Targeting Real chemical accuracy at the EXascale

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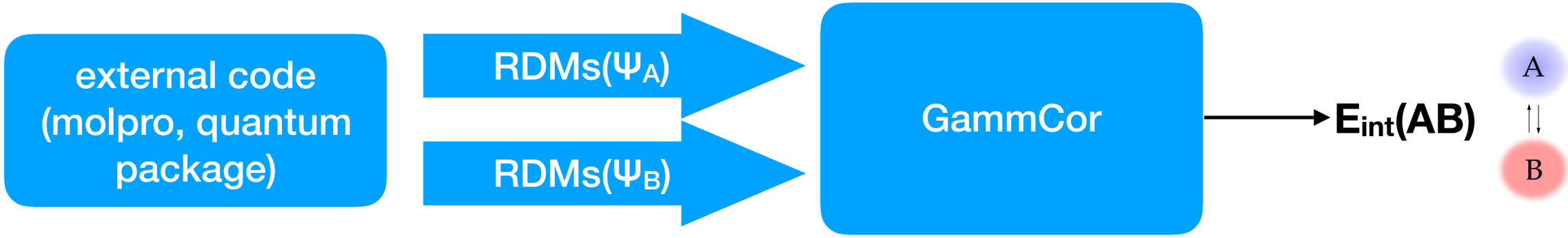
Van der Waals systems: strained and excited

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

Molecular interaction energy calculation with GammCor

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



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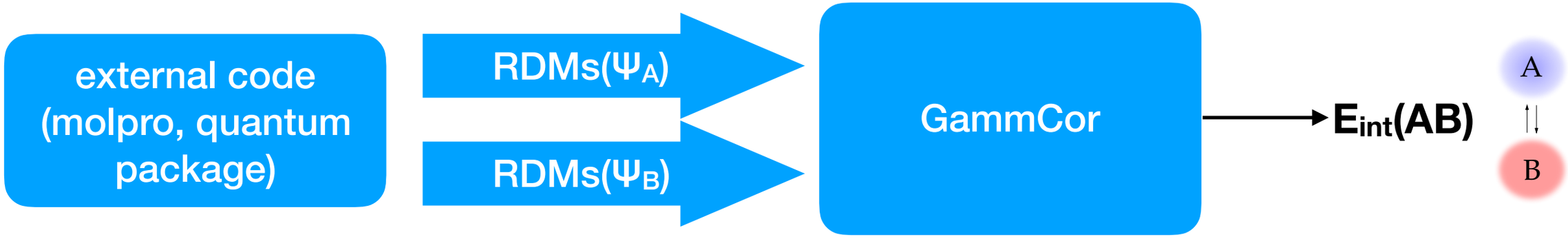


Energy decomposed interaction, e.g. SAPT (symmetry adapted perturbation theory)

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

components of clear physical meaning - give insight into a character of interaction

New algorithms for handling (reading, sorting, transforming) two-electron integrals: savings on scratch space, better efficiency

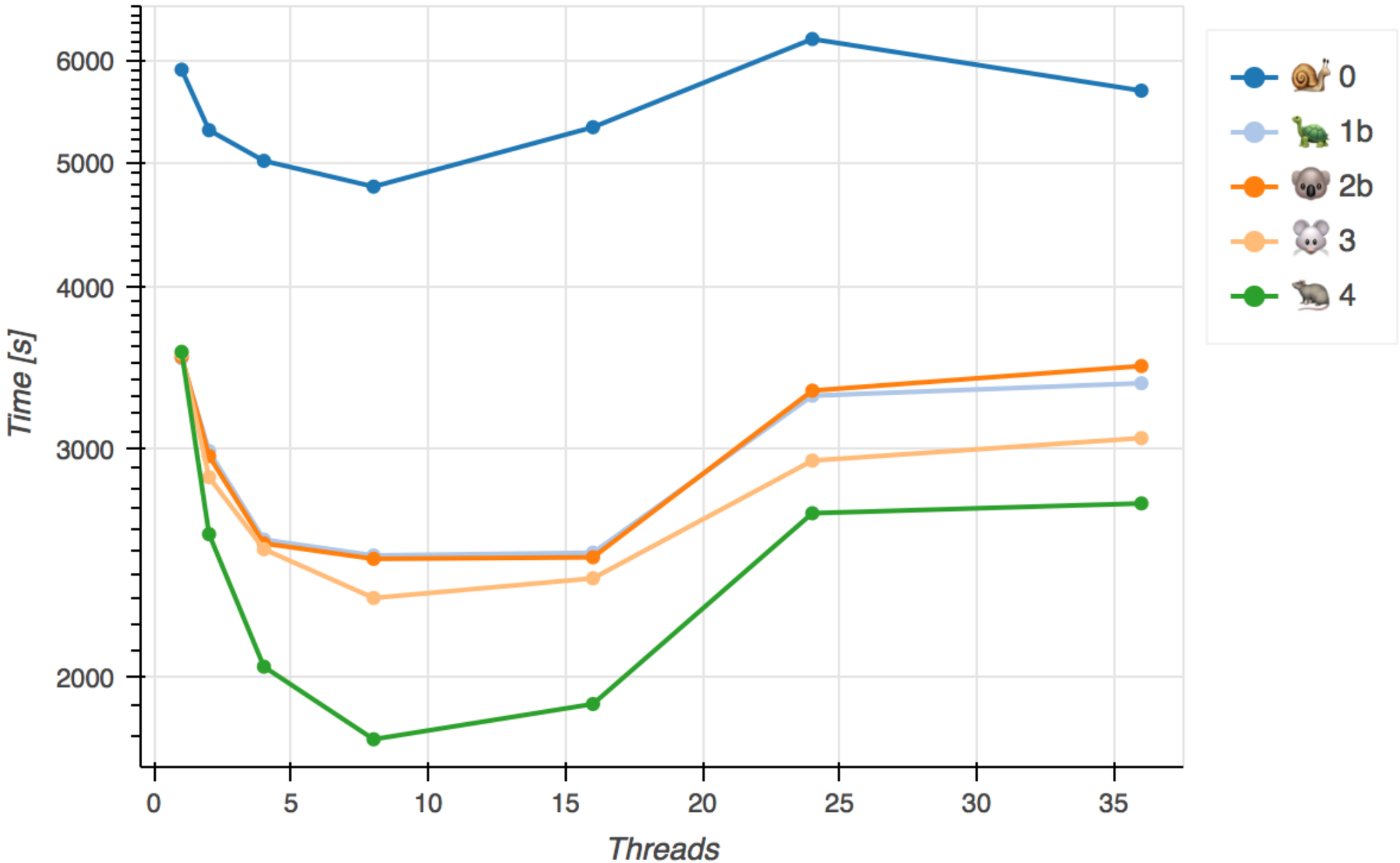
OpenMP directives

OpenMP at the MKL level

Improved vectorization

Computing second-order interaction energy terms: new algorithms based on Cholesky decomposition

LONG 🔵🔵 SAPT: C2H4 Ar, aug-cc-pVQZ, NBasis=428



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Time vs. Thread

Version	1	2	4	8
🐌 0	— 01:38:16	— 01:28:14	— 01:23:33	— 01:19:48
🐢 1b	▼ 00:58:48	▼ 00:49:50	▼ 00:42:34	▼ 00:41:23
🐨 2b	— 00:58:56	— 00:49:24	— 00:42:17	— 00:41:08
🐭 3	— 00:59:16	▼ 00:47:34	— 00:41:51	▼ 00:38:22
🐀 4	— 00:59:28	▼ 00:42:59	▼ 00:33:57	▼ 00:29:50

Dispersion Interactions between Molecules in and out of Equilibrium Geometry:

Visualization and Analysis

THE JOURNAL OF PHYSICAL CHEMISTRY A
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Dispersion Interactions between Molecules in and out of Equilibrium Geometry: Visualization and Analysis

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Piotr H. Kowalski, Agnieszka Krzemińska, Katarzyna Pernal,* and Ewa Pastorczak

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We chose a product of strongly orthogonal geminals as a model (multireference) wavefunction

$$\Psi^{GVB} = \hat{A} \prod_{I=1}^{N/2} \Psi^{I}$$

geminals consist in two orbitals singlet-coupled

$$\Psi^{I}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} \left(c_{I_1} \varphi_{I_1}(\mathbf{r}_1) \varphi_{I_1}(\mathbf{r}_2) + c_{I_2} \varphi_{I_2}(\mathbf{r}_1) \varphi_{I_2}(\mathbf{r}_2) \right) \left(\alpha(\sigma_1) \beta(\sigma_2) - \alpha(\sigma_2) \beta(\sigma_1) \right)$$

GVB orbitals are localized on bonds and lone pairs → intuitive picture, useful for interpretation

Intra-pair correlation → bonds can be broken with GVB

- SAPT(GVB)

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

$$E_{\text{int}}^{\text{SAPT}} = E_{\text{int}}^{\text{SAPT}}(\gamma_{\text{A}}^{\text{GVB}}, \Gamma_{\text{A}}^{\text{GVB}}, \gamma_{\text{B}}^{\text{GVB}}, \Gamma_{\text{B}}^{\text{GVB}})$$

RDMs are computed here from GVB wavefunctions.

