

Transcorrelated method applied to solids: total energy and band structure calculation

Keitaro Sodeyama¹, Rei Sakuma^{2,3}, Shinji Tsuneyuki¹

¹*Department of Physics, University of Tokyo*

²*Research Institute for Computational Sciences, AIST*

³*CREST, Japan Science and Technology Corporation*

sode@cms.phys.s.u-tokyo.ac.jp

In order to calculate electronic structure of solids including electron correlation effects, we have adopted the transcorrelated (TC) method [1-4]. The TC method was first proposed by Boys and Handy in the field of quantum chemistry in 1969. 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 effective Hamiltonian. Some research groups have developed and tested the TC method for atoms and small molecules [1-4], electron gas [5,6] and crystalline semiconductors [6]. For atoms and small molecules, it was reported that the TC method yields accurate total energies. For the crystalline semiconductors, the band gaps calculated by the TC method were greatly improved from those by the Hartree-Fock (HF) method.

In this study, the band gaps and total energies at various lattice constants of crystalline silicon (Si), diamond (C) and silicon carbide (SiC) were calculated by the TC method. The local density approximation (LDA) and HF calculation were also performed to the same systems and compared to the TC results. In the TC method, we used the Jastrow function which was derived from the random phase approximation. The integration over the whole Brillouin zone was replaced by a summation over 32 \mathbf{k} points. Although the convergence of the total energy with increasing the kinetic energy cutoff was slower for the TC method than for the LDA and HF, we have obtained a smooth and almost convergent total energy curves by using energy cutoffs of 49 Ry, 64 Ry and 64 Ry for Si, C and SiC. From the curves, the lattice constants a_0 and bulk moduli B_0 were calculated by the LDA, HF and TC method (Table 1). The comparison between experimental and calculated values of a_0 and B_0 shows that the TC method improves the HF results.

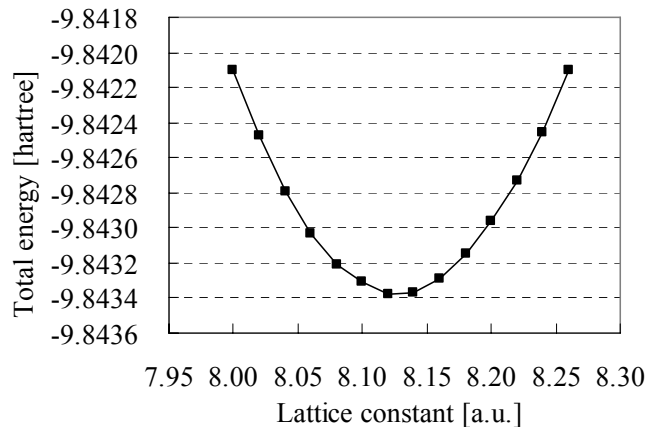


Fig. 1. Total energies of SiC calculated by TC method.

Table 1. Lattice Constants a_0 [Bohr] and bulk moduli B_0 [GPa]

| | | LDA | HF | TC | Expt. |
|-----|-------|-------|-------|-------|-------|
| Si | a_0 | 10.16 | 10.16 | 10.16 | 10.26 |
| | B_0 | 98 | 120 | 103 | 99 |
| C | a_0 | 6.65 | 6.60 | 6.60 | 6.74 |
| | B_0 | 467 | 524 | 501 | 443 |
| SiC | a_0 | 8.15 | 8.08 | 8.13 | 8.24 |
| | B_0 | 228 | 269 | 242 | 225 |

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