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Fingerprints of electron correlation in materials: understanding and predictions from electronic structure theory

Electronic excitations determine the characteristics of materials all over science and technology, from photochemistry to radiation defects, from synchrotron experiments to cancer research. Theory and numerical modelling are valuable tools for the understanding and prediction of many of the important phenomena. During the last decades the field has evolved rapidly, but there are still many challenges. For example, some structures in the excitation spectra of interacting electrons, called quasiparticle peaks, can be directly related to excitations of independent electrons. Others, instead, such as satellites in the photoemission spectra of solids, cannot be understood in such a simple way. They are pure consequences of interaction and correlation, and they cannot be interpreted in a pure bandstructure picture. First principles calculations are in general very efficient in describing bandstructure, especially methods based on many-body perturbation theory such as the so-called GW approximation [1]. However, they often have difficulties to describe quantitatively, or even qualitatively, everything that goes beyond.
In this talk we will see what state-of-the art first principles calculations can today contribute to our understanding, focussing on the main ideas of the underlying theories, their conceptual and technical limitations, and useful comparisons with, and interpretation of, experiment.
We will show ways to go beyond currently used approximations, and we will discuss fingerprints of correlation in photoemission, inelastic x-ray scattering and optical spectra, making close connections between theory and experiment. Systems used for illustration will include models, simple metals and semiconductors, carbon nanostructures and transition metal oxides [2].

The results have been obtained in collaboration with many colleagues in the Theoretical Spectroscopy Group of the Laboratoire des Solides Irradiés and in the European Theoretical Spectroscopy Facility.

[1] L. Hedin, Phys. Rev. 139, A796 (1965).
[2] see e.g. M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011) and Phys. Rev.B 89, 085425 (2014); M. Gatti, G. Panaccione, and L. Reining, Phys. Rev. Lett. 114, 116402 (2015); J. Zhou et al., J. Chem. Phys. 143, 184109 (2015); P. Cudazzo et al., Phys. Rev. Lett. 116, 066803 (2016).