- Dispersion energy descriptor

$$D^{AB}(\mathbf{r}) = \frac{1}{2}\left(D^{A}(\mathbf{r}) + D^{B}(\mathbf{r})\right)$$

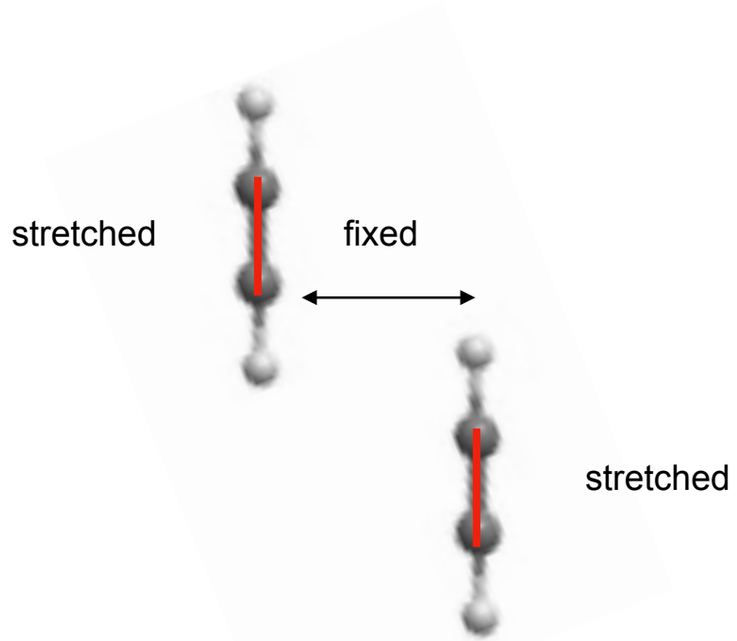
$$\int D^{AB}(\mathbf{r})d\mathbf{r} = E_{disp}^{ERPA}$$

Consistent description of dispersion energy

$$\lim_{R_{AB}\to\infty} E_{disp}^{ERPA} = E_{\text{disp}}^{(2)}$$

Model case: acetylene dimer

Actetylene dimer, $(C_2H_2)_2$ with C-C bond stretched in both monomers.
Inter-monomer distance is kept constant



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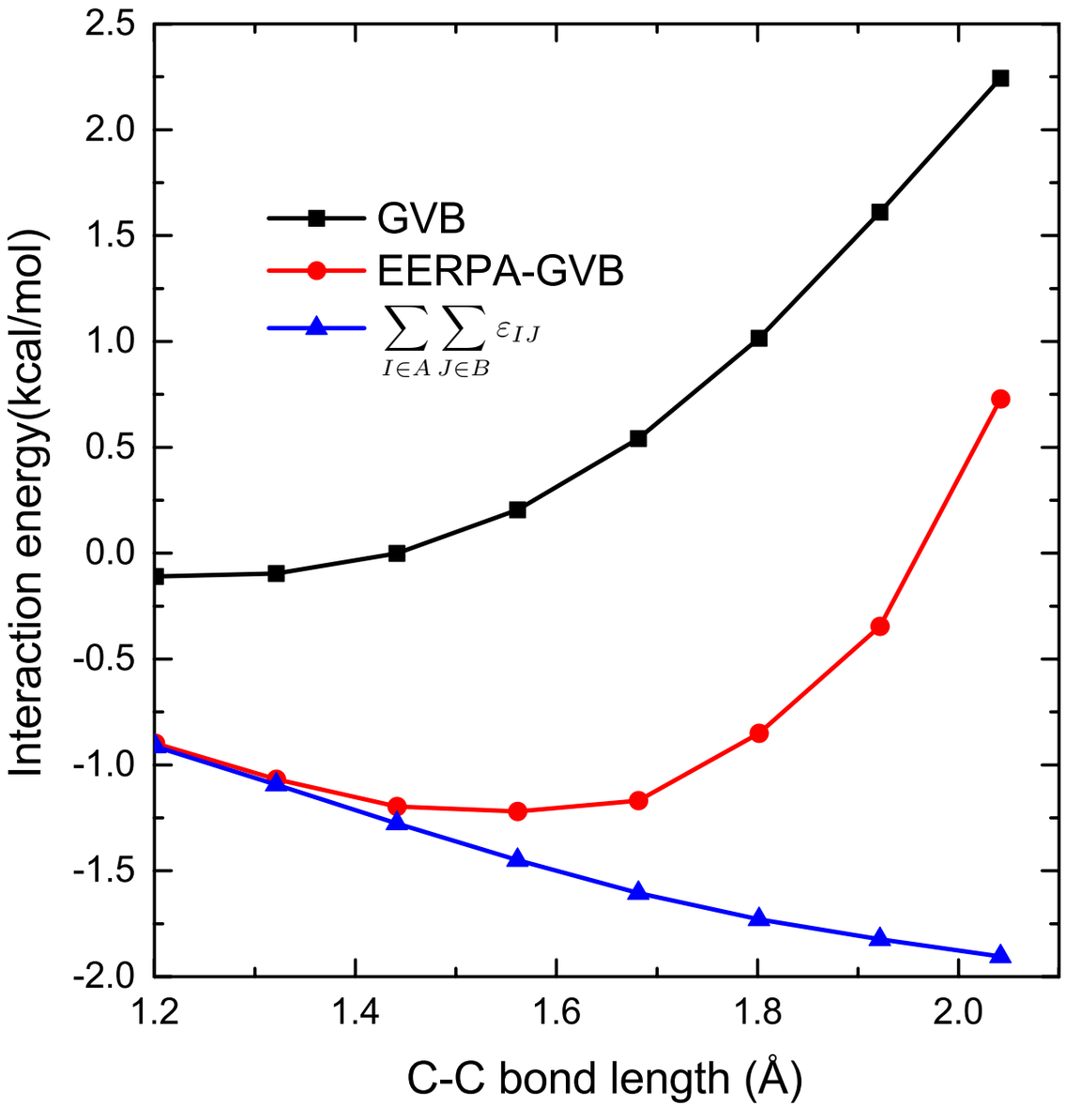

