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New Theoretical Method for Molecular Systems and Nanomolecules JUNHO JEONG, Sengban Patent & Science Laboratory, Albany NY 12205 and State University of New York at Albany, Albany NY 12222 — In general, it has been known that electrons of a molecular system are indistinguishable. However, the total electronic energy computed by the conventional theoretical method, the Hartree Fock Theory or the Density Functional Theory, consists of kinetic and attractive energies on distinguishable electrons and repulsive potential energy on indistinguishable electrons on a molecular system. The other question of the conventional methods is singularity on two-electron integrals because electrons in a molecular system cannot exist at the centre of their nucleus which brings about singularity in free space. The new theoretical method that modified above problems has been applied to hydrogen molecule H_2, and its results have been compared with those of the conventional theoretical methods installed in Gaussian 98 program. The total energies of the conventional methods are much bigger than -1.0 (a.u.) the total energy of hydrogen molecule in the infinite H-H bond distance, and the electron-electron repulsive energies are about 2.911 to 7.728 not 0.0 eV on 1,000 Å H-H bond distance although the energies of the new method agree with the values of the physical concept on H_2.

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