Software Framework for Electronic Structure of Molecules and Solids

Garnet Kin-Lic Chan[1], Toru Shiozaki[2], Edward F. Valeev[3]

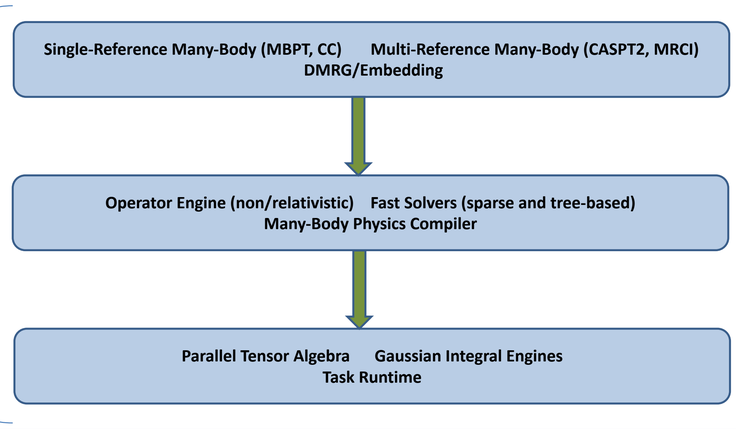
1) Division of Chemistry and Chemical Engineering, California Institute of Technology (2) Department of Chemistry, Northwestern University (3) Department of Chemistry, Virginia Tech

EMoS Framework

is a software suite for treating "Electrons in Molecules and Solids" using Gaussian basis representation.

Objectives:

- Harness the efficient many-body reduced-scaling molecular electronic structure technologies for treating, molecules, solids, and interfaces
- Develop new theoretical methodologies for robust treatment of molecules and solids in ground and excited states
- Develop a coherent software framework featuring an easy-to-use Python frontend and high-efficiency massively-parallel C++ backend



EMoS

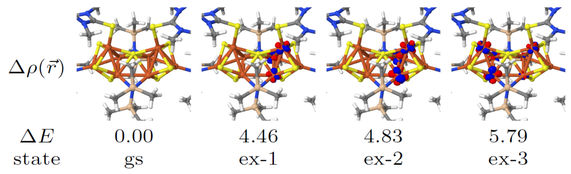
PySCF Python-based Simulations of Chemistry Framework

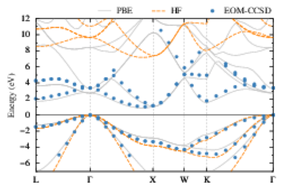
www.pyscf.org

PySCF is a general-purpose electronic structure platform implemented in Python programming language.

Highlights:

•Electronic structure (HF, MCSCF, CI, CC) of ground state and excited states for finite-size and extended systems.
•Properties of ground states (NMR, ZFS, IR spectra).
•Properties of excited states (nuclear gradients, transition dipole moment).





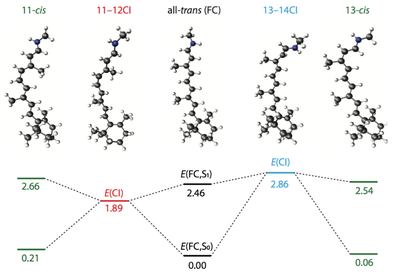
PBC coupled cluster method (CCSD and EOM-IP/EA-CCSD) to reveal the band structures of silicon crystal. The IP and EA spectra of CCSD method show good agreement with DFT (LDA) bands.

BAGEL

Parallel, efficient open-source program
www.nubakery.org

Selected features:

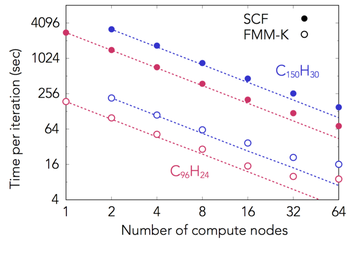
- HF, MP2, CASSCF, CASPT2, MRCI
- Relativistic Dirac Hamiltonian
- Nuclear gradients and derivative couplings

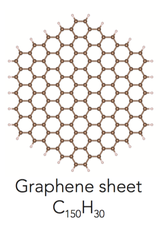


Retinal isomerization dynamics (Mol Phys 2018)

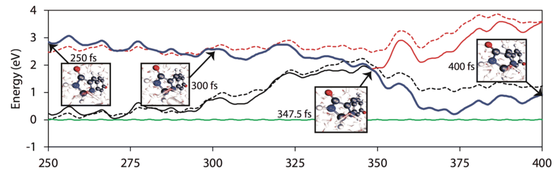
Development under this award:

- XMS-CASPT2 derivative couplings
- XMS-CASPT2 on-the-fly surface hopping dynamics
- FMM-based exact exchange for small-gap systems
- New relativistic CASSCF





Highly scalable FMM-K algorithm



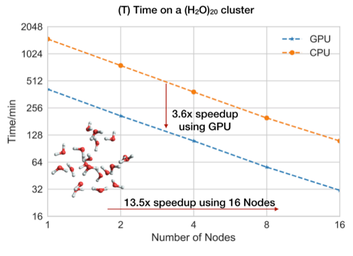
CASPT2 surface hopping dynamics simulations for a GFP model chromophore

MPQC4

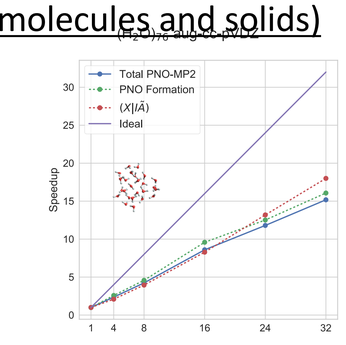
Massively Parallel Quantum Chemistry package
mpqc.org

Highlights:

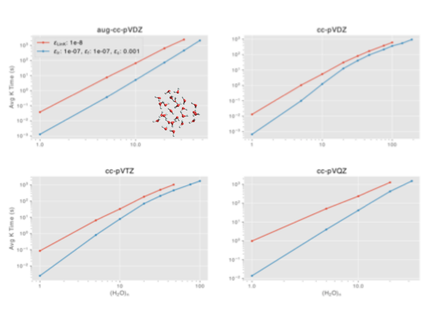
- Designed in C++ from ground-up for maximum parallelism
- Accurate electronic structure of molecules and solids
  - CCSD(T)-F12, CCSDT, EOM-{EE,IP,EA}-CCSD, GF2-F12 (molecules)
  - PNO-MP2 (molecules and *solids*)
  - MA-RI-J (solids)
  - O(N) HF Exchange (molecules and solids)



CCSD(T) code for heterogeneous distributed-memory machines



O(N) PNO-MP2 implementation offers reduced-scaling and excellent strong performance.



Local Density Fitting-based Hartree-Fock exchange greatly reduces cost relative to conventional (LinK) algorithm.

The EMoS Project is supported by NSF Awards 1550456 to Virginia Tech, 1550481 to Northwestern University, and 1657286 to California Institute of Technoogy