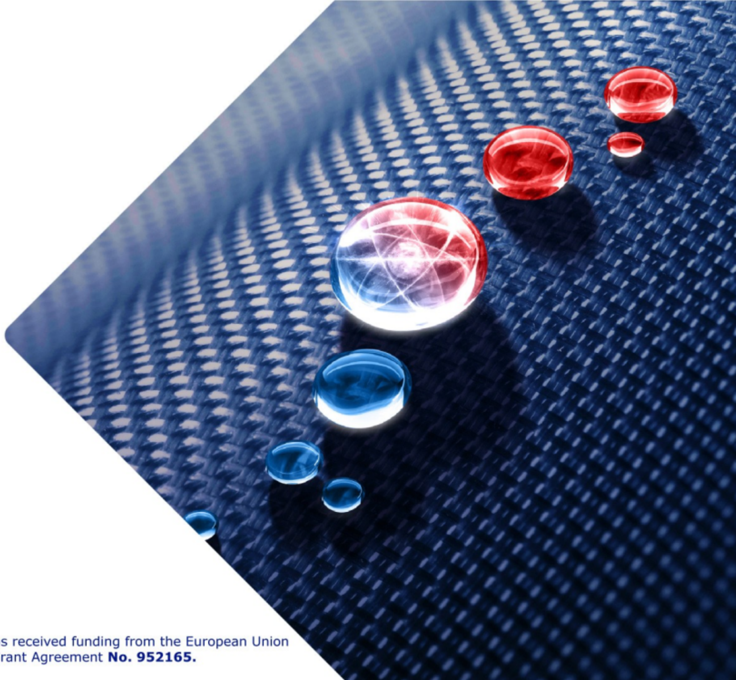
Targeting Real chemical accuracy at the EXascale

Multiconfigurational Symmetry-Adapted Perturbation Theory

Michał Hapka, Kasia Pernal

April 19, 2023



Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

Noncovalent interactions

- physicochemical properties of noncovalent complexes, clusters, and condensed molecular matter
- thermodynamics of nonideal gases
- outcomes of reactive/nonreactive collisions
- IR spectra of molecular clusters

Interaction energy

$$E_{int} = E_{AB} - E_A - E_B$$

- internal coordinates of the monomers A and B used in the calculations of E_A and E_B are the same as within the dimer AB

Molecular Interactions

Interaction energy for weakly interacting subsystems A and B

- Supermolecular approach

$$E_{int} = E_{AB} - E_A - E_B$$

Molecular Interactions

Interaction energy for weakly interacting subsystems A and B

- Supermolecular approach

$$E_{int} = E_{AB} - E_A - E_B$$

- Perturbation-theory approach: expansion in orders of the interaction potential

$$E_{int} = E^{(1)} + E^{(2)} + \ldots$$

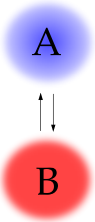
  - E_{int} obtained directly, in a perturbative manner
  - based on monomer properties
  - partitioned into well-defined energy contributions
  - free of basis-set superposition error (BSSE)

Perturbation Theory

$$\hat{H} = \underbrace{\hat{H}_A + \hat{H}_B}_{\hat{H}_0} + \hat{V}$$

$$\hat{V} = \sum_{i \in A} \sum_{k \in B} \frac{1}{r_{ik}} - \sum_{i \in A} \sum_{\beta \in B} \frac{Z_\beta}{|\mathbf{r}_i - \mathbf{R}_\beta|} - \sum_{k \in B} \sum_{\alpha \in A} \frac{Z_\alpha}{|\mathbf{r}_k - \mathbf{R}_\alpha|} + \sum_{\alpha \in A} \sum_{\beta \in B} \frac{Z_\alpha Z_\beta}{R_{\alpha\beta}}$$

- $\hat{V}$ treated as perturbation



$$\Phi_0 = \Phi_A \Phi_B$$

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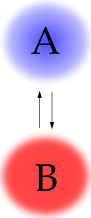

$$\Phi_0 = \Phi_A \Phi_B$$

- Φ_0 violates Pauli principle

Rayleigh-Schrödinger Perturbation Theory

$$E_{\text{int}} = E_{\text{RS}}^{(1)} + E_{\text{RS}}^{(2)} + \dots$$

$$E_{\text{RS}}^{(k)} = \langle \Phi_0 | \hat{V} \Phi_{\text{RS}}^{(k-1)} \rangle$$

