

A unifying approach for calculating excited and ground state properties of correlated systems for the simulation of x-ray spectroscopies.

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Abstract

A scheme is provided to describe local correlation effects of atomic (molecular) multiplet character both in the ground state and the excited state of a system presenting electron correlation features (e.g. transition metal oxides).

The theoretical framework is based on multiple scattering theory, generalized to incorporate configuration interaction effects into the independent particle description. The ensuing picture is one in which either the excited photo-electron in a photoemission experiment or the test electron in the description of ground state properties propagates from site to site by a succession of scattering events with or without change in kinetic energy. This theory is termed Multi-channel Multiple Scattering Theory. The similarity with the process of electron-molecule scattering is underlined, clarifying the concept of channel and providing a clue to the type of optical potential to be used, in which exchange effects are particularly important. This potential will be used to construct an energy functional for the description of ground state properties in the framework of a generalized Kohn-Sham approach, where electron correlation effects can be taken into account, overcoming in this way the limitations of current Density Functional Theory calculations [1]. A comparison with an alternative method to calculate correlation effects, the so-called Dynamical Mean Field theory, will be outlined.

[1] C.R. Natoli et al, Multiple scattering theory for non-local and multichannel potentials, J. Phys.: Condens. Matter **24** (2012) 365501.