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Band structure calculations using the transcorrelated method REI SAKUMA, KEITARO SODEYAMA, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo — We have been developing a new wave-function-based method for calculating the electronic properties of solids. The main feature of this method, called the transcorrelated (TC) method, is a similarity transformation of the Hamiltonian using the Jastrow-Slater trial wave function, which leads to an effective non-hermitian Hamiltonian with three-body interactions. Correlation effects are incorporated in the effective Hamiltonian via the similarity transformation. The wave function is optimized by solving a set of Hartree-Fock-like single particle equations derived by minimizing the variance of the effective Hamiltonian. In this work, the TC method is applied to the band structure calculations of *sp* semiconductors. In the TC method, Koopmans' theorem holds, in which the eigenenergies of the single particle orbitals are interpreted as the ionization energies and electron affinities. By applying the Jastrow function derived from the random phase approximation (RPA), the screening effect is incorporated in the effective Hamiltonian, which significantly reduces the value of band gaps of semiconductors from their Hartree-Fock values.

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