POLISH NATIONAL AGENCY FOR ACADEMIC EXCHANGE

STER PROGRAMME

name of the unit:		symbol:
QUANTUM CHEMISTRY GROUP Institute of Physics, Lodz University of Technology		I-71 http://www.fizyka.p.lodz.pl/en/
head of the unit:	potential promoters:	contact person:
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scope of activities:

We develop quantum chemistry theories, methods, and computational algorithms for electronic structure predictions of atoms and molecules. They are implemented in quantum chemistry programs including our homegrown software GammCor.

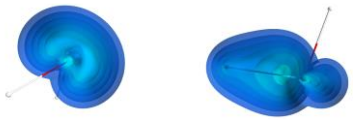
Our fields of interest include:

- electron correlation,
- density function theory
- density matrix functional theory
- molecular interaction theory

We are also interested in real-life problems which quantum-chemical computation methods could help solve. One of such problems is the performance of photoswitches, molecules that undergo reversible structural changes upon irradiation with light of a specific color. Using both computation and experimental results of our collaborators, we try to work out which of the photoswitches' properties determine the essential parameters of their performance.

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B} & \mathcal{A} \end{pmatrix} \begin{pmatrix} \mathbf{X}^\nu \\ \mathbf{Y}^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} -\mathcal{N} & 0 \\ 0 & \mathcal{N} \end{pmatrix} \begin{pmatrix} \mathbf{X}^\nu \\ \mathbf{Y}^\nu \end{pmatrix}$$

Extended Random Phase Approximation equation



Visualization of the dispersion energy density for water dimer.

$$E_{corr}^{ACn_{\max}} = \frac{4}{\pi}\mathrm{Tr}\left[\left(\int_0^\infty \mathrm{d}\omega \sum_{n=1}^{n_{\max}} \frac{\bar{\mathbf{C}}(\omega)^{(n)}}{n!(n+1)}\right)\mathbf{D}^2\right]$$

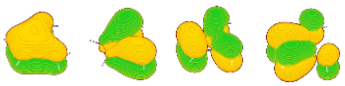
Adiabatic connection formula for the correlation energy applicable to strongly correlated molecules

present activities:

Our current activity focuses on correlation energy methods based on adiabatic connection and random phase approximation theories. We aim at developing accurate and efficient approach to computing correlation energy in strongly correlated systems.

The other mainstream of the research work concerns molecular interactions in multireference systems including electronically excited dimers. For this purpose a novel symmetry adapted perturbation method has been developed and implemented in our code.

Methods combining density functional theory with wavefunction theory either via range-separation of the electron interaction operator or on-top pair density functionals are also actively developed in our group.



(1.95) (1.91) (1.89) (0.11)

Strongly correlated orbitals of C4H2-1,2-(CH2)2 biradical

future activities:

Strongly correlated systems and development of efficient algorithms for computing electron correlation energy.

The portfolio of research groups was created as part of the Programme "STER" – Internationalisation of doctoral schools" as part of the realization of the project "Curriculum for advanced doctoral education & taining – CADET Academy of Lodz University of Technology".

publications:

- M. Hapka, M. Przybytek, K. Pernal: Symmetry-adapted perturbation theory based on multiconfigurational wave function description of monomers, Journal of Chemical Theory and Computation 17, 5538 (2021).
- O. V. Gritsenko, R. van Meer, K. Pernal: Efficient evaluation of electron correlation along the bond-dissociation coordinate in the ground and excited ionic states with dynamic correlation suppression and enhancement functions of the on-top pair density, Physical Review A 98, 062510 (2018).
- E. Pastorczak, K. Pernal: Correlation energy from the adiabatic connection formalism for complete active space wave functions, Journal of Chemical Theory and Computation 14, 3493 (2018).
- **K. Pernal:** Electron correlation from the adiabatic connection for multireference wave functions, Physical Review Letters 120, 013001 (2018).

keywords:

electron correlation, electronic structure methods, density functional theory, strong correlation

list of internship proposals in this research team:

Particle-particle extended random phase approximation for strong correlation.
On-top pair density functionals.