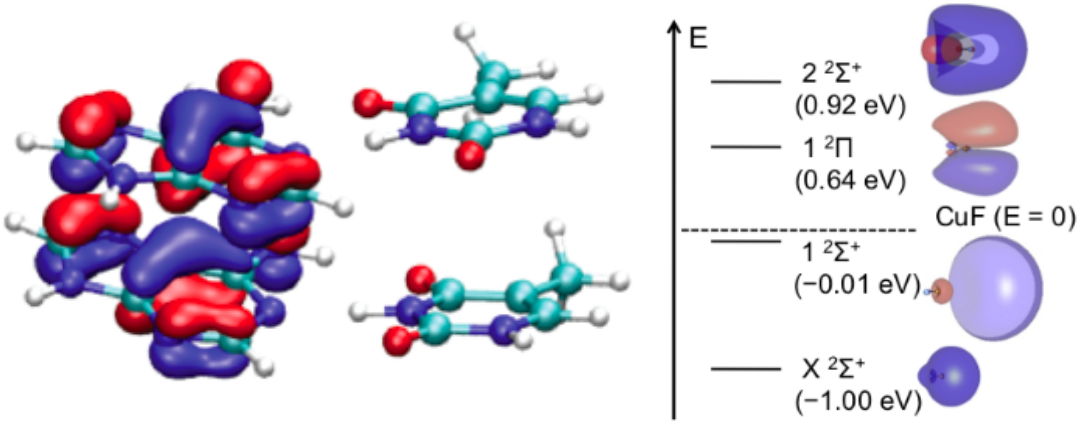
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Post Hartree-Fock Features

Coupled-Cluster, Equation-of-Motion, and Algebraic Diagrammatic Construction Methods

- Significantly enhanced coupled-cluster codes rewritten for better performance on multicore systems;
- Single- and mixed-precision execution, RI and Cholesky decomposition within CC/EOM-CC for improved performance and access to larger molecules;
- Energy, gradient, and properties for CCSD and EOM-CC/ADC methods;
- More properties: two-photon cross-sections, ground- and excited-state (hyper)-polarizabilities, electronic circular dichroism rotatory strengths, non-adiabatic and spin-orbit couplings, Dyson orbitals;
- Complex absorbing potentials within CC/EOM-CC framework for metastable electronic states: Energies, gradients, Dyson orbitals, exciton analysis;
- Approximate EOM-CC methods for larger molecules;
- PCM, QM/MM, and EFP for ADC and EOM-CC wave functions; density embedding for ADC;
- ADC and EOM methods for core-ionized and core-excited states.



New Approaches for Strong Correlation:

- Perfect quadruples and perfect hextuples methods for strong correlation problems;
- Coupled-cluster valence bond (CCVB) and related methods for multiple bond breaking;
- RAS-nSF methods;
- Variational 2RDM methods;
- Incremental and adaptive CI methods.

Request a free trial at www.q-chem.com