第１４回トポロジカル物質科学セミナー
Topological Materials Science Seminar (14)

Orbital doping in hybrid transition metal oxides

Dr. Mario Cuoco
CNR-SPIN, Salerno and Dipartimento di Fisica,
Università di Salerno, Fisciano 84084, Italy

Place: Room 525, Department of Physics, Kyoto University
Date: Aug. 4 (Thu), 2016
Time: 10:30-12:00

Abstract: Transition metal (TM) oxides are fascinating materials characterized by a subtle interplay between charge, spin, and orbital degrees of freedom, which in many cases gives rise to complex types of collective behavior. In this framework, we present how magnetic and orbital patterns in a uniform 4d host are modified by the inclusion of 3d impurities substituting the 4d ions for both insulating and metallic hosts. In particular, for the case of an insulating host, we investigate the changes in spin and orbital patterns induced by magnetic transition-metal ions without an orbital degree of freedom doped in a strongly correlated insulator with spin-orbital order. In this context, we study the 3d ion substitution in 4d transition-metal oxides in the case of $3d^3$ doping at either $3d^2$ or $4d^4$ sites, which realizes orbital dilution in a Mott insulator. Although we concentrate on this doping case as it is known experimentally and more challenging than other oxides due to finite spin-orbit coupling, the conclusions are more general. We derive the effective 3d−4d (or 3d−3d) superexchange in a Mott insulator with different ionic valencies, underlining the emerging structure of the spin-orbital coupling between the impurity and the host sites, and demonstrate that it is qualitatively different from that encountered in the host itself. The impurity either acts as a spin defect accompanied by an orbital vacancy in the spin-orbital structure when the host-impurity coupling is weak or favors doubly occupied active orbitals (orbital polarons) along the 3d−4d bond leading to antiferromagnetic or ferromagnetic spin coupling. [1]

For the case of a metallic host, we show that doping a t_{2g} system can lead to emergent orbitally directional double-exchange effects. We find that, due to the orbital directionality, the competition between antiferromagnetic (AF) and ferromagnetic (FM) correlations in layered systems makes antiferromagnetically coupled FM zigzag stripes and checkerboard clusters the dominant patterns in the phase diagram over a large range of doping. We demonstrate how the breaking of the orbital directionality as well as the inclusion of the Coulomb interaction can significantly affect the zigzag-checkerboard competition and lead to orbital or charge ordering in the ground state. [2]

Finally, I will discuss possible topological phases occurring for the case of doped t_{2g} system.

[Acknowledgements –EU- MSCA-IF project "UFOX"]

1. W. Brzezicki, A. M. Oleś, and M. Cuoco, Phys. Rev. X **5**, 011037 (2015).
2. W. Brzezicki, C. Noce, A. Romano, and M. Cuoco, Phys. Rev. Lett. **114**, 247002 (2015).

Host: Y Maeno [Kyoto Univ. Core Research Group A01]
(075-753-3783 / maeno@scphys.kyoto-u.ac.jp)