

Spin-orbital excitations in correlated materials: a theoretical spectroscopy approach

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Collaborations: TEMPO and GALAXIES beamlines at SOLEIL

Strongly correlated materials display remarkable properties, such as metal-insulator transitions or superconductivity with high critical temperatures, that make them very attractive for new technological applications. On the fundamental level, understanding the electronic properties of these materials is still today a great challenge for both theory and experiments.

Concerning theory, very promising methods are based on Green's functions within ab initio many-body perturbation theory. Green's-functions methods allow an analysis in direct contact with experiments, giving the possibility to work in direct collaboration with experimentalists. The goal of this thesis is to address the role played by the spin and orbital degrees of freedom in the determination of the electronic and optical properties of strongly correlated materials. Prototypical compounds will be studied using Green's-functions methods and the calculated spectra will be compared with measurements that will be done by our experimental colleagues. A tight collaboration with experimentalists from the synchrotron Soleil and other theoreticians from the European Theoretical Spectroscopy Facility (see <http://www.etsf.eu>) is an important aspect of the thesis work.