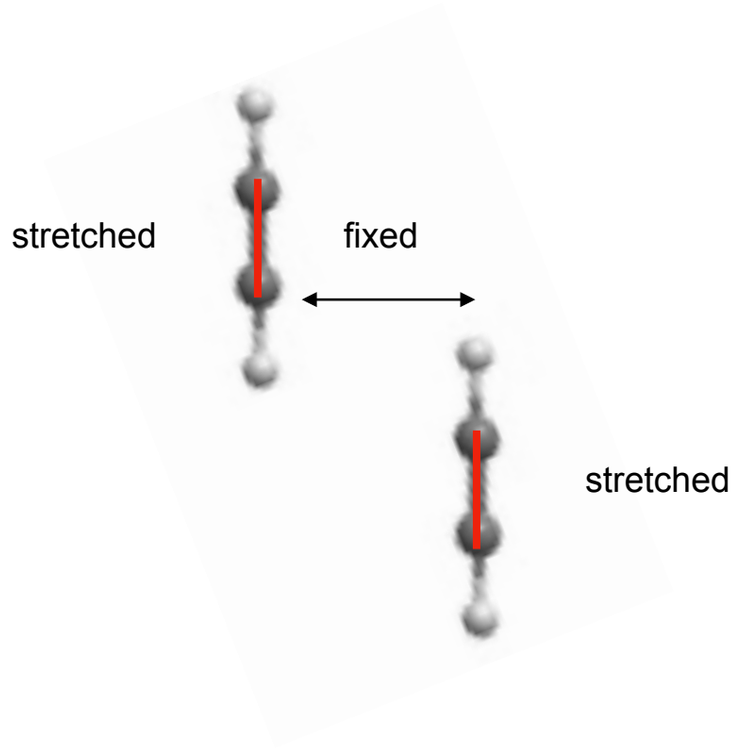

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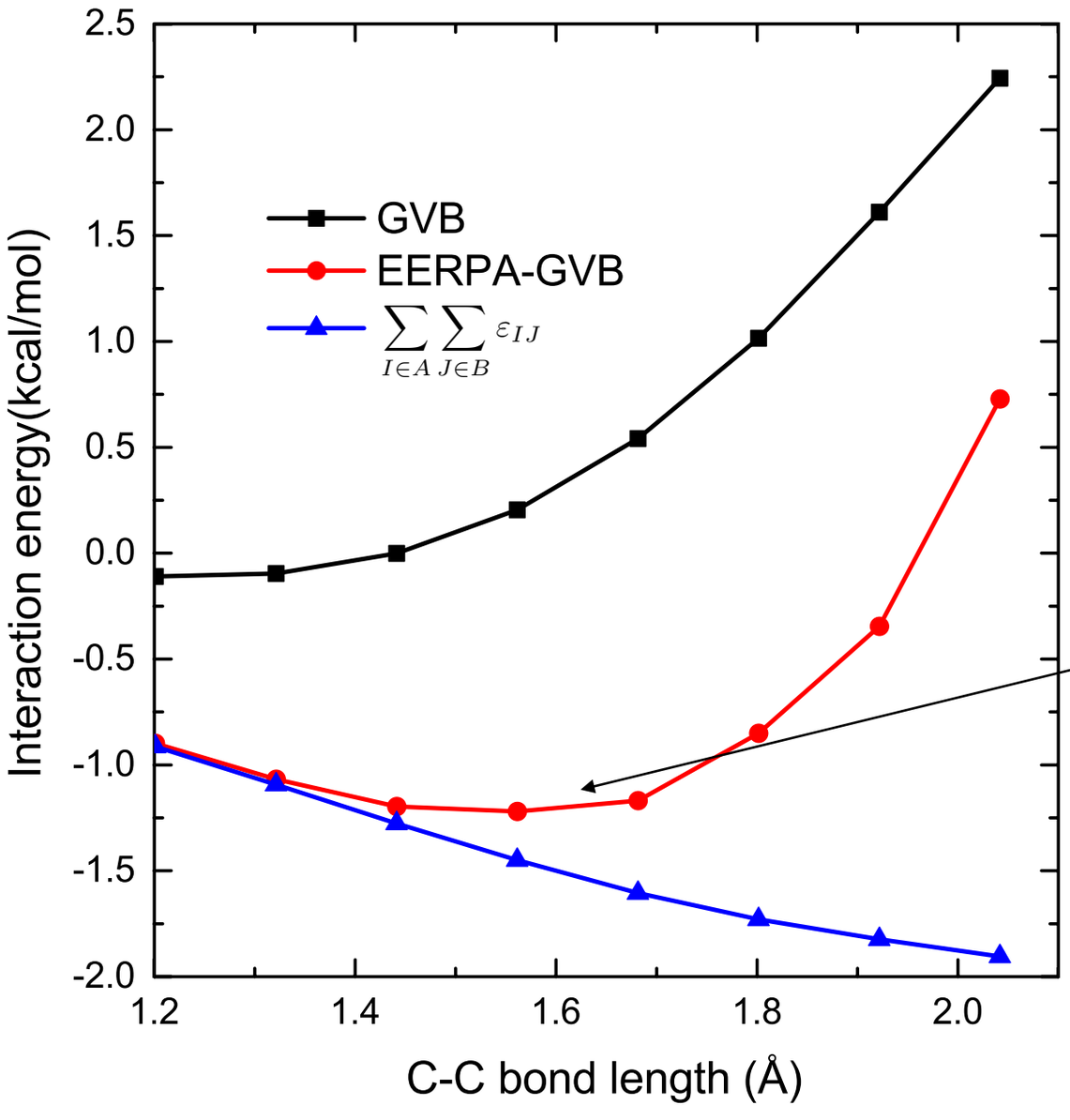

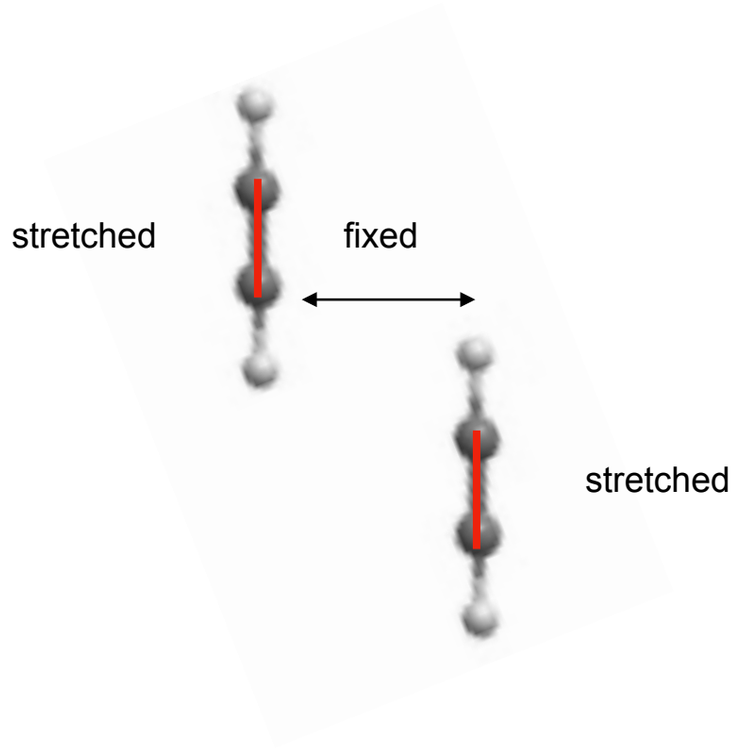

when bonds are stretched, interaction energy passes through the minimum

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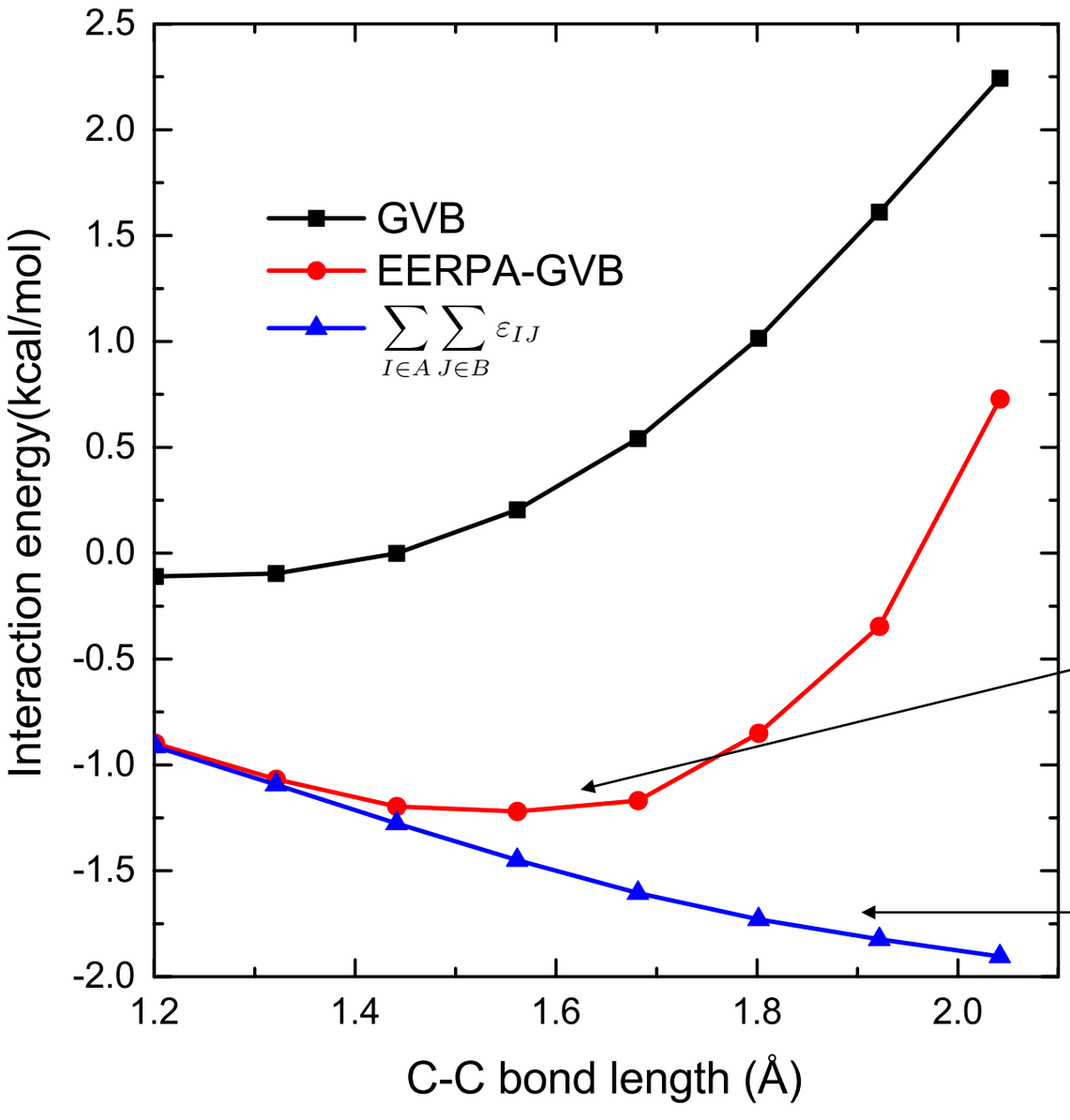
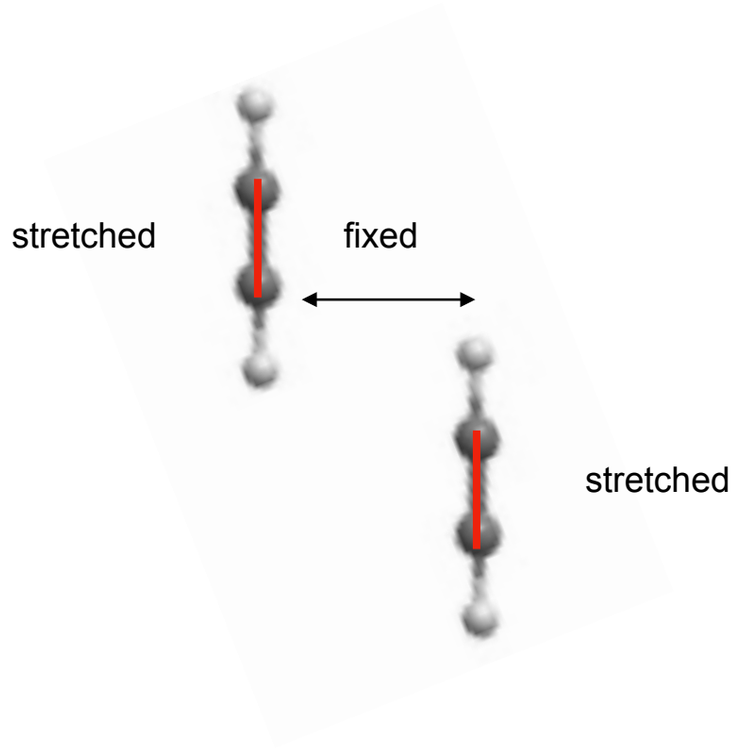
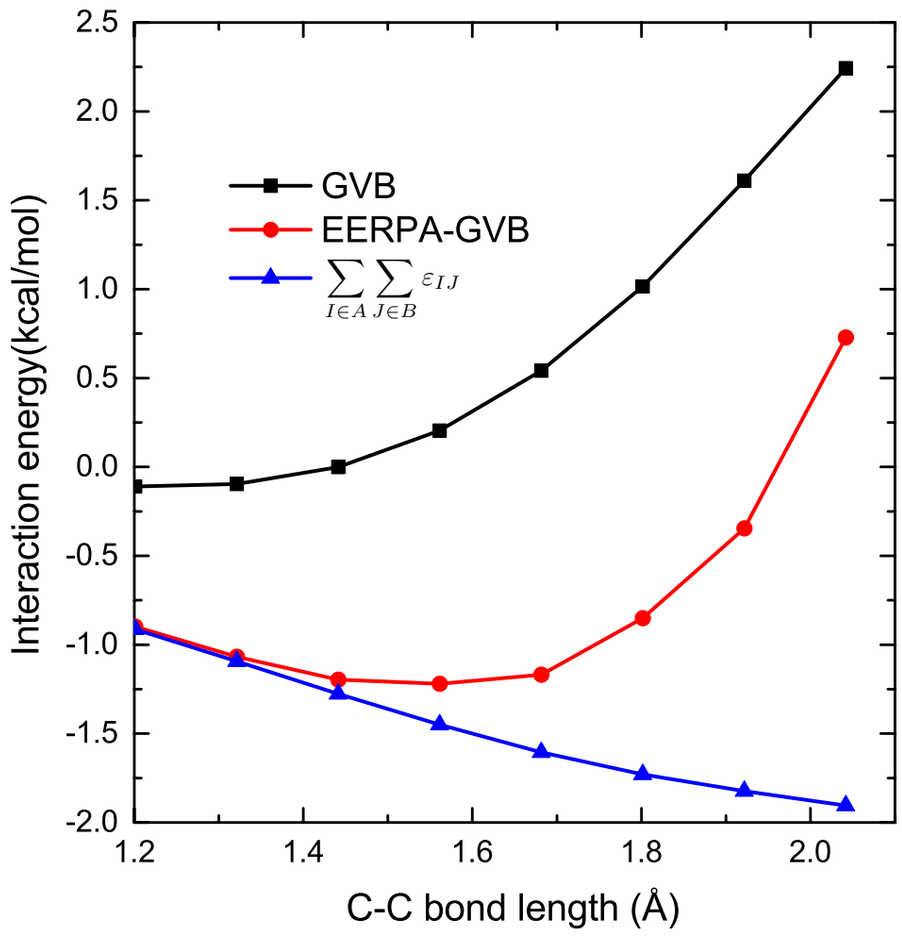




