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The transition metal oxides are emerging as the natural playground where the intriguing effects induced by electron correlations can be addressed. Since the s electron of the transition metals are transferred to the oxygen ions, the remaining electrons near the Fermi level have strongly correlated d character and are responsible for the physical properties of the transition metal oxides. These electron correlations, together with dimensionality and relativistic effect, play a crucial role in the formation and the competition of different electronic, magnetic and structural phases, giving rise to a rich phase diagram: Mott insulators, charge, spin and orbital orderings, metal-insulator transitions, multiferroics and superconductivity. The investigation of correlated electron physics usually refers to 3d transition metal oxides, mainly because of high-temperature superconductivity in the cuprates and in the iron-pnictides, and colossal magneto-resistance in manganites, but also because the highly extended 4d-shells would a priori suggest a weaker ratio between the intra-atomic Coulomb interaction and the electron bandwidth. Nevertheless, the extension of the 4d-shells also points towards a strong coupling between the 4d-orbitals and the neighbouring oxygen orbitals, implying that these transition metal oxides have the tendency to form distorted structure with respect to the ideal one. As a consequence, the change in the Metal-Oxygen-Metal bond angle often leads to a narrowing of the d-bandwidth, bringing the system on the verge of a metal-insulator transition or into an insulating state. Hence, 4d materials share common features with 3d systems having additionally a significant sensitivity of the electronic states to the lattice structure, effective dimensionality and, most importantly, to relativistic effects due to stronger spin-orbit coupling.

The main purpose of this thesis is a study of the mechanisms and the fundamental interactions that control the formation and the competition of different magnetic and structural phase driven by the electronic correlations, dimensionality and relativistic effects in Ru-, Cr- and Mn- based perovskite systems, also considering what happens in hybrid or eutectic structures.

The mean field theory of itinerant uniform ferro/ metamagnetism and its consequences are introduced. We present two analytically solvable models: the M^6 Landau theory and the full analytical solution of one-dimensional tight binding density of state. We compute the analytical thermodynamic functional, the phase diagram, the quantum critical endpoint and the critical magnetic field. Necessary and sufficient conditions to have itinerant metamagnetism are examined. We analyse the interface Sr_2RuO_4-$Sr_3Ru_2O_7$. We study the modification of the electronic structure induced by nanometric inclusions of Sr_2RuO_4 embedded as *c*-axis stacking fault in $Sr_3Ru_2O_7$ and viceversa. The change of the density of states near the Fermi level is investigated as a function of the electron density, the strength of the charge transfer at the interfaces between the inclusion and the host, and of the distance from the inclusion. Then, we examine how the tendency towards long range orders is affected by the presence of the nanometric inclusions. This is done by looking at the basic criteria for broken symmetry states such as superconductivity, ferromagnetism and metamagnetism. We show that, according to the strength of the charge transfer coupling, the ordered phases may be enhanced or hindered, as a consequence of the interplay between the host and the inclusion, and we clarify the role played by the orbital degree of freedom showing an orbital selective behaviour within the t_{2g} bands. A discussion on the connections between the theoretical outcome and the experimental observations is also presented. We study the effect of electronic correlation at interface Sr_2RuO_4-$Sr_3Ru_2O_7$. We study in detail the role of the electronic correlation in systems based on nanometric inclusions of Sr_2RuO_4 embedded as *c*-axis stacking fault in $Sr_3Ru_2O_7$ and viceversa. The metamagnetic properties in mean field theory approach using the realistic density of state are analyzed. We study the analysis of the electronic reconstruction at the interface Sr_2RuO_4-$Sr_3Ru_2O_7$. We study the fermiology of Sr_2RuO_4 and $Sr_3Ru_2O_7$ from first principles: comparison, main features and calculation of effective hopping Ru-Ru are performed. Effect of the octahedral rotation and dimensionality are analyzed studying ab-initio the interface Sr_2RuO_4-$Sr_3Ru_2O_7$. We show that the rotations strongly reduce the main hopping parameter of the d_{xy} band, making near the Van Hove singularity to the Fermi level. We study the tetragonal-monoclinic transition in the compound $KCrF_3$. We present the electronic structure and the volume relaxation study for the $KCrF_3$ in the two different crystalline phases. Following the usual definition of the e_g orbital $\mid \theta >= \cos\frac{\theta}{2}|3z^2-1\rangle + \sin\frac{\theta}{2}|x^2-y^2\rangle$, the calculation of the orbital gives $\theta = 110.5^\circ$ for the tetragonal structure, that is similar to $LaMnO_3$. For the monoclinic phase, we find $\theta = 120.9^\circ$ and 102.2° for the two types of octahedron. We discuss similarities with $KCuF_3$ and $LaMnO_3$ in the orbital order. We deepen the study of $KCrF_3$ studying the low-energy physics and the non-collinear properties of its antiferromagnetic ground state. We present and compare the hopping parameters for the cubic, tetragonal and monoclinic structures of $KCrF_3$ using the e_g basis and the Maximally localised Wannier functions. Moreover, we analyse the strength of electronic

