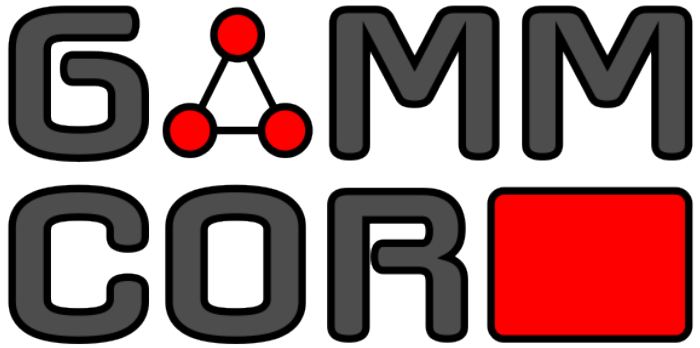
GammCor: electron correlation and molecular interaction calculations

Authors: K. Pernal[1], M. Hapka[2], M. Modrzejewski[2], M. Przybytek[2]

[1]Lodz University of Technology, Poland

[2]University of Warsaw, Poland



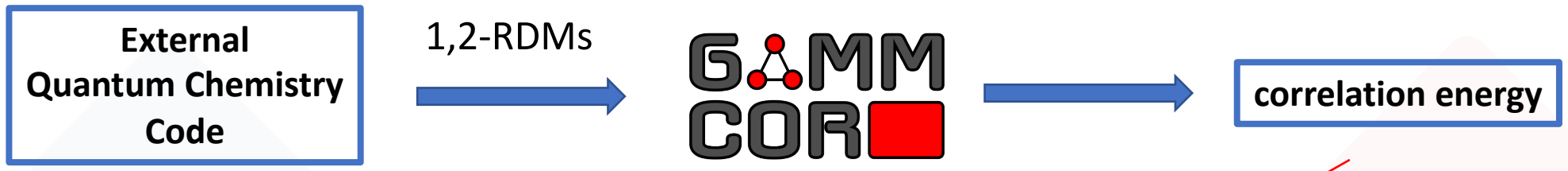
https://github.com/pernalk/GAMMCOR

All methods implemented in GammCor rely on one- and two-electron reduced density matrices

Interfaced with: Molpro, Dalton, Quantum Package, Orca

Compatible with **TREXIO** library

Electron correlation energy from GammCor



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

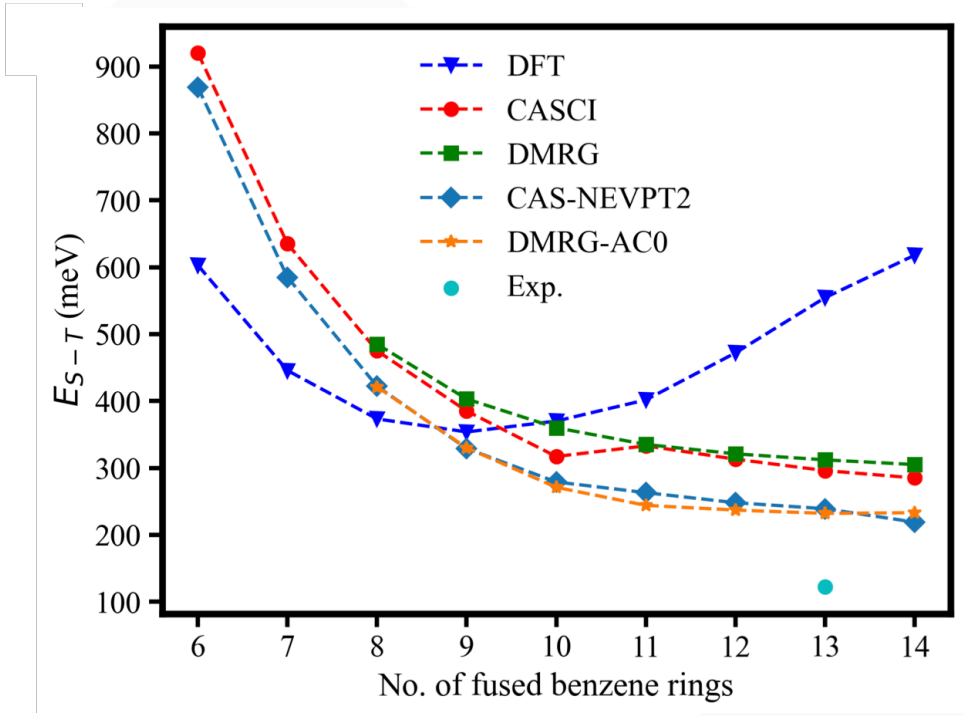
unique feature: dynamic correlation energy using adiabatic connection method is applicable to more than 50 active orbitals (basis set size limit is over 1000)

