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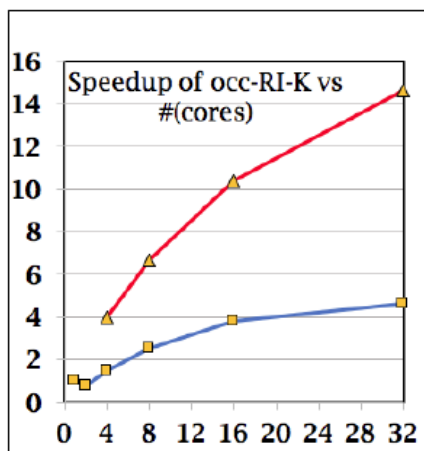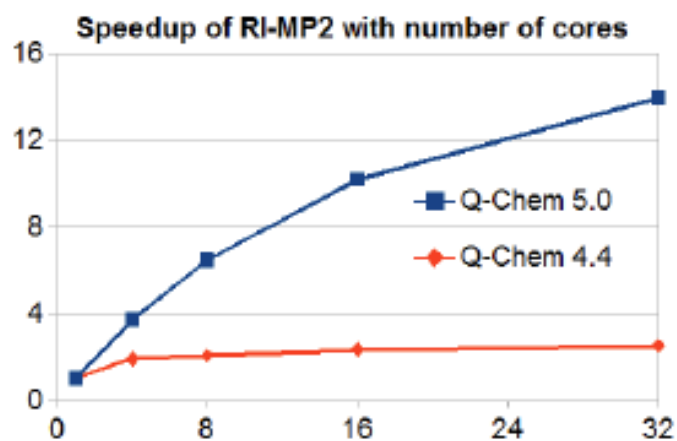A Quantum Leap Into the Future of Chemistry

Computational Efficiency

(a) Parallel scaling for Diamon-doid_octahedral (148 atoms, red line) and Vitamin E (81 atoms, blue line)

(b) Parallel scaling for vitamin E molecule (cc-pVDZ, 81 atoms, 684 basis functions)

- **Resolution-of-the-Identity Algorithms for SCF and Post-SCF Calculations:**
  - occ-RI-K algorithm for Hartree-Fock exchange;
  - RI-SCF gradient;
  - I-MP2, SCS-MP2, SOSMP2 methods;
  - RI-CCSD and RI-EOM energies and gradients.

- **Fast Algorithms for DFT Calculations:**
  - Algorithms for Coulomb (Continuous Fast Multipole Method, J engine, Fourier Transform Coulomb, Quantum Ewald Mesh);
  - Algorithms for Hartree-Fock exchange (LinK, ARIK) and numerical integration (mrXC).

- **Fast Algorithms for Perturbation Theory Calculations:**
  - Fast integral transformations, RI approximation, scaling of different spin components, Laplace transform, dual basis extrapolation, and the use of localized orbitals.

- **Fast Algorithms for Coupled-Cluster Calculations:**
  - Enhanced by a modern tensor library, RI approximation, Cholesky decomposition, single-precision execution, frozen natural orbitals.

- **Efficient Implementation on Shared-Memory Multicore Machines; GPU acceleration via BrianQC module; Cloud-Enabled.**

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