when bonds are stretched, interaction energy passes through the minimum

the value of dispersion energy keeps on increasing

SAPT analysis



r_{CC}/Å	1.20	1.56	1.80	1.92
GVB	-0.33	0.20	1.01	1.61
EERPA-GVB	-1.16	-1.22	-0.85	-0.35
SAPT(GVB)	-1.07	-1.18	-0.79	-0.50
$E^{(1)}_{elst}$	-1.05	-2.50	-3.04	-3.22
$E^{(1)}_{exch}$	0.83	3.04	4.27	4.86
$E^{(2)}_{ind}$	-0.22	-1.07	-1.61	-1.87
$E^{(2)}_{exch-ind}$	0.16	0.90	1.41	1.66
$E^{(2)}_{disp}$	-0.87	-1.84	-2.22	-2.39
$E^{(2)}_{exch-disp}$	0.08	0.29	0.40	0.45
$E^{(2)}_{disp}+E^{(2)}_{exch-disp}$	-0.79	-1.55	-1.82	-1.93
$\sum_{I\in A}\sum_{J\in B}\varepsilon_{IJ}$	-0.91	-1.45	-1.73	-1.82

Interaction energies and their components of acetylene dimer for different C-C bond lengths in kcal/mol

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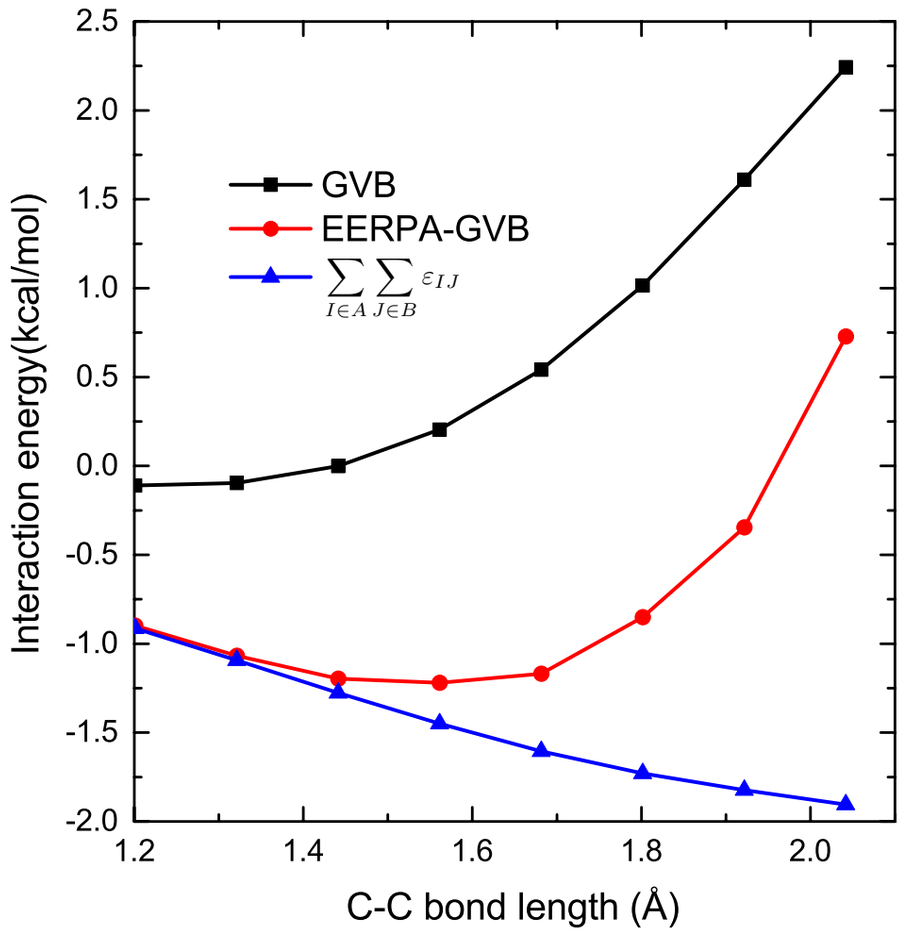

dispersion increases → interaction is strengthened

r_{CC}/Å	1.20	1.56	1.80	1.92
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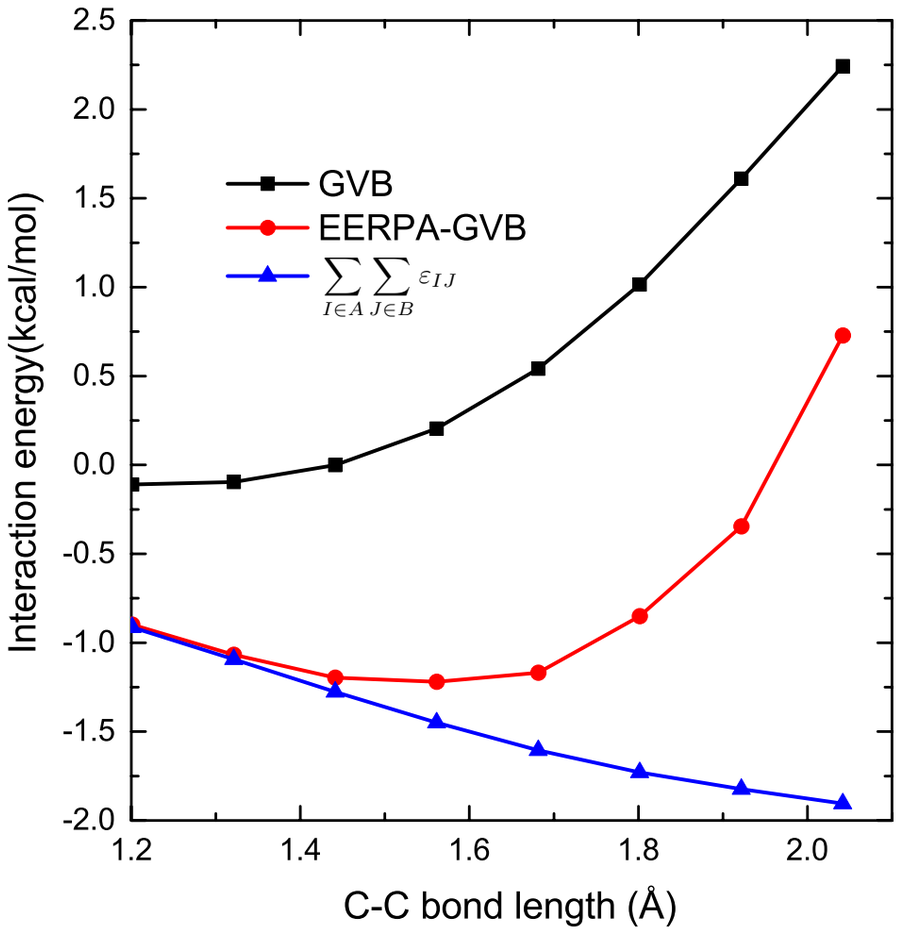

