GammCor: electron correlation and molecular interaction calculations

Authors: K. Pernal, M. Hapka, M. Modrzejewski, M. Przybytek

- Electron correlation energy for strongly correlated molecules
  unique feature: capable of treating ~10^2 strongly correlated electrons
- Molecular interaction energy decomposed into physically meaningful components
  unique features: applicable to electronically excited systems (local excitons), open-shell molecules, and molecules out of equilibrium geometries; visualization of dispersion energy density in real space.

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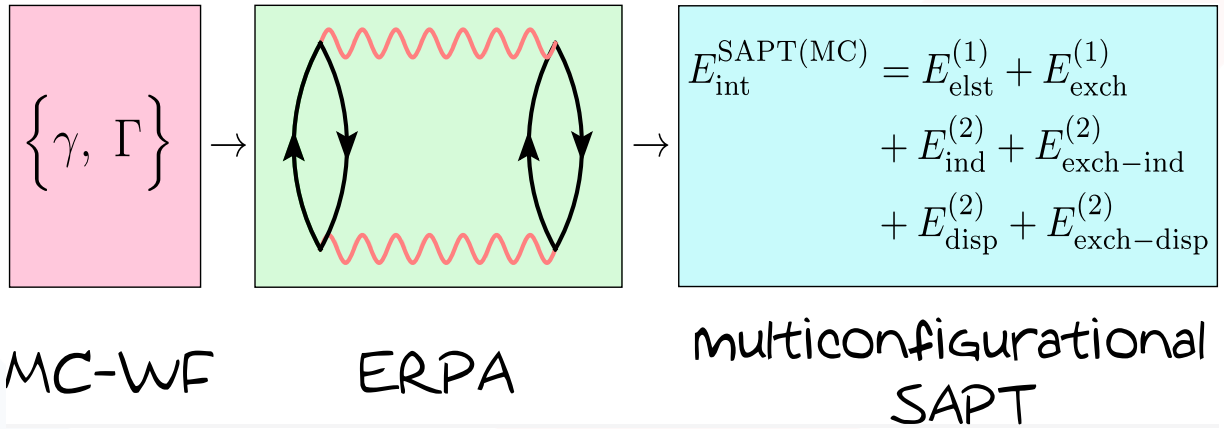
Interoperability with other codes:

- Requires 1- and particle reduced density matrices
- Compatible with **TREXIO** library
- Interfaced with: Molpro, Dalton, Quantum Package, Orca

Interaction energy in molecular complexes with localized excitons



M. Hapka et al., J. Chem. Theory Comput., 17, 5538 (2021)

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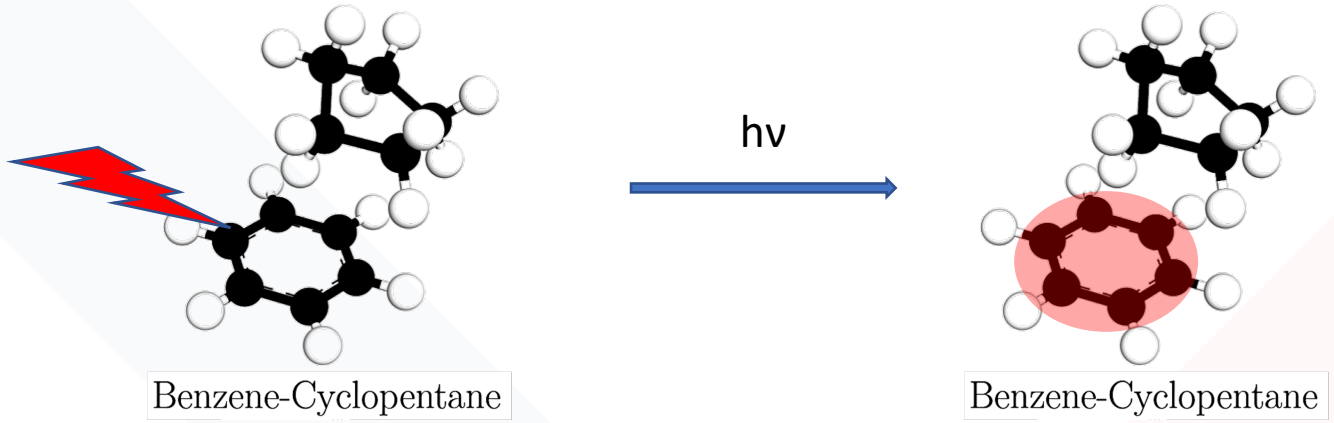


E_{int} changes by 0.15 kcal/mol. Mainly electrostatic and dispersion interaction effects.

