First Principles Electronic Structure Calculations for Strongly Correlated Systems

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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.