSNO of $x$=0 is antiferromagnetic insulator where each Ni ion is $Ni^{2+}$. In the LSNO ($x$=1/3), hole is localized on the $x^2$-$y^2$ orbital of $Ni^{3+}$ site. In the result of LSNO ($x$=1) by using LSDA+U method, hole is doped into $3z^2$-1 orbitals of Ni ions due to the strong on-site Coulomb interaction in contrast to hole in LSNO ($x$=1/3). In real LSNO ($x$>1/2), hole is doped into $3z^2$-1 orbital. The LSDA+U result, however, becomes an unrealistic antiferromagnetic metal. A real ground state should be paramagnetic metal and its wavefunction a linear combination of Slater determinants with different spin configurations. In the result of LSNO ($x$=1/2) by using LSDA+U, hole is not localized on specific site. Consequently, the system is metal. The real LSNO ($x$=1/2) shows charge and spin stripe order and is insulator. It is more puzzling than the case of LSNO ($x$=1), because the wavefunction of band insulator is well described with a single Slater determinant.

In the LSNO, two $e_g$ orbitals of Ni ion are relevant. We constructed double orbital extended Hubbard model Hamiltonian for $x$=1/2 system based on the LDA calculation and solved its exact ground state. On-site Coulomb and exchange interaction parameters $U$ and $J$ are imported from LSDA+U calculation. The ground state changes depending on the value of inter-site Coulomb interaction $V$. The ground state with $0<V<0.41$ does not show charge order while $0.41<V<1$ does. We chose the value $V$=0.5eV, which is consistent with that of 0.34eV in RPA calculation of $LaMnO_3$. [3] Charge and spin order are discussed by using charge-charge and spin-spin correlation function respectively. And the transport property is discussed by using single particle spectral function.

Analytic continuation of the ground state wavefunction at $V$=0.5eV to $V$=0eV causes degenerated single electron state at Fermi level. Thus the inter-site Coulomb interaction stabilizes charge order and causes energy gap opening at Fermi energy. Spin order in real LSNO ($x$=1/2) is understood by introducing anisotropy of second nearest neighbor hopping integrals, which is different from usual Jahn-Teller mechanism, into the model Hamiltonian. The LSDA+U result does not shows charge order, since it does not include the correlation effect induced by $V$, such as self-interaction of $Ni^{2+}$ $x^2$-$y^2$ orbital with its tail on $Ni^{3+}$ site.

[1] H. Yoshizawa, T. Kakeshita, R. Kajimoto, T. Tanabe, T. Katsufuji, and Y. Tokura, Phys. Rev. **B61**, R854 (2000).
[2] S. Yamamoto and T. Fujiwara, arXiv:0704.3323v1 [cond-mat.str-el].
[3] Y. Nohara, A. Yamasaki, S. Kobayashi, and T. Fujiwara, Phys. Rev. **B74**, 064417 (2006).