Theory of Ca - $L_{2,3}$ edge – XAS using novel multichannel multiple scattering method

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A new computational method for X-ray absorption spectroscopy (XAS) is presented that allows taking account of atomic multiplet-like electron correlation effects in condensed systems, on the basis of *ab initio* electron structure calculations. It is built on the multi-channel extension of multiple scattering theory by Natoli *et al*. [1] and the eigen-channel R-matrix method [2]. Here, we present an application of the new method to the Ca $L_{2,3}$ near-edge XAS. At this absorption edge, the experimentally observed lineshape, in particular the branching ratio, deviates strongly (and systematically) from that obtained from the standard, one-electron approach to XAS. The failure of one-electron theory can be attributed to a strong interference between the L_2 and L_3 absorption channels, due to the Coulomb and exchange interaction between the photo-electron and the 2p core-hole. The pure multiplet-like part of this interaction (described by Slater-integrals F^k, G^k, $k>0$) can be taken into account in the new method without introducing any adjustable parameters. This interaction changes the branching ratio to roughly 1:1 in good agreement with experiment. The remaining differences in peak positions and details of the lineshape can be corrected for by taking into account the screened monopole part of the Coulomb interaction (related to F^0).

References:

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