- the RS series either diverges or converges too slowly
- in systems containing atoms other than hydrogen and helium, RS diverges
    - even the lowest energy physical states are buried in a continuum of unbound, unphysical states

P. Claverie, Int. J. Quantum Chem. 5 273 (1970); W. H. Adams Int. J. Quantum Chem. S24 531 (1990)

Rayleigh-Schrödinger PT: LiH example

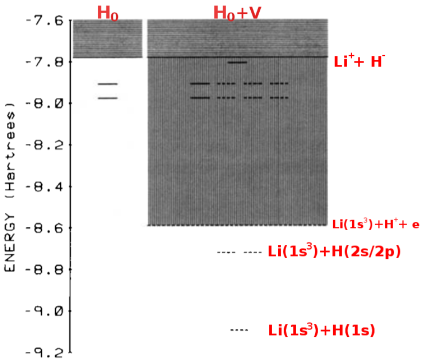

Figure 2. Energy level diagram showing selected eigenvalues of $\hat{H}^0$ and $\hat{H}^0 + \hat{V}$ for $^1\Sigma^+$ States of LiH at $R = \infty$. The closely spaced vertical lines represent the unphysical continuum. The other conventions are explained in the caption to Figure 1. The two lowest energy, unphysical levels of $\hat{H}^0 + \hat{V}$ are also represented on the right. The single physical state just below the continuum correlates with no state of $\hat{H}^0$.

W. H. Adams *Int. J. Quantum Chem.* S24 531 (1990)

Rayleigh-Schrödinger PT: LiH example

- Electrons assigned initially to the system A can fall into the Coulomb wells of the system B by means of the strong nucleus-electron attraction, ejecting some other electrons into the continuum

Interaction operator $\hat{V}$

$$\hat{V} = -\sum_{i\in A}\sum_{\beta\in B}\frac{Z_\beta}{r_{i\beta}} - \sum_{k\in B}\sum_{\alpha\in A}\frac{Z_\alpha}{r_{k\alpha}} + \sum_{i\in A}\sum_{k\in B}\frac{1}{r_{ik}} + \sum_{\alpha\in A}\sum_{\beta\in B}\frac{Z_\alpha Z_\beta}{R_{\alpha\beta}}$$

Symmetry-adapted Perturbation Theory

Key idea behind SAPT

- replace $\Phi_A \Phi_B \rightarrow \hat{A}(\Phi_A \Phi_B)$

Symmetrized Rayleigh-Schrödinger Theory (SRS)

$$E_{\mathrm{RS}}^{(k)} = \langle \Phi_0 | \hat{V} \Phi_{\mathrm{RS}}^{(k-1)} \rangle$$

$$E_{\mathrm{SRS}}^{(k)} = \frac{\langle \Phi_0 | \hat{V} \mathcal{A} \Phi_{\mathrm{RS}}^{(k-1)} \rangle}{\langle \Phi_0 | \mathcal{A} \Phi_{\mathrm{RS}}^{(k-1)} \rangle}$$

Symmetry-adapted Perturbation Theory

- **SRS**: B. Jeziorski, K. Szalewicz, G. Chałasiński, *Int. J. Quant. Chem.*, **14**, 271 (1978)

- **HS**: J. O. Hirschfelder, R. Silbey, *J. Chem. Phys.*, **45**, 2188, (1966)
- **MSMA**: J. N. Murrell, G. Shaw, *J. Chem. Phys.*, **46** 1768 (1967); J. I. Musher, A. T. Amos, *Phys. Rev.*, **164**, 31, (1967)
- **ELHAV**: R. Eisenschitz, F. London, *Z. Phys.* **60**, 491, (1930); J. Hirschfelder, *Chem. Phys. Lett.* **1** 363 (1967); A. van der Avoird, *J. Chem. Phys.* **47** 3649 (1967)
- **JK**: B. Jeziorski, W. Kołos, *Int. J. Quant. Chem.*, **12-S1**, 91, (1977)