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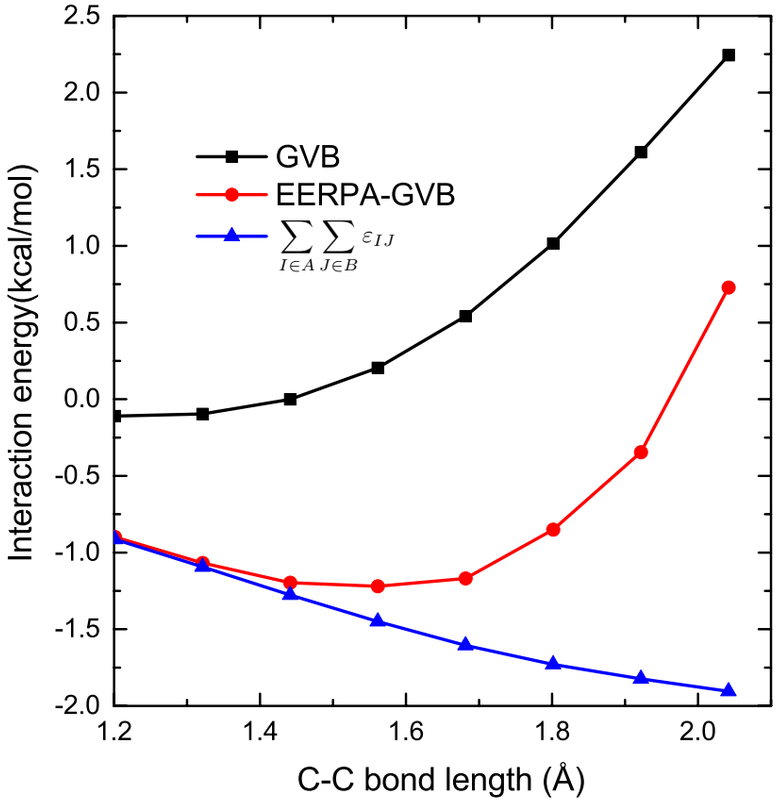
dispersion increases → interaction is strengthened

exchange energy also increases and for sufficiently large C-C bond
it is not compensated by electrostatic energy → interaction is weakened

Dispersion energy density, $D^{AB}(\mathbf{r})$, analysis



r_{CC}/Å	1.20	1.56	1.80	1.92
C-H (far)	2	2	1	1
C-H (close)	35	27	24	23
C-C	63	71	75	76

Contributions to the dispersion energy from fragments of the monomers, in %.

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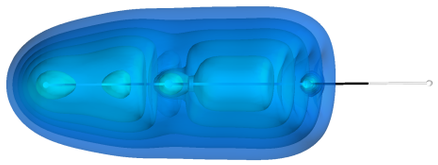
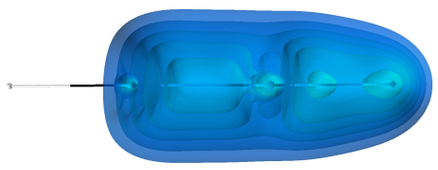
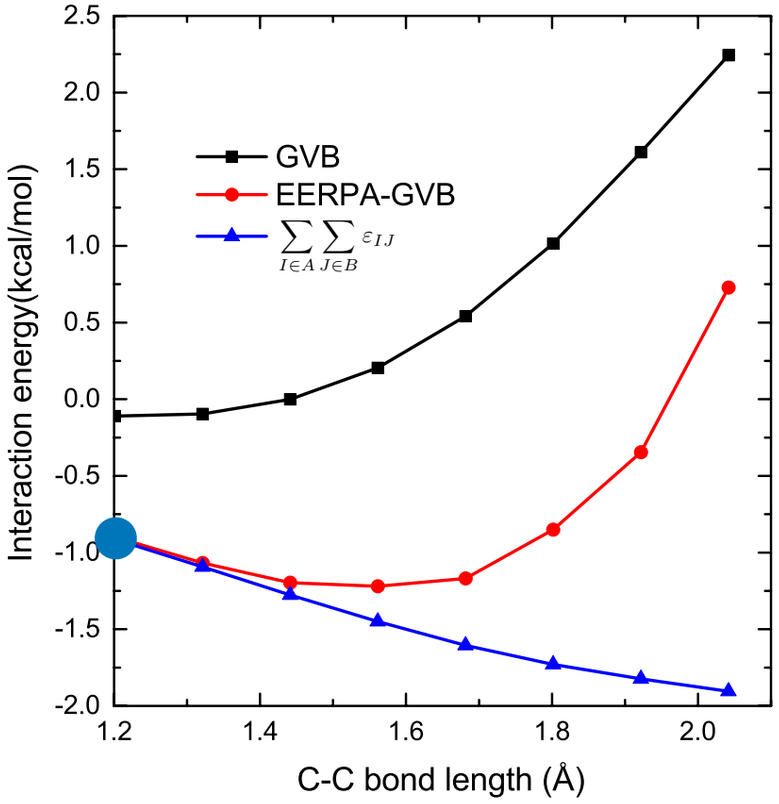


C-C bond length: 1.20





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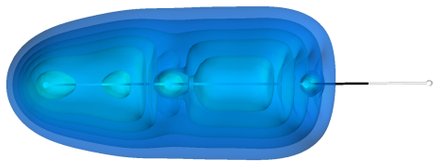

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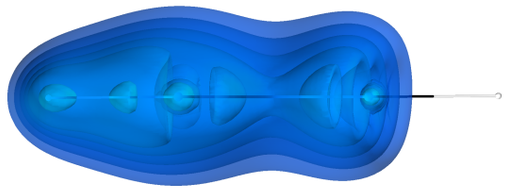
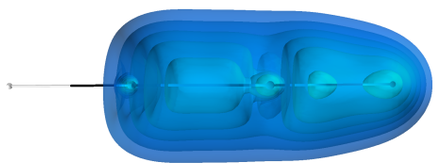
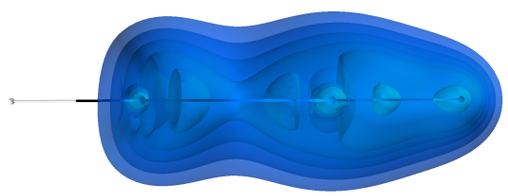
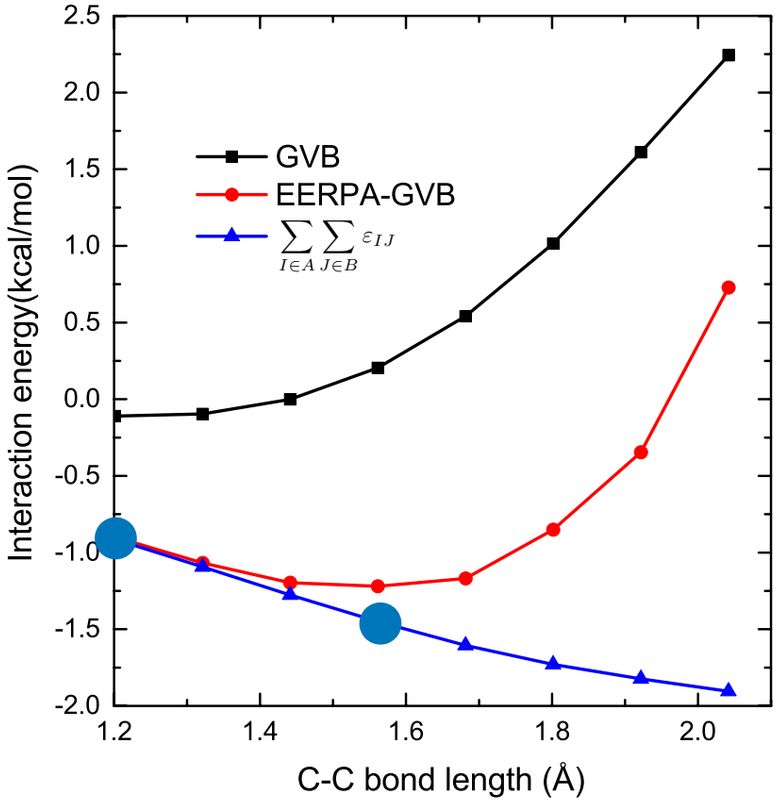


C-C bond length: 1.56







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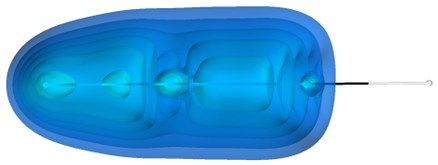

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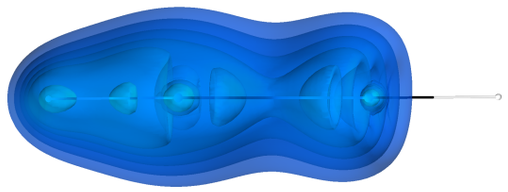

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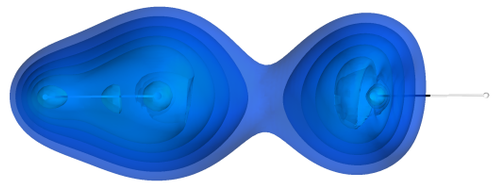

