LDA+DMFT method with Iterative Perturbation Theory and its application to ferromagnetic bcc-Fe, fcc-Ni and anti-ferromagnetic NiO

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Many physical properties in strongly correlated systems have been studied quite extensively both experimentally and theoretically. These are not well described, however, by the local density approximation (LDA) method and we need more sophisticated approaches with dynamical correlation effects.

The LDA+DMFT[2] are proposed in order to combine LDA with the dynamical mean field theory (DMFT).[1] Many LDA+DMFT methods adopt the projected effective Hamiltonian of the Wannier function. With the use of projected effective Hamiltonian with fixed Wannier function, one can not discribe a change of hybridization mixing by strong Coulomb interaction. The aim of our research is to construct a novel LDA+DMFT method which can treat a variety of realistic materials in strongly correlated systems, such as multi-atom (compound) cases, spin-polarized cases and the cases including strong hybridization between s, p and d bands.

In our research, our LDA+DMFT method has used the full-LDA Hamiltonian without projecting onto any kind of effective Hamiltonian and adopted the Iterative Perturbation Theory (IPT)[3-4] as a solver for the mapped single impurity problem. We then apply our LDA+DMFT method to ferromagnetic bcc-Fe and fcc-Ni as a test of transition metals, and to anti-ferromagnetic NiO as an example of transition metal oxide.[5] The energy spectra obtained by the LDA+DMFT are shown in Fig.1. For Fe and Ni, occupied 3d band width in the LDA+DMFT is narrower than the LDA and Ni 6eV satellite is observed. For NiO, band gap is 4.3 eV, the occupied satellite peak based on Ni 3d bands is observed and the system becomes the charge-transfer insulator. These effects obtained by the LDA+DMFT are in good agreement with experimental XPS result.

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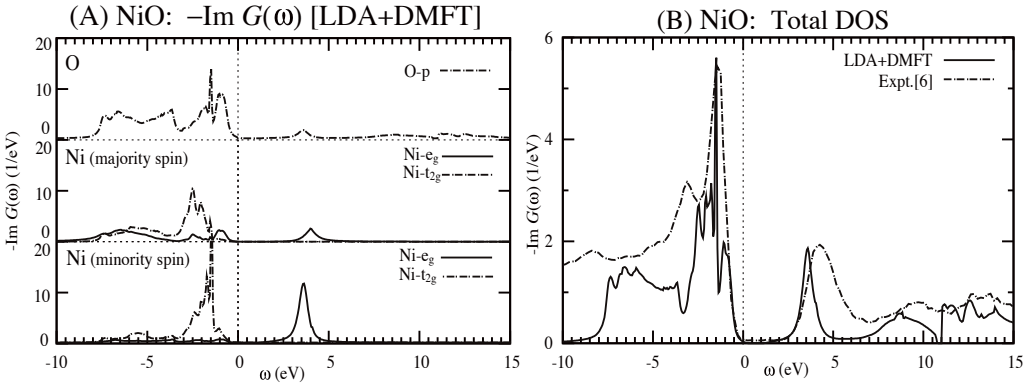

Fig.1: Energy spectrum for NiO obtained by the LDA+DMFT.
(A) Partial DOS. (B) Total DOS with the experimental XPS spectrum.[8]