MS051.O03

FPMS code with an interface to 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 materials. 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 neighbouring 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 by use of multiple scattering theory in order to have right picture for XANES framework for such low-lying energy 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 special 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 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 pass self-consistent charge density and potential calculated by electronic structure codes to multiple scattering calculations. For the first application, it was implemented especially for using VASP outputs and applied for Graphene systems. [3] Recently it was also extended to manage Gaussian09 code and applied to Angle resolved photoemission spectroscopy (ARPES). Further, ES2MS is merged into FPMS code, thus the codes became as a suite package. We demonstrates several examples in order to see the effect of SCF charge density and the potential on XANES spectra calculated by this last version of FPMS.

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Keywords: XANES, full potential, multiple scattering