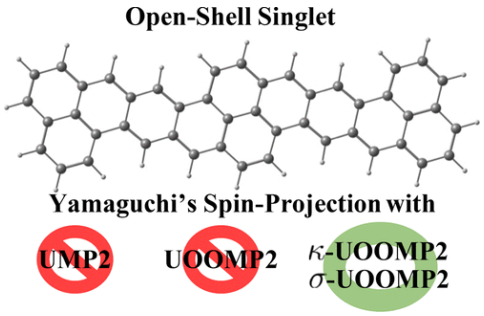
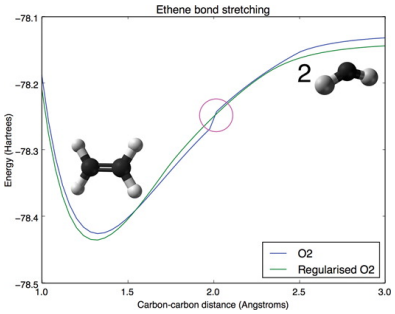
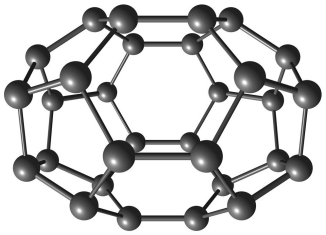
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Regularized Orbital-Optimized Møller-Plesset Perturbation Theory for Strongly Correlated Species

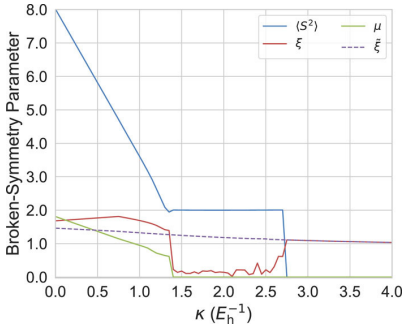




- Unrestricted Hartree-Fock (UHF) may exhibit artificial spin-symmetry-breaking in open-shell systems, and using UHF orbitals for correlated wave function calculations could lead to incorrect energetics and properties.
- Orbital-optimized MP2 (OOMP2) restores spin-symmetry and removes the discontinuity in the first-order properties at the onset of symmetry-breaking in MP2.
- Orbital optimization in OOMP2 could produce very small energy denominators which make the total energy diverge. In addition, OOMP2 may unphysically prefer restricted solutions and remove the Coulson-Fischer point from potential energy curves.
- Q-Chem offers several regularization schemes (κ-OOMP2 and σ-OOMP2) to fix the above issues. Combined with approximate spin-projection, these regularized OOMP2 methods are powerful and economical tools for studying strongly correlated systems.



(a) C_{30} (D_{5h} symmetry), a strongly correlated molecular cluster of which symmetry-breaking is essential



(b) Measures of symmetry breaking parameters as functions of the regularization strength of C_{30}

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