Lattice, Charge, Spin, and Orbital Ordering of Insulating $La_{0.5}Ca_{0.5}MnO_3$

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Doped manganites are known to show very rich behavior due to complex interplay and competition of lattice, orbital, charge, and spin degree of freedom. Specifically, at half-doping the system shows insulating phase with zig-zag orbital ordering and CE-type magnetic ordering, with stripe-like charge ordering. The underlying mechanism of the formation of this structure still remain unresolved. Additionally, recent experiment indicates that charge disproportion seems to be extremely small between the 3+ and 4+ manganese.

In this work, insulating phases of $La_{1-x}Ca_xMnO_3$ at x=0, 0.5, and 1 are studied and compared, employing density functional theory within LDA+U approximation, and recently developed energy-resolved symmetry-respecting construction of Wannier functions. The resulting electronic structure agrees very well with resonant inelastic soft X-ray scattering, and shows the observed lattice, orbital, spin and charge ordering[1,2]. Interestingly, the charge disproportion against doping is found to depend very weakly on the amount of doping; even in fully doped $CaMnO_3$, about half of the hoped holes do not reside in the manganese sites. This unexpected behavior can be understood as consequence of the large p-d hybridization. The major portion of the doped holes actually reside in the oxygen sites that surround the Mn^{4+} sites, forming Wannier states of the same symmetry as the expected Mn^{4+} e_g-states. This resolves the current dilemma and suggests that a charge-transfer insulator may be a more appropriate description of the doped manganites.

This work demonstrates the usefulness of LDA+U approximation and and the derived Wannier functions in the study of strongly correlated systems.

[1] S. Grenier, *et al.* Phys. Rev. B **69**, 134419 (2004).

[2] K.J. Thomas, *et al.* Phys. Rev. Lett. **92**, 237204-1 (2004).