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Diffusion Monte Carlo calculations of solids using transcorrelated trial wave functions YOSHIYUKI YAMAMOTO, Department of Physics, The University of Tokyo, RYO MAEZONO, School of Information Science, JAIST, MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo, ISSP, The University of Tokyo — Diffusion Monte Carlo (DMC) method is an *ab initio* wave-function theory that can treat correlated quantum systems to high accuracy within reasonable computational time, and enables us to calculate large systems such as solids. For electronic systems, DMC suffers from the fermion-sign problem, and in order to avoid it we have to use the fixed-node approximation. The amount of fixed-node error depends on the quality of the nodal structure of the trial wave function that we prepare in advance. A promising trial wave function is that of transcorrelated (TC) method, which is one of the wave-function theories. In this method, wave functions are approximated as the Slater-Jastrow form and the orbitals in the Slater determinant are relaxed by solving one-electron equations of similarity-transformed Hamiltonian. The nodal structure of the Slater-Jastrow wave function is determined by its determinantal part, so we can optimize the nodal structure of the Slater-Jastrow wave function by TC method. In this talk, we will present the fixed-node DMC energies of solids using TC trial wave functions and compare the energies with those using trial wave functions constructed from density functional theory and Hartree-Fock method.

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