Symmetry-adapted Perturbation Theory

- **SRS**: B. Jeziorski, K. Szalewicz, G. Chałasiński, *Int. J. Quant. Chem.*, **14**, 271 (1978)
  - **SRS** is the only SAPT vartiant applicable to many-electron systems
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Symmetry-adapted Perturbation Theory

Advantages of SRS

- dramatic improvement of low-order interaction energies
  - accounts for electron exchange: tunnelling of electrons between monomers
- correct asymptotic behavior through all orders
- clear physical interpretation of low-order energy corrections

Interaction energy decomposition in SRS

$$E^{(k)}_{\mathrm{SRS}} = E^{(k)}_{\mathrm{RS}} + E^{(k)}_{\mathrm{exch}}$$

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Interaction energy decomposition in SAPT

$$E^{(k)}_{\mathrm{SAPT}} = E^{(k)}_{\mathrm{RS}} + E^{(k)}_{\mathrm{exch}}$$

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Interaction energy decomposition in SAPT

$$\begin{aligned} E_{\text{int}}^{\text{SAPT}} = {} & E_{\text{elst}}^{(1)} + E_{\text{exch}}^{(1)} \\ & + E_{\text{ind}}^{(2)} + E_{\text{exch-ind}}^{(2)} + E_{\text{disp}}^{(2)} + E_{\text{exch-disp}}^{(2)} \end{aligned}$$

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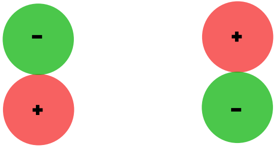
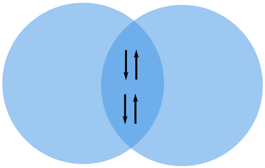
$$E_{\mathrm{int}}^{\mathrm{SAPT}} = E_{\mathrm{elst}}^{(1)} + E_{\mathrm{exch}}^{(1)} + E_{\mathrm{ind}}^{(2)} + E_{\mathrm{exch-ind}}^{(2)} + E_{\mathrm{disp}}^{(2)} + E_{\mathrm{exch-disp}}^{(2)}$$



$$E_{\mathrm{elst}}^{(1)} = \int\int \frac{\rho_A(\mathrm{r}_1)\rho_B(\mathrm{r}_2)}{|\mathrm{r}_1 - \mathrm{r}_2|}\mathrm{d}\mathrm{r}_1\mathrm{d}\mathrm{r}_2$$

- represents the energy of electrostatic (Coulombic) interaction of the monomer’s charge distributions

$$E_{\rm int}^{\rm SAPT} = E_{\rm elst}^{(1)} + E_{\rm exch}^{(1)} + E_{\rm ind}^{(2)} + E_{\rm exch-ind}^{(2)} + E_{\rm disp}^{(2)} + E_{\rm exch-disp}^{(2)}$$



$$E^{(1)} = \frac{\langle \Phi_0 | \hat{V} \hat{\mathcal{A}} \Phi_0 \rangle}{\langle \hat{\mathcal{A}} \Phi_0 | \hat{\mathcal{A}} \Phi_0 \rangle}$$

$$E_{\rm exch}^{(1)} = E^{(1)} - E_{\rm elst}^{(1)}$$

- energetic effect due to Pauli repulsion

$$E_{\mathrm{int}}^{\mathrm{SAPT}} = E_{\mathrm{elst}}^{(1)} + E_{\mathrm{exch}}^{(1)} + E_{\mathrm{ind}}^{(2)} + E_{\mathrm{exch-ind}}^{(2)} + E_{\mathrm{disp}}^{(2)} + E_{\mathrm{exch-disp}}^{(2)}$$