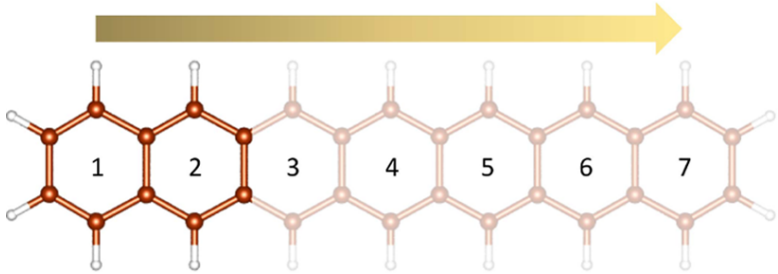
recent development: Cholesky-decomposed two-electron integrals on-the-fly

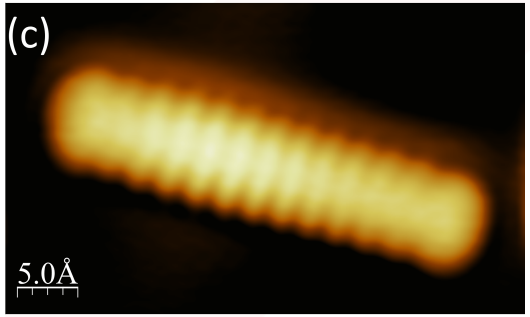
P. Beran et al., J. Chem. Theory Comput., 17, 7575 (2021)

State-of-the-art calculations with GammCor

Calculations for the ST gaps for polyacenes up to n=14 fused benzene rings : 58 electrons in 58 π orbitals