SAPT(MC) in GammCor: up to 10^2 electrons in 10^3 basis set functions.

Wavefunctions for monomers: CASSCF, CI.

M.R. Jangrouei et al., J. Chem. Theory Comput., 18, 3497 (2022)

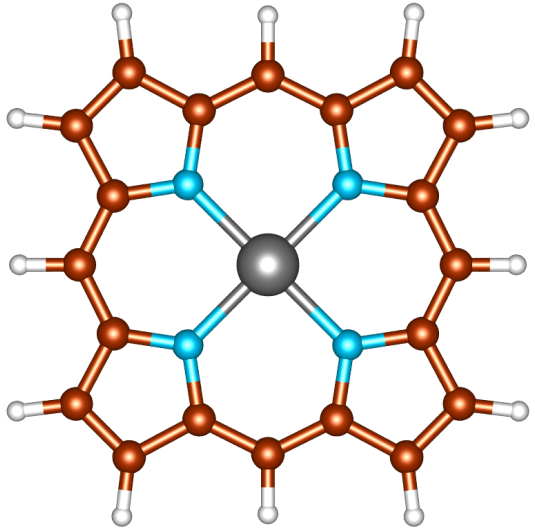
Density Matrix Renormalization Group with **Dynamical Correlation via Adiabatic Connection**

$$E = E^{\mathrm{DMRG}} + E^{\mathrm{AC}}_{\mathrm{corr}}$$

MOLMPS

GAMMCOR

1,2-RDMs



P. Beran et al., J. Chem. Theory Comput., 17, 7575 (2021)

GAMMCOR

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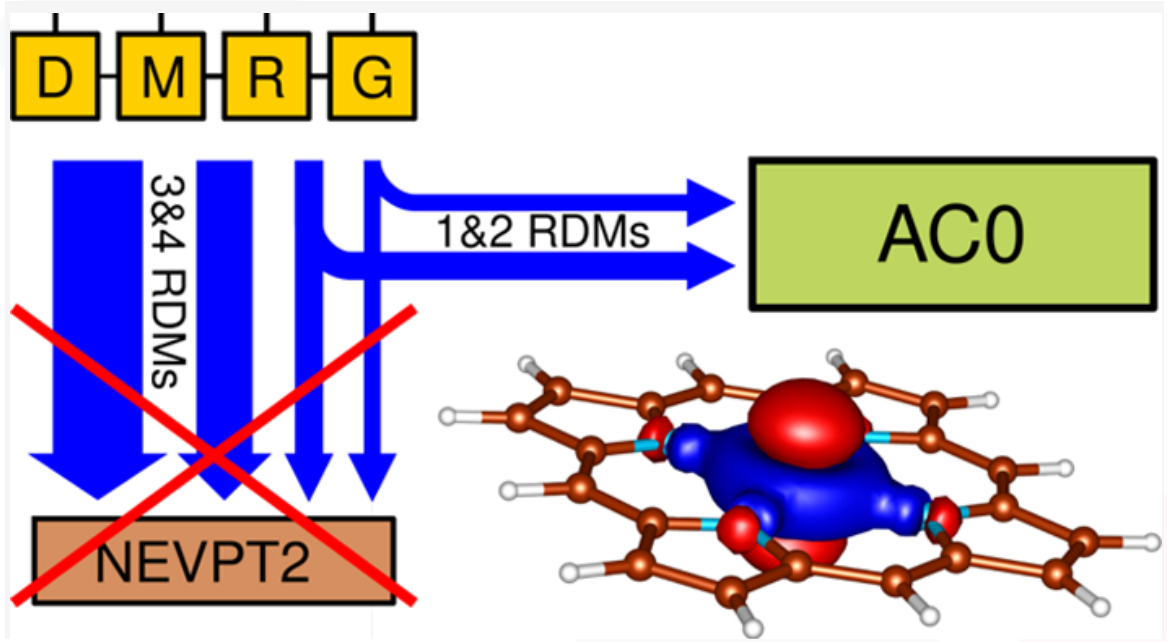

Fe(II)-porphyrin

Quintet-Triplet energy gap

40 active electrons in 42 orbitals

Wall Time of AC0 calc.: ~10^3 sec.

P. Beran et al., J. Chem. Theory Comput., 17, 7575 (2021)