DFT-CI calculations for RIXS and RIXS-MCD

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Resonant inelastic x-ray scattering (RIXS) has attracted much attention in past 10 years. RIXS is a photon-in/photon-out spectroscopy, which enable us track all electronic and other elementary excitations in materials by tuning incident and outgoing photon energies. Recent developments of high-resolution monochromator and detector enable us to measure the RIXS spectra in high-energy resolution. Recently, magnetic circular dichroism (MCD) of RIXS has been investigated which is a promising new probe for identifying magnetic structures of materials. On the other hand, the interpretation of the fine structures in the RIXS and RIXS-MCD is not straightforward because of the complexity of transition channels. The reliable theoretical calculations are necessary for interpreting and extracting information about the electronic, atomic and magnetic structures from experimental spectra.

The spectral shapes of RIXS and RIXS-MCD at the *K*-pre-edge and $L_{2,3}$-edges of 3d transition metals (TMs) are dominated by the multiplet structures which originate from the strong electronic correlations between 3d electrons and 2p core-hole. Therefore, the single-particle approximation including the density functional theory (DFT) cannot reproduce the experimental spectra in general. In this work, we applied the *ab-initio* configuration interaction method using the four-component molecular orbitals obtained by relativistic density functional calculations (DFT- CI) for simulating the multiplet structures appearing in RIXS and RIXS-MCD in TM compounds. The RIXS spectra in arbitrary geometries can be calculated following the Kramers-Heisenberg formula using the many-electron wavefunctions obtained by the DFT-CI method. This approach is succeeded to reproduce the experimental *K*-pre-edge and $L_{2,3}$-edge RIXS of TMs and to reveal the origin of RIXS features. The RIXS-MCD can also be calculated by introducing the Zeeman terms in the CI Hamiltonian. In this talk, the use cases of the DFT-CI method to interpret RIXS and RIXS-MCD in simple TM oxides will be demonstrated.

References

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