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Solid-state calculations using the second-order Møller-Plesset perturbation theory combined with the transcorrelated method
MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, ISSP, The University of Tokyo — Recently, wave-function theory has been actively applied to solid-state calculations, where the Hartree-Fock (HF) method is used as a starting point. Transcorrelated (TC) method [1-5] is expected to be an attractive alternative to the HF method, in which the total wave function is assumed to be the Jastrow-Slater-type wave function, and the many-body Hamiltonian is similarity-transformed by the Jastrow factor. Then the electron correlation effects are taken into account through the similarity-transformed Hamiltonian. However, the band gaps calculated using the TC method have about 1 or 2 eV errors for some semiconductors. For improving accuracy, we apply the second-order Møller-Plesset (MP2) perturbation theory to the similarity-transformed Hamiltonian, and will show that the band structures of solids are corrected well with the same level of computational cost as that for conventional MP2 applied to the HF method.

[1] S. F. Boys and N. C. Handy, Proc. R. Soc. London Ser. A 309, 209 (1969).
[2] S. Ten-no, Chem. Phys. Lett. 330, 169 (2000).
[3] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. 119, 10015 (2003).
[4] R. Sakuma and S. Tsuneyuki, J. Phys. Soc. Jpn. 75, 103705 (2006).
[5] M. Ochi, K. Sodeyama, R. Sakuma, and S. Tsuneyuki, J. Chem. Phys. 136, 094108 (2012).

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