

Low-Loss EELS: Simulations and Applications

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The low-loss region of the EEL spectrum ($< \sim 50$ eV) provides information about composition, electronic structure and optical properties. Despite this wealth of information it has not found as wide application in the study of materials as the ionization edges and, in particular, the energy-loss near-edge structures (ELNES) have. In the low-loss region, interband transitions and plasmon losses are observed. The unoccupied density of states (DOS) and the occupied DOS are both important and influence the spectrum. There is also some interaction between collective and single-electron excitations. This region is often therefore more complex and difficult to interpret than the ELNES.

Recent years have seen significant improvements in the *ab initio* calculations used to simulate energy loss near edge structure (ELNES) and these are now widely used. In many cases the agreement between experimental and calculated ELNES with these methods is very good. The success of these calculations of ELNES, leads us to question whether *ab initio* calculations can also provide accurate simulations of low-loss EELS. Given the difficulties of directly relating electronic structure to features in the low-loss EELS, there is an even greater need for calculations as an aid to interpretation than there is for ELNES.

Recently, it has been shown that *ab initio* calculations can predict and explain the low-loss EELS spectrum very well for many materials [1-3]. Ground-state density function theory (DFT) and the random phase approximation (RPA), also called the independent quasiparticle approximation, have been used. At the same time the improvements in spectrometer design and the introduction of monochromators mean that the experimental information in the low loss region is more readily available and reliable. In addition, the move towards spectrum imaging modes, where signal levels are low, may also prompt more studies using low-loss EELS.

This paper will discuss and present examples of applications of DFT-RPA calculations to low-loss EELS. Examples will be given where it may be necessary to go beyond DFT-LDA to using more sophisticated approaches such as time-dependent DFT, GW calculations and the Bethe-Salpeter approach. Some examples of recent experimental interest (Ni-sulfides, GaN based materials, Ti-Ca oxides) will be presented and the relative usefulness of the low-loss and core-loss signals in these examples will be discussed.

References

- [1] P. Moreau and M. C. Cheynet, *Ultramicroscopy*, 94 (2003) 293
- [2] M. Launay, F. Boucher and P. Moreau, *Phys. Rev. B*, 69 (2004) 035101
- [3] V. J. Keast, *J. Electron Spectrosc. Rel. Phen.* (2005) in press.