Electronic structure of NiO and MnO by GW approximation starting from LSDA+U

Yoshiro Nohara[A] and Takeo Fujiwara[ABC]
Department of Applied Physics, University of Tokyo[A],
Center for Research and Development of Higher Education, University of Tokyo[B],
and Core Research of Evolutional Science and Technology, Science and Technology Agency (CREST-JST)[C]
nohara@coral.t.u-tokyo.ac.jp

GW approximation (GWA) is now widely used for various insulator, semiconductors and transition metal oxides. This method achieves a great success in case that the L(S)DA wavefunctions are good starting ones. However, GWA could not present spectrum with experimental results in case that real wavefunctions are believed to be more localized than those of LSDA.

We proposed a novel GWA, named U+GWA, [1] and, in the present paper, apply to antiferromagnetic NiO and MnO. U+GWA starts from the LSDA+U Hamiltonian and obtain one-electron wavefunctions. After that, one can calculate the exchange energy with screened Coulomb interactions by RPA. Then the exchange-correlation energy should be subtracted from the resultant self-energy. Therefore, if one can proceed the self-consistent calculation, the results should coincide with the standard GWA, though we should stop the procedure at the first step calculation.

We apply U+GWA to NiO and MnO and obtain energy spectra with a good agreement with the experimentally observed XPS and BIS. The E-k curves of NiO are also in good agreement with the ARPES.[2] The quasi-particle's band gap and magnetic moment in the transition metal ion are also in a good agreement with the experimental values.[3][4][5]

We also discuss the screened Coulomb interactions (W) in these materials. W is separated into the part of d-d screening and the rest. The d-d interaction in NiO is smaller than that in MnO, since the number of d-electrons is larger in NiO.

[1] S. Kobayashi, Y. Nohara, and T. Fujiwara, now in preparation.
[2] Z.-X. Shen, R. S. List, D. S. Dessau, B. O. Wells, O. Jepsen, A. J. Arko, R. Barttlet, C. K. Shih, F. Parmigiani, J. C. Huang, and P. A. P.Lindberg, Phys. Rev. B **44**, 3604 (1991).
[3] G. A. Sawatzky and J. W. Allen, Phys. Rev. Lett. **53**, 2339 (1984)
[4] J. van Elp, R. H. Potze, H. Eskes, R. Berger, and G. A. Sawatzky, Phys. Rev. B **44**, 1530 (1991)
[5] A. K. Cheetham and D. A. O. Hope, Phys. Rev. B **27**, 6964 (1983)