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Orbital selectivity and isostructural phase transitions in $AMnO_3$ – perovskites

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Venue: ”Alexandru Ioan Cuza” University, Corp H, Room H1;
Date: Friday, 8th December 2017, 14.00-15.30 pm

ABSTRACT

Oxides with perovskite structure-type containing Mn ions are well known for interesting physical phenomena, such as colossal magnetoresistance, insulator-metal transition, ferroelectricity coexisting with long range magnetic order, orbital and charge ordering, etc. DFT+DMFT methods are applied to LaMnO3 and BiMnO3, which are the most studied materials in the AMnO3 class. Unusual electronic states with orbital selectivity are found, such as Site- and Orbital- Selective Mott state, Orbital- Selective Mott state and Mott-Band state. Some of these novel states are an alter- native explanation to the previously proposed orbital disordered states, which are relevant to the phenomenology of colossal magnetoresistance phenomena. In this talk I will describe the electronic properties of these states and I will argue that these novel states are a consequence of the interplay between the orbital and electronic degrees of freedom of the manganese correlated d-electrons, the sp-electrons of the A ions and the lattice. I will show that our results are in agreement with temperature dependent resonant x-ray scattering measurements, which up to present could not be explained by other theoretical models. Using DFT+DMFT, I will propose an alternative description to the accepted Jahn-Teller phase transition mechanism in these materials. In addition, I will show that the properties of these novel orbital selective electronic states can be predicted by DFT+DMFT. This is possible due to the recent theoretical developments of forces for structural relaxations in correlated materials within the DFT+DMFT, which allows one to quantitatively study the couplings between structural and electronic degree of freedom in correlated materials.

Everybody is Welcome!