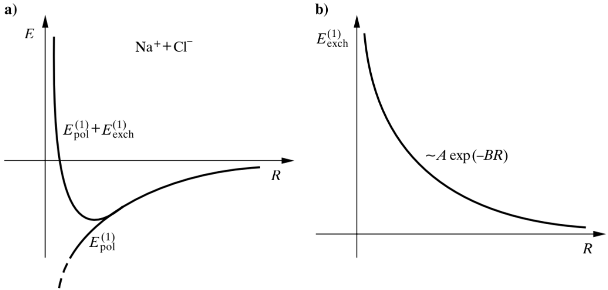
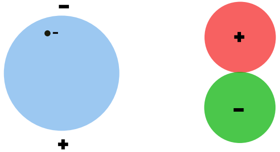


Fig. 13.9. Interaction energy of Na^+ and Cl^-. The polarization approximation gives an absurdity for small separations: the subsystems attract very strongly (mainly because of the electrostatic interaction), while they have had to repel very strongly. The absurdity is removed when the valence repulsion is taken into account (a). Fig. (b) shows the valence repulsion alone modelled by the term $A\exp(-BR)$, where A and B are positive constants.

L. Piela *Ideas of Quantum Chemistry* (2007)

$$E^{\mathrm{SAPT}}_{\mathrm{int}} = E^{(1)}_{\mathrm{elst}} + E^{(1)}_{\mathrm{exch}} + E^{(2)}_{\mathrm{ind}} + E^{(2)}_{\mathrm{exch-ind}} + E^{(2)}_{\mathrm{disp}} + E^{(2)}_{\mathrm{exch-disp}}$$



- electrostatic potential of unperturbed monomer B modifies the wave function of monomer A
- $E^{(2)}_{\mathrm{ind}}$: energetic effect of mutual polarization of the monomers by the field of their interacting partner

$$E_{\mathrm{int}}^{\mathrm{SAPT}} = E_{\mathrm{elst}}^{(1)} + E_{\mathrm{exch}}^{(1)} + E_{\mathrm{ind}}^{(2)} + E_{\mathrm{exch-ind}}^{(2)} + E_{\mathrm{disp}}^{(2)} + E_{\mathrm{exch-disp}}^{(2)}$$

- correlation of instantaneous multipole moments of the monomers (intermolecular, stabilizing effect)

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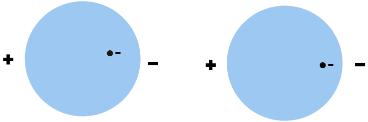

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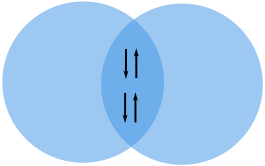

$$E_{\mathrm{exch}}^{(2)} = E_{\mathrm{exch-ind}}^{(2)} + E_{\mathrm{exch-disp}}^{(2)}$$

- $E_{\mathrm{exch-ind}}^{(2)}$ dampens a major part of $E_{\mathrm{ind}}^{(2)}$
- $E_{\mathrm{exch-disp}}^{(2)}$ dampens a few percent of $E_{\mathrm{disp}}^{(2)}$

$E_{\mathrm{int}}^{\mathrm{SAPT}} = E_{\mathrm{elst}}^{(1)} + E_{\mathrm{exch}}^{(1)} + E_{\mathrm{ind}}^{(2)} + E_{\mathrm{exch-ind}}^{(2)} + E_{\mathrm{disp}}^{(2)} + E_{\mathrm{exch-disp}}^{(2)}$

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- $E_{\mathrm{exch-disp}}^{(2)}$ dampens a few percent of $E_{\mathrm{disp}}^{(2)}$

Example: benzene dimer (kcal/mol)

aug-cc-pVDZ	S	T
$E_{\mathrm{ind}}^{(2)}$	-1.84	-1.36
$E_{\mathrm{exch-ind}}^{(2)}$	1.69	1.13
$E_{\mathrm{disp}}^{(2)}$	-6.26	-4.60
$E_{\mathrm{exch-disp}}^{(2)}$	0.88	0.61

A. Hesselmann, G. Jansen, M. Schütz, *J. Chem. Phys.* **122** (2005)

SAPT

$$E_{\text{int}}^{\text{SAPT}} = E_{\text{elst}}^{(1)} + E_{\text{exch}}^{(1)} + E_{\text{ind}}^{(2)} + E_{\text{exch-ind}}^{(2)} + E_{\text{disp}}^{(2)} + E_{\text{exch-disp}}^{(2)}$$

Advantages of SAPT

- Van der Waals minimum: accurate to within few percent
- many flavors of SAPT
    - different approaches to recover correlation within monomers
    - SAPT(CCSD), SAPT(DFT), SAPT0, SAPT2, SAPT-F12, ...