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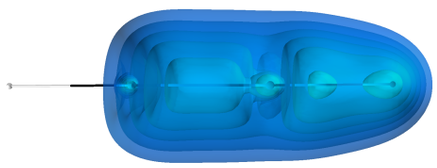

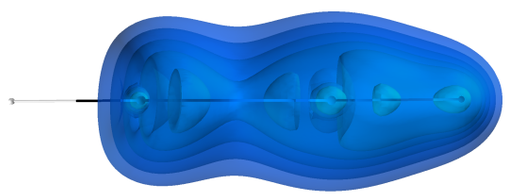

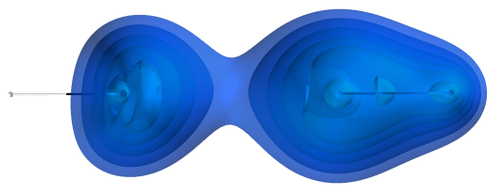

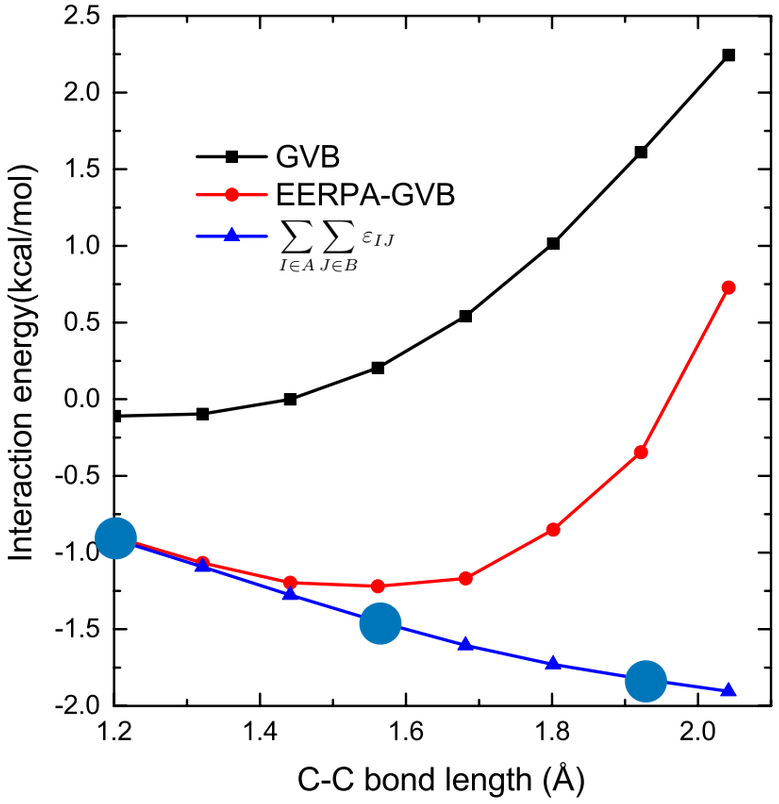

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Contributions to the dispersion energy from fragments of the monomers, in %.

Dispersion interactions in exciton-localised states. Theory and applications to $\pi - \pi^*$ and $n - \pi^*$ excited states

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‡*Faculty of Chemistry, University of Warsaw, ul. L. Pasteura 1, 02-093 Warsaw, Poland*

Dispersion interaction for systems in ground state

- For ground-state weakly interacting systems, dispersion energy follows from the famous Casimir-Polder formula

$$E^{(2)}_{\mathrm{disp}}(A_I B_J) = -\frac{1}{2\pi}\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}'_1 \int \mathrm{d}\mathbf{r}_2 \int \mathrm{d}\mathbf{r}'_2 \frac{1}{r_{12}}\frac{1}{r'_{12}} \int_0^\infty \mathrm{d}\omega \chi_+^{A_I}(\mathbf{r}_1, \mathbf{r}'_1; i\omega)\chi_+^{B_J}(\mathbf{r}_2, \mathbf{r}'_2; i\omega)$$

- Dispersion energy is negative (attractive interaction)

Dispersion interaction for systems with localized excitons

- Generalization of the Casimir-Polder formula for systems with localized excitons

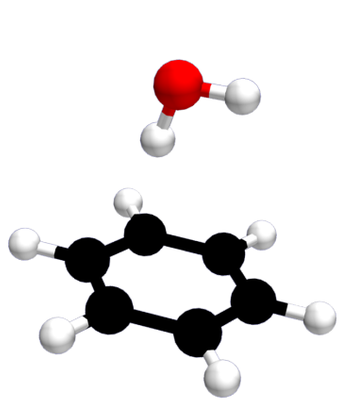
$$E^{(2)}_{\mathrm{disp}}(A_I B_J) = -\frac{1}{2\pi}\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}'_1 \int \mathrm{d}\mathbf{r}_2 \int \mathrm{d}\mathbf{r}'_2 \frac{1}{r_{12}}\frac{1}{r'_{12}} \int_0^\infty \mathrm{d}\omega \chi_+^{A_I}(\mathbf{r}_1,\mathbf{r}'_1;i\omega)\chi_+^{B_J}(\mathbf{r}_2,\mathbf{r}'_2;i\omega)$$

$$+ \sum_{\mu<I,\nu<J} W_{\mu\nu}^{A_I B_J} + \sum_{\mu>I,\nu<J} W_{\mu\nu}^{A_I B_J} + \sum_{\mu<I,\nu>J} W_{\mu\nu}^{A_I B_J}$$

$$W_{\mu\nu}^{A_I B_J} = -\frac{1}{\omega_\mu^{A_I} + \omega_\nu^{B_J}} \left(\int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2 \frac{\rho_\mu^{A_I}(\mathbf{r}_1)\rho_\nu^{B_J}(\mathbf{r}_2)}{r_{12}} \right)^2$$

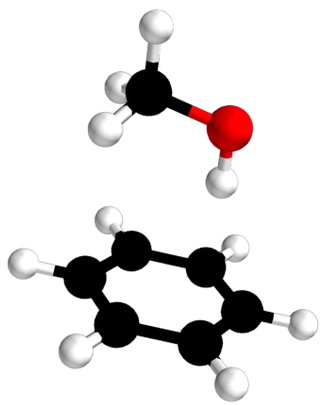
The extra terms (non-Casimir-Polder) are positive for multiple localized excitons - repulsive forces resulting from long-range correlation.

- Studied dimers included excitons on: benzene (pi-pi*), pyridine (pi-pi*) or peptide (n-pi*)



