Full Potential Multiple Scattering theory for X-ray Absorption Spectroscopy with Electronic Structure codes

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X-ray Absorption Near Edge Spectra (XANES) is a powerful tool to investigate electronic and geometrical structures of a material. It can be complementary used with Extended X-ray Absorption Fine Structures (EXAFS) which reflects mainly one dimensional information of the structure, namely distances between the photo-absorption atom and neighboring atoms. EXAFS is usually explained by a simple single scattering theory. XANES may be naturally interpreted itself as an extension of EXAFS towards to lower energy region. Hence we include higher order scatterings via multiple scattering in order to have right picture for XANES framework for such low energy lying continuum states. However, spherical average of scattering atoms, the so-called Muffin-Tin approximation, is widely adapted for the sake of simplicity of the theory and efficiency of numerical computation. In some specific cases such as low dimensional systems and systems having large interstitial space, e.g. diamond and layered structure, this approximation causes serious errors.

We developed FPMS code [1] that does not use this approximation instead separate the space by truncated spheres and Voronoi cells in order to avoid overlapping of spheres and remove the interstitial region. These non-spherical cells are used as scattering sites for multiple scattering calculation. In addition, we implemented ES2MS [2] code that is an interface to transfer self-consistent charge density and potential calculated by electronic structure codes to multiple scattering calculations. It was implemented for various codes, such as VASP [3], Gaussian09 [4] and MOLCAS [5] .Further, ES2MS is merged into FPMS code, thus the codes became as a suite package. We demonstrates several examples of the effect of SCF charge density and the potential for XANES spectra calculated by this last version of FPMS.

References

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