SAPT

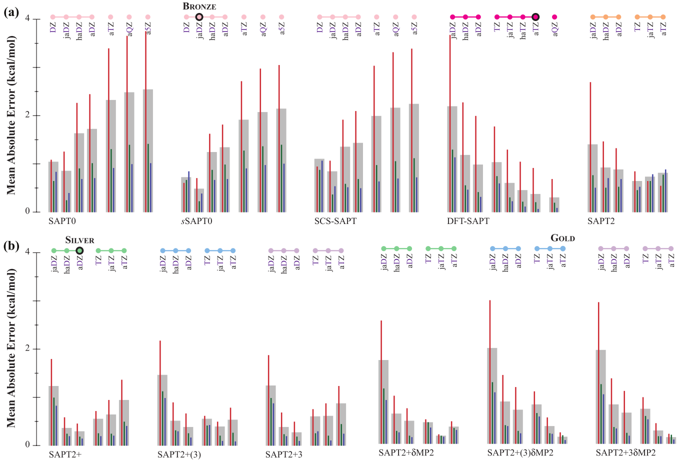


FIG. 2. Performance of SAPT methods. For each technique considered among (a) zeroth- and second-order truncations, (b) higher, triples-including truncations, and (c) higher truncations with δMP2 corrections, the MAE averaged over four databases is plotted (gray) for smaller to larger basis sets. Subset MAE values are shown as inset bars for hydrogen-bonding (red), mixed-influence (green), and dispersion-dominated (blue) NCI motifs. Colored circles correspond to computational cost traces in Fig. 3, and black-bordered colored circles indicate Pauling points[44] in SAPT theory.

T. M. Parker et al. JCP 140, 094106 (2014)

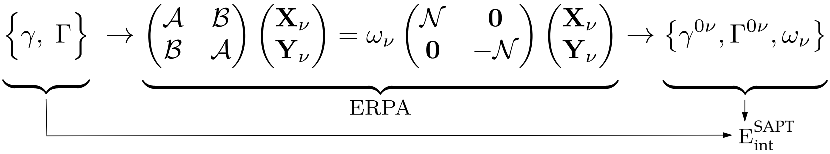
Multiconfigurational SAPT

Motivation

- existing SAPT formulations based on single-reference treatment of the monomers
- lack of formalism for systems described with multireference wavefunctions
    - interactions between excited-state molecules
    - out-of-equilibrium geometries
    - transition-metal complexes
    - ...

M. Hapka, M. Przybytek, K. Pernal, J. Chem. Theory Comput., 17, 5538 (2021)

Multiconfigurational SAPT



$$\underbrace{\left\{\gamma,\ \Gamma\right\}} \rightarrow \underbrace{\begin{pmatrix}\mathcal{A} & \mathcal{B}\\ \mathcal{B} & \mathcal{A}\end{pmatrix}\begin{pmatrix}\mathbf{X}_\nu\\ \mathbf{Y}_\nu\end{pmatrix} = \omega_\nu\begin{pmatrix}\mathcal{N} & \mathbf{0}\\ \mathbf{0} & -\mathcal{N}\end{pmatrix}\begin{pmatrix}\mathbf{X}_\nu\\ \mathbf{Y}_\nu\end{pmatrix}}_{\text{ERPA}} \rightarrow \underbrace{\{\gamma^{0\nu},\Gamma^{0\nu},\omega_\nu\}}$$

$$\mathrm{E}_{\text{int}}^{\text{SAPT}}$$

- takes as input one- and two-particle reduced density matrices (γ, Γ) of the monomers
- based on response properties from extended random phase approximation (ERPA)
- general: may be applied with any MC wavefunction (CAS, GVB-PP, DMRG, **CIPSI**, ...)

