

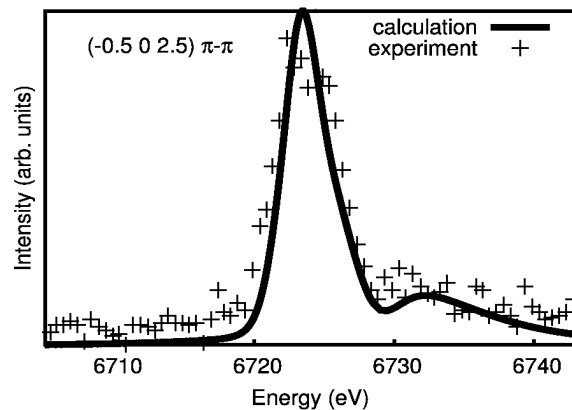
X-ray Absorption Spectroscopies Beyond the Mono-electronic Approach

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The simulation of X-ray absorption (XANES) and resonant X-ray diffraction (RXD) phenomena is often mandatory to interpret the experimental data. The FDMNES package^{1,2} is an *ab initio*, self-consistent, real space code that calculates the XANES and RXD spectra and yields a user-friendly output. When mono-electronic, according to the golden rule, the spectra is some projection of the local density of states calculated in the presence of the core hole. This approach is suitable when the electronic states probed by the photoelectron are delocalized. If this is not the case, and when the effect of the core hole is strong, some new theory, at the same time multi-electronic and multi-atomic, is needed.

Within this context, we are presenting new developments in FDMNES, in the form of a multi-electronic, multi-atomic alternative to the standard calculations. All by sticking to our tensorial formalism, we implemented a time dependent density functional theory (TDDFT) method, in the limits of the linear response and by considering the spin-orbit coupling in a fully relativistic way. Correlation, local fields and interaction with the core hole are described within the exchange - correlation kernel, which plays a key role in the TDDFT. We analyse the contribution of all the above effects to the calculated signal on specific RXD signals. We present our TDDFT results for the branching ratio for the $L_{2,3}$ edges of the transition elements.



Theory and experiment for the $(-0.5\ 0\ 2.5)\ \pi - \pi$ reflection at the Nd L_2 edge in NdMg. Calculations prove the orbital ordering expected in the low temperature phase of NdMg.

We equally discuss the RXD $L_{2,3}$ edges experimental compared to theoretical results proving a double electric and magnetic ordering (antiferroquadrupolar and antiferromagnetic) in the NdMg compound. We argue the importance of considering the spin-orbit coupling into our calculations. We discuss the suitability of the approximations on the form of the potential – the muffin tin approximation versus the full potential method.

References

¹Y. Joly, D. Cabaret, H. Renevier, and C.R. Natoli: *Electron population analysis by full-potential x-ray absorption simulations* in Phys. Rev. Lett. **82**, 2398 (1999)

²O. Bunău and Y. Joly: *Self-consistent aspects of X-ray absorption calculations* in Journal of Physics: Condensed Matter **21**, 345501 (2009)

³ O. Bunău, R.M. Galéra, M. Amara, Y. Joly, S. Luca and C. Detlefs: *Resonant magnetic and multipolar scattering in the antiferroquadrupolar phase of NdMg: a study at the Nd $L_{2,3}$ edges* submitted to Phys. Rev. B

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