First Principles Electronic Structure Calculations for Strongly Correlated Systems

Takeo Fujiwara\textsuperscript{1,2,3}, Oki Miura\textsuperscript{1} and Yoshiro Nohara\textsuperscript{1}

\textsuperscript{1}Department of Applied Physics, The University of Tokyo, Tokyo 113-8656,
\textsuperscript{2}Center for Research and Development of Higher Education, The University of Tokyo, Tokyo 113-8656,
\textsuperscript{3}Core Research for Evolutional Science and Technology, Japan Science and Technology Corporation (CREST-JST), Japan
fujiwara@coral.t.u-tokyo.ac.jp

We are proposing two novel methods of the electronic structure calculation for strongly correlated
electron systems. First one is a novel GW Approximation method named $U+GWA$, starting from
the LSDA+U method. is proposed, where we can start the GW Approximation with more
localized wave functions. Second one is a novel LDA+DMFT with the iterative perturbation
theory (IPT).

GWA is the first term approximation of the many-body perturbation series and the self-energy
is replaced by the lowest order term of the exchange energy with the dynamically screened
interaction of the random phase approximation (RPA). In fact, this approach is successful if LSDA
would give reasonably good starting wave-functions, though it may not be always true. Several
trials of partially self-consistent treatment have been proposed to improve the quasi-particle band
structure. The essence of these methodologies exists how to obtain localized wave-functions in
transition metal oxides. Another possibility would be an establishment of a methodology to start
from some unperturbed Hamiltonian which gives localized wave-functions. $U+GWA$ is a novel
methodology starting from the LSDA+U method. Examples of calculated results will be shown
for antiferromagnetic NiO and $V_2O_3$ and we will show a good agreement of the band gap and
spectrum with those of experiments.

We also propose a novel LDA+DMFT method with IPT in order to include all orbitals s, p and
d, instead of projection onto Wannier type wave-functions. IPT is an approximation method for
the self-energy of many-body Green’s function, an interpolation method of the self-energy
between that of the strong U limit and that of the high frequency limit. IPT is actually quite
efficient in the calculation of multi-orbital case and the case of many atoms in a unit cell. Since
our LDA+DMFT can change the hybridization mixing as a result of strong Coulomb interaction, it
can establish a character of the charge-transfer type antiferromagnetic insulator of NiO with a
good agreement of the value of the band gap and spectrum.