ERPA: K. Chatterjee, K. Pernal, *J. Chem. Phys.* 137 (2012)

Multiconfigurational SAPT

$$\underbrace{\left\{\gamma,\ \Gamma\right\}} \rightarrow \underbrace{\begin{pmatrix}\mathcal{A} & \mathcal{B}\\ \mathcal{B} & \mathcal{A}\end{pmatrix}\begin{pmatrix}\mathbf{X}_\nu\\ \mathbf{Y}_\nu\end{pmatrix} = \omega_\nu \begin{pmatrix}\mathcal{N} & \mathbf{0}\\ \mathbf{0} & -\mathcal{N}\end{pmatrix}\begin{pmatrix}\mathbf{X}_\nu\\ \mathbf{Y}_\nu\end{pmatrix}}_{\text{ERPA}} \rightarrow \underbrace{\{\gamma^{0\nu},\Gamma^{0\nu},\omega_\nu\}}$$

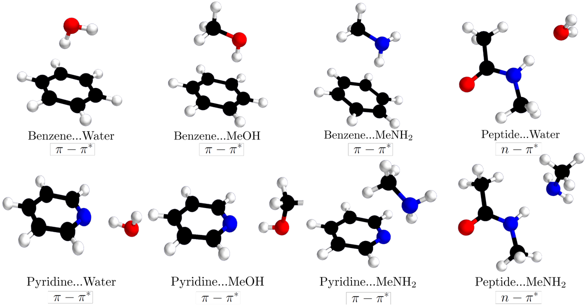
$$\downarrow$$

$$\mathrm{E}_{\text{int}}^{\text{SAPT}}$$

- valid for ground and excited states (singlet and high-spin states)
- N^6 scaling with system size ($n_{\mathrm{OCC}}^3 n_{\mathrm{SEC}}^3$)
  - N^5 algorithm for $E_{\mathrm{disp}}^{(2)}$

M. Hapka, M. Przybytek, K. Pernal, JCTC, 15, 6712 (2019), 17, 5538 (2021)

Example: excited-state complexes



Benzene...Water $\pi - \pi^*$

Benzene...MeOH $\pi - \pi^*$

Benzene...$MeNH_2$ $\pi - \pi^*$

Peptide...Water $n - \pi^*$

Pyridine...Water $\pi - \pi^*$

Pyridine...MeOH $\pi - \pi^*$

Pyridine...$MeNH_2$ $\pi - \pi^*$

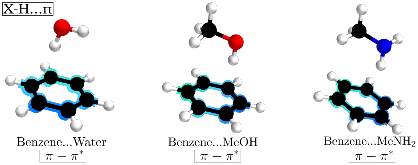
Peptide...$MeNH_2$ $n - \pi^*$

- How does E_{int} change upon excitation?

S66: J. Řezáč et al., *J. Chem. Theory Comput.* 7, 2427 (2011)

M. R. Jangrouei et al., *J. Chem. Theory Comput.*, 18(6), 3497-3511 (2022)

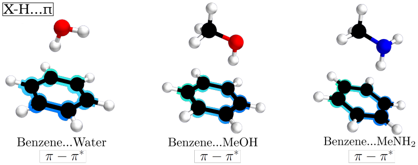
Benzene$\cdots H_2O$, $\cdots$MeOH, $\cdots MeNH_2$



	$E_{es} - E_{gs}$		
	H_2O	MeOH	$MeNH_2$
$\Delta E^{(1)}_{elst}$	0.88	0.98	0.54
$\Delta E^{(1)}_{exch}$	−0.35	−0.45	−0.25
$\Delta E^{(2)}_{ind}$	0.11	0.15	0.08
$\Delta E^{(2)}_{exch-ind}$	−0.05	−0.08	−0.03
$\Delta E^{(2)}_{disp}$	0.17	0.24	0.22
$\Delta E^{(2)}_{exch-disp}$	−0.05	−0.07	−0.05
ΔE^{SAPT}_{int}	0.72	0.77	0.50

