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Total energy calculations using the transcorrelated method: wavefunction approach for solids KEITARO SODEYAMA, REI SAKUMA, SHINJI TSUNEYUKI, Department of Physics, 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 this 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 orbital energies are optimized by solving a set of Hartree-Fock(HF)-like equations derived by minimizing the variance of the H_{TC}. In this study, the total energies of crystalline silicon and carbon are calculated by the TC methods at various lattice constants. The bulk moduli of silicon by HF and TC methods were 115 and 102 GPa. Those of carbon were 524 and 501 GPa. Comparing with the experimental values of 99.2 and 443 GPa, the TC method, which includes the electron correlation effect in the framework of wavefunction approach, improves the HF results.

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