A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

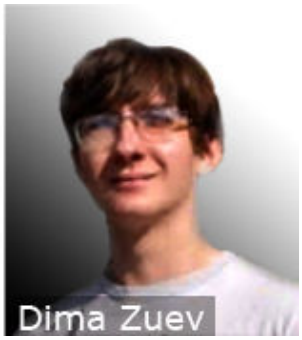
Frozen Natural Orbital (FNO) Approach

Developers: Anna Krylov, Arie Landau and Dima Zuev

The FNO approach allows substantial truncation (by about half) of the virtual orbital space thereby reducing the computational effort in CC and IP-CC calculations. For ionization energies, 30-70% reduction of the virtual space yields errors below 1 kcal/mol. For moderate-size systems, we observe 3-4 fold speed up. The reduced disc and memory usage allows access to larger systems. Only Q-Chem features the FNO truncation for IP-CC as well as more robust population-based truncation criteria and e extrapolation scheme.

Publication: A. Landau, K. Khistyaev, S. Dolgikh, A. Krylov, "Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism", J. Chem. Phys **132**, 014109 (2010).

For more information on how to use this feature, refer to the Q-Chem Manual:
For CC: Section 5.9;
For EOM-IP-CC: Section 6.62 and 6.65



For more new features, visit:
www.q-chem.com/whatsNew4.html

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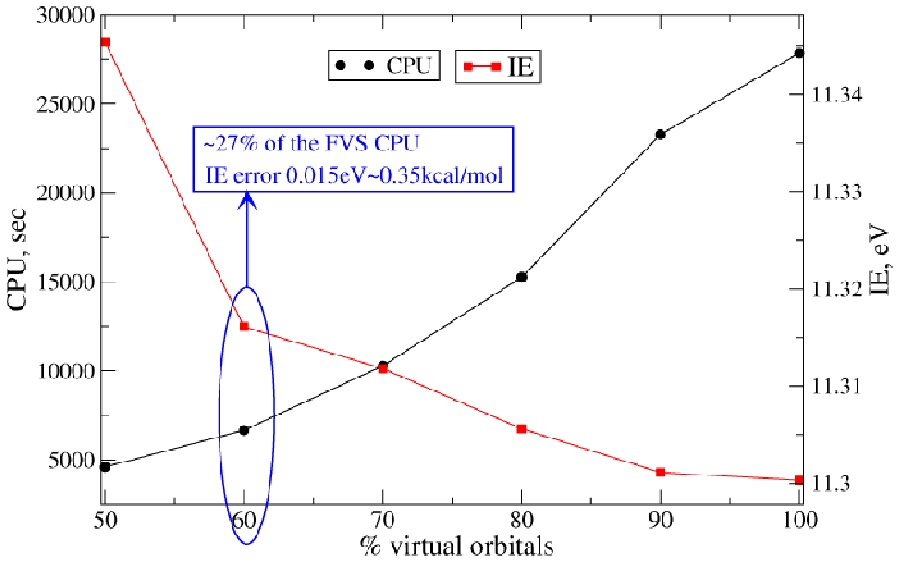
What's New in Q-Chem

Frozen Natural Orbital (FNO) Approach (continued)



The picture shows CPU (black circles) and the lowest IE of water dimer (red squares) as a function of the percentage of virtual natural orbitals retained in the EOM-IP-CC(2,3)/cc-pVZ+dff calculation. As the size of virtual space increases, the CPU increases and IE approaches the FVS value. The calculation using 60% of the virtual orbitals requires only about 27% of the FVS CPU time, while the error in the IE (relative to the FVS value) is less than 0.5 kcal/mol.

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