電子波動関数の動径解を用いた 共鳴非弾性散乱スペクトルの第一原理分光学計算

First principle spectroscopic calculation for RIXS through Radial part solutions of Electron distribution wavefuncion

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We developed the method to calculate reasonable Coulomb repulsion with Hartree-Fock type radial differential equation. Calculation is conducted by Density Functional Theory (DFT) employing Norm Conserving Pseudo potential (NCP) and expanded on Plane wave basis (PW). After the projection on the symmetry adapted Wannier function (WF) [1], we extract radial part of such calculation results [2]. Yielded radial part solutions are not the function of radial distance dependent but the one of position vector dependent. Slater Integrals derived from these calculations are well defined as first principle and reasonable than those of Cowan code [3], which is manipulated for fitting to experimental results.

We report RIXS spectral calculation results which applied this method for typical strong correlation material, NiO calculated through occupation representation calculation code e.g. Quanty [4].

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