Application of High Accuracy Calculation for the Study UV-Visible Absorption Spectra of Gold Dimer

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The absorption UV-visible spectra of gold dimer is investigated using the multiconfigurational exact molecular mean-field intermediate Hamiltonian Fock-space Coupled Cluster (IHFSCC). The most accurate description of the system was achieved explicitly including spin Coulomb type integrals (SS/SS) and including Gaunt interaction (DOOSSSS-GAUNT). Calculated spectra showed similarities when are compared to experimental data gas neon matrix.