🟩 - stabilization 🟥 + destab. kcal/mol

Benzene$\cdots H_2O$, $\cdots$MeOH, $\cdots MeNH_2$



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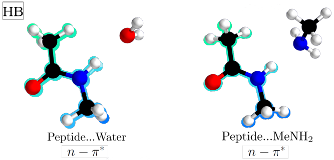
$\Delta E^{(2)}_{ind}$	0.11	0.15	0.08
$\Delta E^{(2)}_{exch-ind}$	-0.05	-0.08	-0.03
$\Delta E^{(2)}_{disp}$	0.17	0.24	0.22
$\Delta E^{(2)}_{exch-disp}$	-0.05	-0.07	-0.05
ΔE^{SAPT}_{int}	0.72	0.77	0.50

- stabilization + destab. kcal/mol

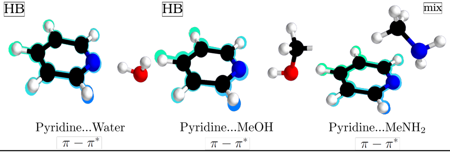
Peptide$\cdots$ H_2O, $\cdots$ $MeNH_2$



	$E_{es} - E_{gs}$	
	H_2O	$MeNH_2$
$\Delta E^{(1)}_{elst}$	0.71	0.71
$\Delta E^{(1)}_{exch}$	-0.03	0.05
$\Delta E^{(2)}_{ind}$	0.12	-0.12
$\Delta E^{(2)}_{exch-ind}$	-0.03	0.32
$\Delta E^{(2)}_{disp}$	-0.01	-0.10
$\Delta E^{(2)}_{exch-disp}$	0.01	0.05
ΔE^{SAPT}_{int}	0.77	0.91

🟩 - stabilization	🟥 + destab.	kcal/mol

Pyridine$\cdots H_2O$, $\cdots$MeOH, $\cdots MeNH_2$



Pyridine...Water $\pi - \pi^*$

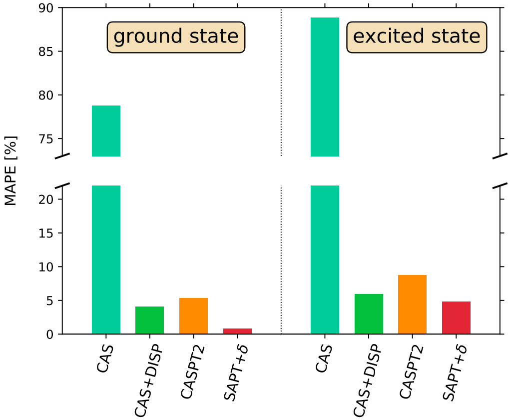
Pyridine...MeOH $\pi - \pi^*$

Pyridine...$MeNH_2$ $\pi - \pi^*$

	$E_{es} - E_{gs}$		
	H_2O	MeOH	$MeNH_2$
$\Delta E^{(1)}_{elst}$	0.04	0.03	0.17
$\Delta E^{(1)}_{exch}$	0.02	0.02	-0.15
$\Delta E^{(2)}_{ind}$	0.02	0.02	0.04
$\Delta E^{(2)}_{exch-ind}$	0.01	0.01	−0.04
$\Delta E^{(2)}_{disp}$	0.02	0.04	0.15
$\Delta E^{(2)}_{exch-disp}$	0.00	0.00	−0.03
ΔE^{SAPT}_{int}	0.03	0.04	0.14

- stabilization   + destab.   kcal/mol

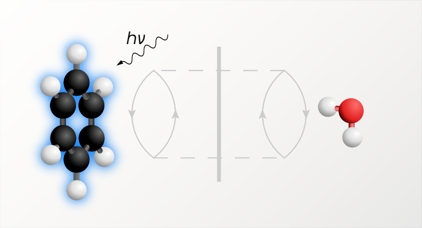
E_{int} for excited-state complexes



- SAPT > CAS+DISP > CASPT2

M. R. Jangrouei et al., *J. Chem. Theory Comput.*, 18(6), 3497-3511 (2022)

Multiconfigurational SAPT



GammCor, `https://github.com/pernalk/GAMMCOR`

Tutorial

- interactions between excited-state molecules
- out-of-equilibrium geometries

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TREX
Targeting Real chemical accuracy at the EXascale

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Thank you for your attention!