4P-112

Mean-field second-order Moller-Plesset perturbation theory

Tran Nguyen Lan[1] and Takeshi Yanai[1, 2]
[1] The Graduate University for Advanced Studies
[2] Institute for Molecular Science

We use the canonical transformation to include the dynamic correlation effect at the MP2 level on the molecular Hamiltonian under the one-particle (mean-field) formalism. The cumulant decomposition plays the key role to do this purpose. By this way, we will obtain a new correlated Hamiltonian. Therefore, the wave function and eigenvalues after relaxation due to correlation field can be obtained by resolving the Schrodinger equation with this new Hamiltonian. Several tests have been done to show advantages of our theory.