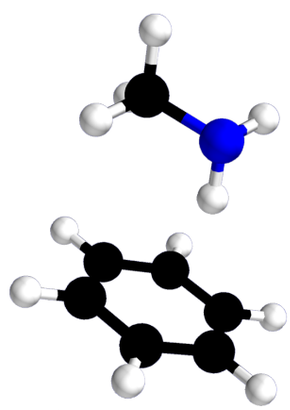
Benzene...Water

$\pi - \pi^*$



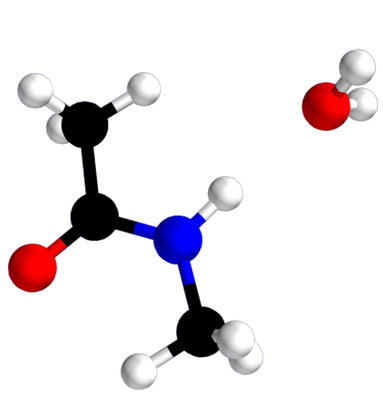
Benzene...MeOH

$\pi - \pi^*$



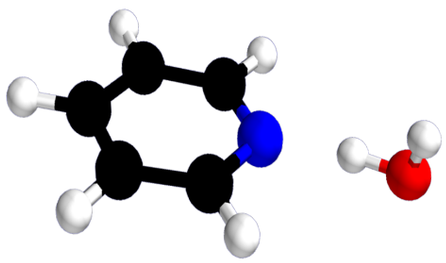
Benzene...$MeNH_2$

$\pi - \pi^*$



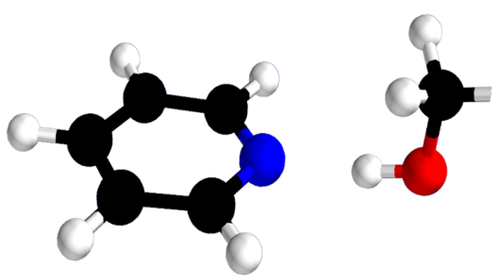
Peptide...Water

$n - \pi^*$



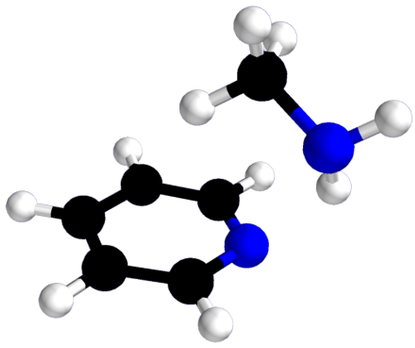
Pyridine...Water

$\pi - \pi^*$



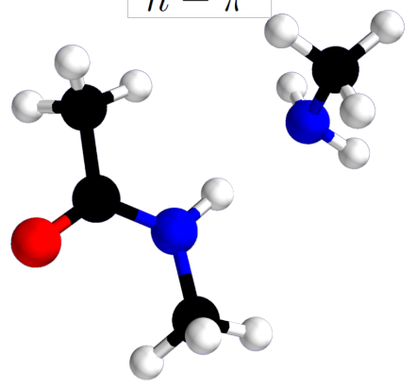
Pyridine...MeOH

$\pi - \pi^*$



Pyridine...$MeNH_2$

$\pi - \pi^*$

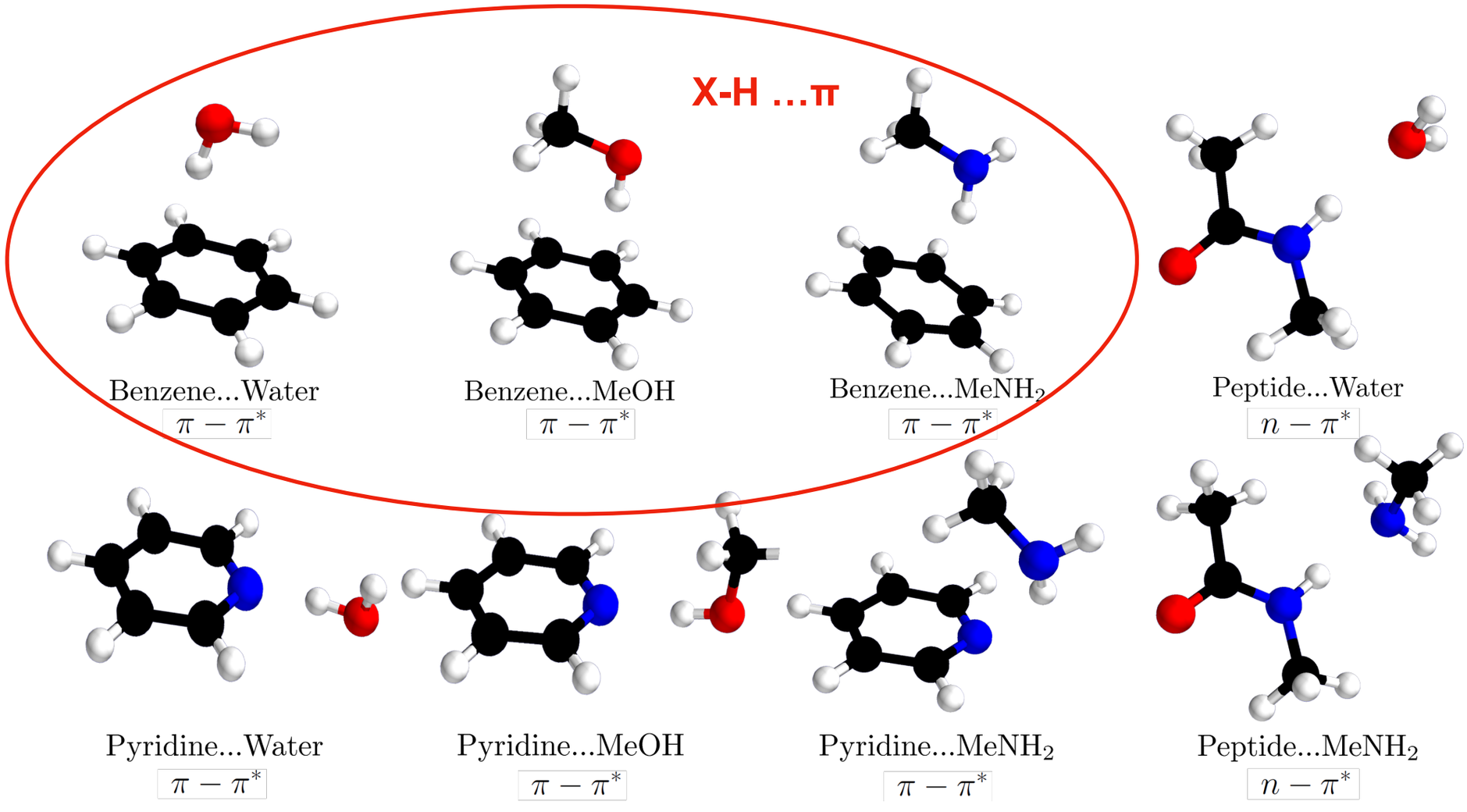


Peptide...$MeNH_2$

$n - \pi^*$

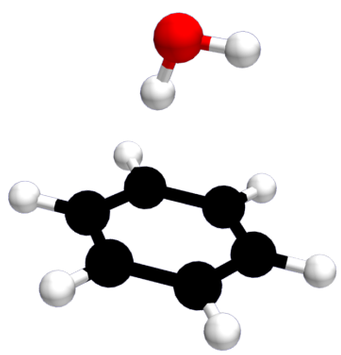
- SAPT(CAS) only needs 1,2-RDMs of monomers
- We have used CASSCF wavefunctions to obtain RDMs of monomers

- Interactions of the studied systems are of different types:



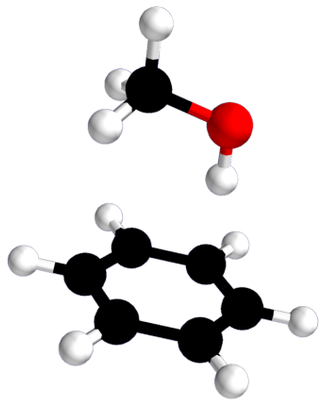
- Interactions of the studied systems are of different types:

H-bond



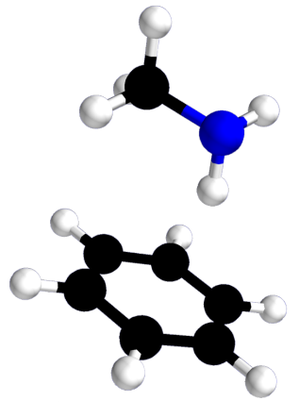
Benzene...Water

$\pi - \pi^*$



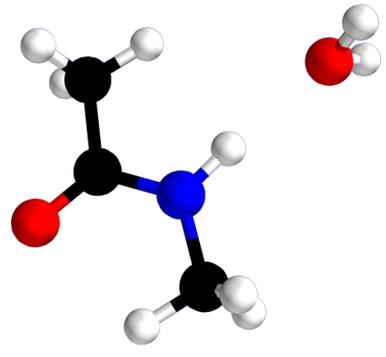
Benzene...MeOH

$\pi - \pi^*$



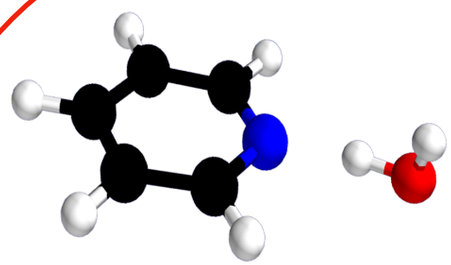
Benzene...$MeNH_2$

$\pi - \pi^*$



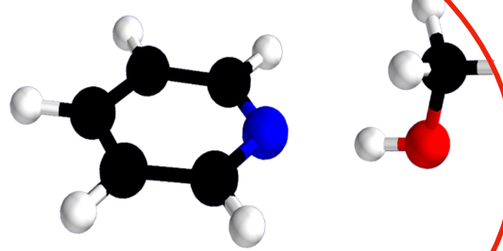
Peptide...Water

$n - \pi^*$



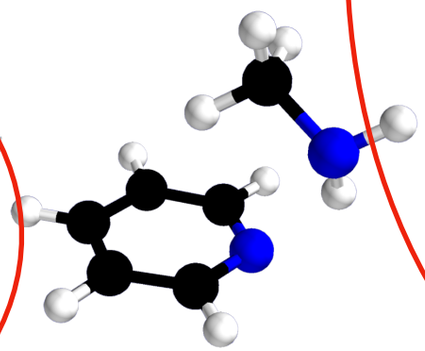
Pyridine...Water

$\pi - \pi^*$



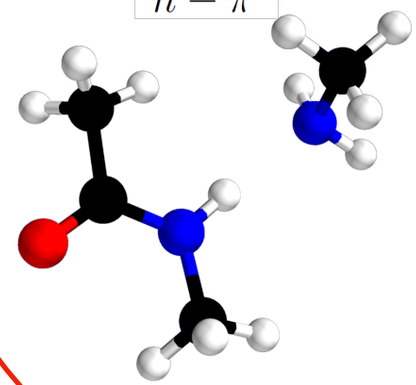
Pyridine...MeOH

$\pi - \pi^*$



Pyridine...$MeNH_2$

$\pi - \pi^*$



Peptide...$MeNH_2$

$n - \pi^*$

Table 4: Interaction energies in kcal·mol^{-1} for $\pi-\pi^*$ (benzene and pyridine complexes) and $n-\pi^*$ (peptide complexes) excited states. The SAPT acronym refers to SAPT(CAS) results including the δ_{CAS} correction [see Eq. (54)]. The Est. EOM-CCSD(T) values from Ref. 19 are given as reference in the last column. Mean unsigned errors (MUE) and mean absolute percentage errors (MA%E) are computed with respect to the reference.