correlation using the Cococcioni method based on linear response approach. Although, the atomic number of chromium is relatively small, it is observed experimentally that the spin-orbit effect can play a non trivial role at low temperature. We go beyond the spin collinear approximation, the spin-orbit coupling and the weak ferromagnetism are also examined. Finally, we study from first principles the magnetic, electronic, orbital and structural properties of the $LaMnO_3$ doped with gallium atoms. The gallium atoms reduce the Jahn-Teller effect, and accordingly reduce the charge gap. Surprisingly, the system does not go towards a metallic phase. The doping tends to reduce the orbital order by weakening the antiferromagnetic phase and by favoring an unusual insulating ferromagnetic phase due to the effect of the correlated disorder. It is also presented a general discussion on the results obtained and some comments on prospective and open questions.

Gli ossidi di metalli di transizione sono un laboratorio naturale dove gli effetti indotti dalle correlazioni elettroniche possono essere osservati. Siccome gli elettroni s dei metalli di transizione sono trasferiti sugli ioni ossigeno, i restanti elettroni vicino al livello di Fermi hanno un carattere d fortemente correlato e sono responsabili delle proprietà fisiche dei metalli di transizione. Queste correlazioni elettroniche, insieme con la dimensionalità ed effetti relativistici, giocano un ruolo cruciale nella formazione e competizione delle differenti fasi elettroniche, magnetiche e strutturali dando origine ad un ricco diagramma di fase: isolanti di Mott, ordini di carica, spin ed orbitale, transizioni metallo-isolante, multiferroici e superconduttività. L'investigazione della fisica degli elettroni correlati solitamanete si riferisce ai ossidi di metalli 3d, principalemte a causa della superconduttività ad alta temperatura nei composti a base di rame e ferro-pnictidi, e della magneto-resistenza colossale nelle manganiti, ma anche perchè gli estesi elettroni 4d potrebbero a priori suggerire un rapporto tra la repulsione di Coulomb e le ampiezze di bande più debole. Tuttavia, l'estensione degli orbitali 4d anche porta un forte accoppiamente tra gli elettreoni 4d e gli orbitali degli ossigeni vicini, implicando che questi ossidi hanno una tendenza a formare strutture distorte. Come conseguenza, il cambio negli angoli del legame Metallo-Ossigeno-Metallo spesso porta ad un assottigliamento della ampiezza di band d, portando il sistema vicino alla transizione metallo-isolante. Quindi i materiali 4d condividono dei fattori comuni con i sistemi 3d presentando addizionali e significanti dipendenze degli stati elettronici dalla struttura reticolare, dimensionalità effettiva e, ancor più importante, da effetti relativistici dovuti al forte accoppiamento spin-orbitale

Il principale scopo di questa tesi è lo studio dei meccanismi e delle interazioni fondamentali che controllano la formazione e la competizione delle differenti fasi magnetiche e strutturali guidate dalla correlazione elettroniche, dimensionalità ed effetti relativistici in sistemi peroskitici basati su rutenio, cromo e manganese, anche considerando cosa accade nelle eterostrutture.