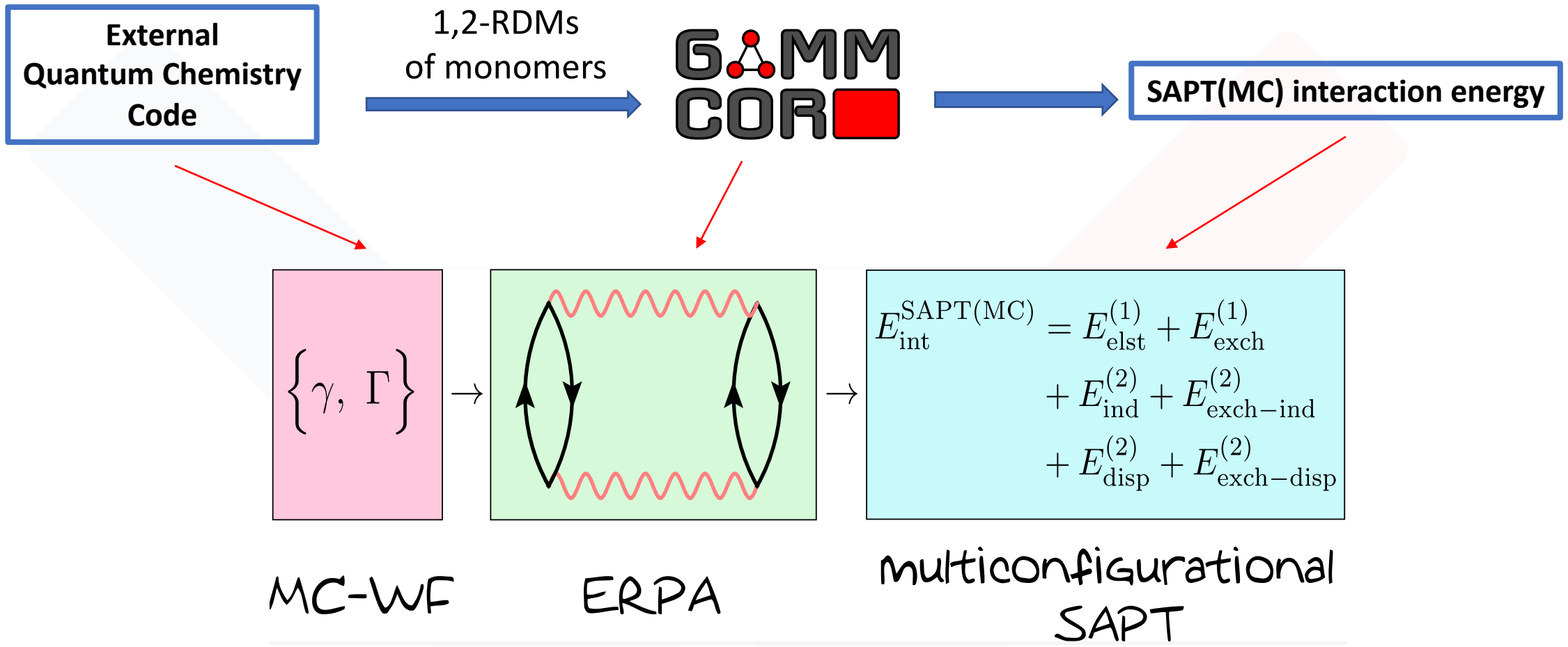


On-surface synthesized tridecacene

First experimental proof of open-shell biradical character of a long polyacene (tridecacene).

Zuzak et al., Angew. Chem. Int. Ed. 2024, 63, e202317091

Molecular interactions with GammCor



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

Molecular interactions with GammCor

unique features:

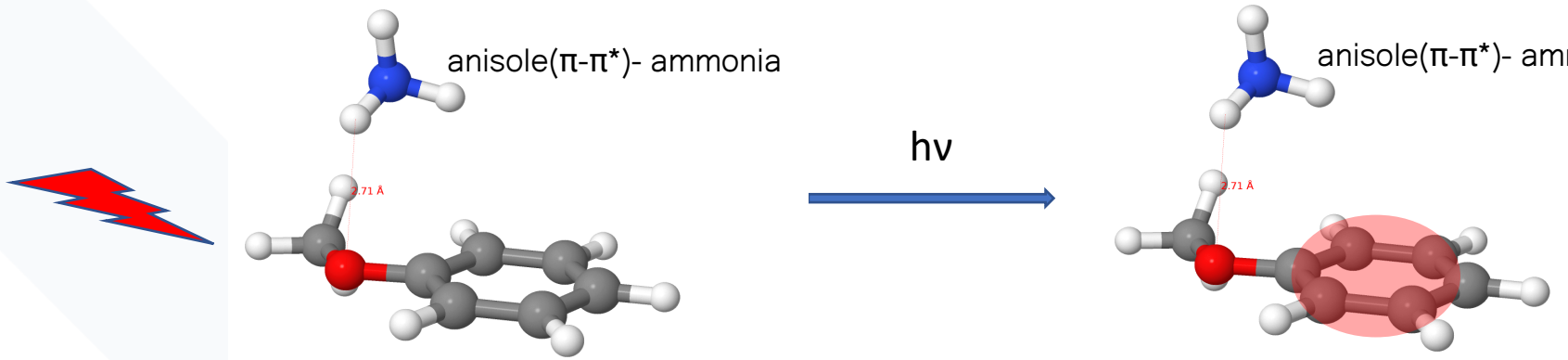
- only 1,2-RDMs from wavefunction calculations are needed;
- applicable to electronically excited systems (local excitons), open-shell molecules, and molecules out of equilibrium geometries

recent developments:

- Cholesky-decomposed two-electron integrals on-the-fly
- Reduced-scaling algorithm for dispersion energy

Hapka et al., J. Phys. Chem. Lett. 14, 6895 (2023)

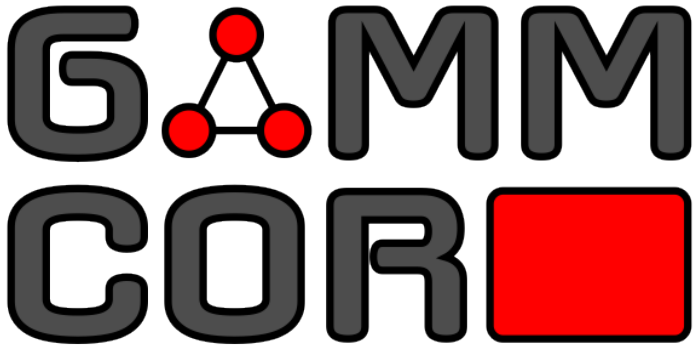
Interaction energy in molecular complexes with localized excitons



Interaction energy increases after excitation due to electrostatic, dispersion, and induction effects.

SAPT(MC) in GammCor: 1226 basis set functions.

Wavefunctions for monomers: CASSCF.



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Installation guide and user manual available at:

https://qchem.gitlab.io/gammcor-manual/