Ab-Initio Theory of Resonant X-Ray Scattering

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We present a first principles formalism for resonant scattering of circularly polarised x-rays from solids using a minimal amount of mathematics. The theory is split into two parts. Firstly, a good description of the electronic structure of the underlying material is necessary. In our theory this is provided by self-interaction corrected density functional theory and implemented using the fully relativistic LMTO method. Secondly, the theory of the spectroscopy is implemented using standard time dependent perturbation theory to second order in the electron-photon interaction vertex. Using this method *f*-electrons can be described as either localized or delocalized allowing us to study the effect of electron localization and valency of rare earths and their ordered compounds in the x-ray diffraction spectra. Furthermore, being fully relativistic spin-orbit coupling, spin-polarisation and crystal field effects are all treated on an equal footing. Furthermore, in the examples we have looked at all three of Hund's rules are satisfied in the ground state of the material.

The theory will be illustrated with applications to several example materials. These examples will be used to demonstrate the properties of materials that can be deduced from the resonant x-ray spectra. Finally direct comparison with some recent experimental results will be made.