Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Acceleration of the transcorrelated method for solids KEITARO SODEYAMA, MASAYUKI OCHI, University of Tokyo, REI SAKUMA, Chiba University, SHINJI TSUNEYUKI, University of Tokyo — To calculate the electronic structures of solids including electron correlation effects, we have developed the transcorrelated (TC) method. In the TC method, a many-body wave function is represented by a correlated wave function $F\Phi$, where Φ is a single Slater determinant and F is a Jastrow function, $F = \exp[-\sum_{i<j} u_{ij}]$. u_{ij} is a two-body function called Jastrow factor. The many-body Hamiltonian H is similarity transformed to an effective Hamiltonian $H_{TC} = F^{-1}HF$ with up-to-three-body interaction. One-electron orbitals in the Slater determinant Φ and their orbital energies are optimized by solving a set of Hartree-Fock-like single particle equations derived by minimizing the variance of the H_{TC}. We have confirmed that the total energy calculations for solids using the TC method were feasible enough to determine the lattice constants and bulk moduli. However, it required a lot of computational time for solid that scales as $O(N_k^3 N_{band}^4)$. In this presentation, we will demonstrate that the CPU cost can be reduced by orders of magnitude after revising the algorithm.

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Date submitted: 25 Nov 2009 Electronic form version 1.4