Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Fock exchange in FLAPW method TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Fock exchange potential has distinct features which cannnot be seen in the LDA exchange potential. (i) It is self-interaction free potential and (ii) nonlocal potential and thus state-dependent potential. With appropriate correlation effects added, these two features may produce significantly improved results over the conventional LDA results, as one can witness in the GW calculations. Massidda et al. (1993) proposed a way to calculate Fock exchange potential of extended solids within the FLAPW method. Their idea was to apply Weinert's Poisson solver to infinite lattice summation as is done for the Hartree potential calculation. Due to the long range nature of Coulomb interaction, one encounters singularity problem in this process. They handled it by simply extending Gygi's prescription (1986), which was originally developed for the norm-conserving pseudopotential framework. In this paper, we present our formula in calculating Fock exchange matrix of solids based on the FLAPW method. Following Massidda's idea, we use Weinert's Poisson solver. However, in treating the Coulomb singularity, we have developed more accurate way: the occupied eigenfunctions in Fock operator are expanded upto the second order in terms of q vector based on the $k \cdot p$ perturbation theory, whearas Gygi's way corresponds to the zeroth order expansion. With this higher order expansion, one can achieve faster convergence for the Brillouin zone integration appearing in the Fock operator.

Tatsuya Shishidou
Hiroshima University

Date submitted: 20 Nov 2007 Electronic form version 1.4