	CAS	CAS +DISP	AC0 -CAS	lrAC0 -CAS	CASPT2	CAS -reVV10	SAPT	LC-BOP +LRD	ref.
benzene-water	0.11	-2.43	-2.39	-2.82	-3.12	-2.93	-2.51	-2.88	-2.67
benzene-MeOH	0.96	-3.15	-2.62	-3.74	-3.42	-4.03	-3.25	-3.55	-3.49
benzene-$MeNH_2$	1.51	-2.57	-2.40	-3.00	-3.24	-3.46	-2.62	-2.74	-2.80
pyridine-water	-4.20	-7.41	-6.61	-7.34	-7.90	-6.37	-6.91	-7.96	-7.15
pyridine-MeOH	-4.01	-7.97	-6.72	-7.91	-7.21	-6.98	-7.44	-8.37	-7.70
pyridine-$MeNH_2$	0.61	-3.73	-3.43	-4.11	-3.96	-4.24	-3.82	-4.06	-4.19
peptide-water	-2.23	-4.70	-4.23	-4.52	-4.92	-4.29	-4.36	-4.81	-4.63
peptide-$MeNH_2$	-2.08	-6.76	-6.18	-6.82	-7.28	-6.23	-6.40	-6.97	-6.82
MUE	3.77	0.24	0.61	0.15	0.40	0.49	0.23	0.28	-
MA%E	88.83	5.93	13.27	3.70	8.74	10.77	4.85	5.12	-

We have shown that SAPT(CAS) yields interaction energy of good accuracy.

	$E^{(1)}_{\text{elst}}$	$E^{(1)}_{\text{exch}}$	$E^{(2)}_{\text{ind}}$	$E^{(2)}_{\text{exch-ind}}$	$E^{(2)}_{\text{disp}}$	$E^{(2)}_{\text{exch-disp}}$	$E^{\text{SAPT}}_{\text{int}}$	$\varepsilon^{1\to0}_{\text{disp}}$
benzene-water	−1.85	2.82	−1.23	0.65	−2.88	0.33	−2.16	−0.04
benzene-MeOH	−2.10	4.07	−1.57	0.96	−4.63	0.52	−2.76	−0.06
benzene-$MeNH_2$	−1.68	3.73	−1.12	0.88	−4.62	0.54	−2.28	−0.02
pyridine-water	−11.23	10.66	−5.17	2.96	−4.05	0.84	−5.99	−0.07
pyridine-MeOH	−11.79	11.79	−5.92	3.53	−4.95	0.99	−6.37	−0.08
pyridine-$MeNH_2$	−3.89	5.46	−1.79	1.30	−5.01	0.66	−3.27	−0.08
peptide-water	−5.99	5.33	−1.95	1.01	−2.93	0.46	−4.09	0.00
peptide-$MeNH_2$	−9.84	10.91	−5.04	3.35	−5.78	1.10	−5.30	0.00

	$\Delta E^{(1)}_{\text{elst}}$	$\Delta E^{(1)}_{\text{exch}}$	$\Delta E^{(2)}_{\text{ind}}$	$\Delta E^{(2)}_{\text{exch-ind}}$	$\Delta E^{(2)}_{\text{disp}}$	$\Delta E^{(2)}_{\text{exch-disp}}$	$\Delta E^{\text{SAPT}}_{\text{int}}$
benzene-water	0.88	−0.35	0.11	−0.05	0.17	−0.05	0.72
benzene-MeOH	0.98	−0.45	0.15	−0.08	0.24	−0.07	0.77
benzene-$MeNH_2$	0.54	−0.25	0.08	−0.03	0.22	−0.05	0.50
pyridine-water	−0.04	0.02	0.02	0.01	0.02	0.00	0.03
pyridine-MeOH	−0.03	0.02	0.02	0.01	0.04	0.00	0.04
pyridine-$MeNH_2$	0.17	−0.15	0.04	−0.04	0.15	−0.03	0.14
peptide-water	0.71	−0.03	0.12	−0.03	−0.01	0.01	0.77
peptide-$MeNH_2$	0.71	0.05	−0.12	0.32	−0.10	0.05	0.91

Generation of an exciton on benzene weakens the X-H…π bond.

Surprise: it is not only due to electrostatic but also decreased dispersion.

	$E^{(1)}_{\text{elst}}$	$E^{(1)}_{\text{exch}}$	$E^{(2)}_{\text{ind}}$	$E^{(2)}_{\text{exch-ind}}$	$E^{(2)}_{\text{disp}}$	$E^{(2)}_{\text{exch-disp}}$	$E^{\text{SAPT}}_{\text{int}}$	$\varepsilon^{1\to0}_{\text{disp}}$
benzene-water	−1.85	2.82	−1.23	0.65	−2.88	0.33	−2.16	−0.04
benzene-MeOH	−2.10	4.07	−1.57	0.96	−4.63	0.52	−2.76	−0.06
benzene-$MeNH_2$	−1.68	3.73	−1.12	0.88	−4.62	0.54	−2.28	−0.02
pyridine-water	−11.23	10.66	−5.17	2.96	−4.05	0.84	−5.99	−0.07
pyridine-MeOH	−11.79	11.79	−5.92	3.53	−4.95	0.99	−6.37	−0.08
pyridine-$MeNH_2$	−3.89	5.46	−1.79	1.30	−5.01	0.66	−3.27	−0.08
peptide-water	−5.99	5.33	−1.95	1.01	−2.93	0.46	−4.09	0.00
peptide-$MeNH_2$	−9.84	10.91	−5.04	3.35	−5.78	1.10	−5.30	0.00

	$\Delta E^{(1)}_{\text{elst}}$	$\Delta E^{(1)}_{\text{exch}}$	$\Delta E^{(2)}_{\text{ind}}$	$\Delta E^{(2)}_{\text{exch-ind}}$	$\Delta E^{(2)}_{\text{disp}}$	$\Delta E^{(2)}_{\text{exch-disp}}$	$\Delta E^{\text{SAPT}}_{\text{int}}$
benzene-water	0.88	−0.35	0.11	−0.05	0.17	−0.05	0.72
benzene-MeOH	0.98	−0.45	0.15	−0.08	0.24	−0.07	0.77
benzene-$MeNH_2$	0.54	−0.25	0.08	−0.03	0.22	−0.05	0.50
pyridine-water	−0.04	0.02	0.02	0.01	0.02	0.00	0.03
pyridine-MeOH	−0.03	0.02	0.02	0.01	0.04	0.00	0.04
pyridine-$MeNH_2$	0.17	−0.15	0.04	−0.04	0.15	−0.03	0.14
peptide-water	0.71	−0.03	0.12	−0.03	−0.01	0.01	0.77
peptide-$MeNH_2$	0.71	0.05	−0.12	0.32	−0.10	0.05	0.91

H-bonds are weakened when n-pi* exciton is generated.

It is mainly the electrostatic effect: electron density is removed from H-bond acceptor (N atom).

	$E^{(1)}_{\text{elst}}$	$E^{(1)}_{\text{exch}}$	$E^{(2)}_{\text{ind}}$	$E^{(2)}_{\text{exch-ind}}$	$E^{(2)}_{\text{disp}}$	$E^{(2)}_{\text{exch-disp}}$	$E^{\text{SAPT}}_{\text{int}}$	$\varepsilon^{1\to0}_{\text{disp}}$
benzene-water	−1.85	2.82	−1.23	0.65	−2.88	0.33	−2.16	−0.04
benzene-MeOH	−2.10	4.07	−1.57	0.96	−4.63	0.52	−2.76	−0.06
benzene-$MeNH_2$	−1.68	3.73	−1.12	0.88	−4.62	0.54	−2.28	−0.02
pyridine-water	−11.23	10.66	−5.17	2.96	−4.05	0.84	−5.99	−0.07
pyridine-MeOH	−11.79	11.79	−5.92	3.53	−4.95	0.99	−6.37	−0.08
pyridine-$MeNH_2$	−3.89	5.46	−1.79	1.30	−5.01	0.66	−3.27	−0.08
peptide-water	−5.99	5.33	−1.95	1.01	−2.93	0.46	−4.09	0.00
peptide-$MeNH_2$	−9.84	10.91	−5.04	3.35	−5.78	1.10	−5.30	0.00

	$\Delta E^{(1)}_{\text{elst}}$	$\Delta E^{(1)}_{\text{exch}}$	$\Delta E^{(2)}_{\text{ind}}$	$\Delta E^{(2)}_{\text{exch-ind}}$	$\Delta E^{(2)}_{\text{disp}}$	$\Delta E^{(2)}_{\text{exch-disp}}$	$\Delta E^{\text{SAPT}}_{\text{int}}$
benzene-water	0.88	−0.35	0.11	−0.05	0.17	−0.05	0.72
benzene-MeOH	0.98	−0.45	0.15	−0.08	0.24	−0.07	0.77
benzene-$MeNH_2$	0.54	−0.25	0.08	−0.03	0.22	−0.05	0.50
pyridine-water	−0.04	0.02	0.02	0.01	0.02	0.00	0.03
pyridine-MeOH	−0.03	0.02	0.02	0.01	0.04	0.00	0.04
pyridine-$MeNH_2$	0.17	−0.15	0.04	−0.04	0.15	−0.03	0.14
peptide-water	0.71	−0.03	0.12	−0.03	−0.01	0.01	0.77
peptide-$MeNH_2$	0.71	0.05	−0.12	0.32	−0.10	0.05	0.91

H-bonds are **not** weakened when pi-pi* exciton is generated on pyridine.

Electrostatic energy not affected: electron density on H-bond acceptor (N atom) not changed.

Future GammCor development enabling new applications

Handing (I/O) large files (integrals) has remained a bottleneck restricting the size of systems we can compute.

We are developing a new Cholesky-based algorithm for computing second-order exchange-polarization terms.

Combination of SAPT with CIPSI (gammcor and quantum package via trexio) opens a way for improving the accuracy of SAPT.

Systems with local excitons of biological importance: nucleobase dimers