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Transcorrelated method applied to covalent and ionic solids: total energy and band structure calculation KEITARO SODEYAMA, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo, REI SAKUMA, JST-CREST, AIST — 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, the band gaps and total energies of covalent and ionic solids were calculated by the TC method at various lattice constants. The local density approximation (LDA) and HF calculations were also performed to the same systems and compared to the TC results. In covalent solids such as silicon carbide, the lattice constant and bulk modulus calculated by the TC method were not largely different from the LDA results. In ionic solids such as lithium hydride, we found that the lattice constant, bulk modulus and band gap calculated by the TC method were closer to the experimental results than the LDA results.

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