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Transcorrelated method applied to solids: numerical assessment of the SCF effect KEITARO SODEYAMA, 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 which was first proposed by Boys and Handy. In the TC method, the 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 and their orbital energies are optimized by solving a set of Hartree-Fock (HF)-like single particle equations derived by minimizing the variance of the H_{TC}. In this study, we have investigated the effect of the self-consistent field (SCF) approach which was used in solving the HF-like single particle equations in the TC method. For this purpose, band gaps of Si, SiC, and LiF were calculated as a one-shot perturbation by using the unperturbed LDA orbitals as initial guess orbitals. The difference between the one-shot TC and conventional SCF TC results is small for Si but large for SiC, and especially large for LiF. From this result, we found that the SCF effect was important for strongly polarized solids such as LiF because the initial LDA orbitals were poorly described for such polarized solids.

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