Theoretical Chemistry Team

HEAD:

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GROUP MEMBERS:

Prof. Joanna Sadlej, PhD DSc (emeritus);
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RESEARCH PROFILE:

Our research focuses on different aspects of light-molecules interactions. In particular, we apply and develop methods of quantum chemistry to study stability, spectroscopic properties, and photoreaction mechanisms of molecular and supramolecular systems. Our special focus is also set on Nuclear Magnetic Resonance and chiralooptical spectroscopic parameters. For up-to-date information, please visit our webpages: *tct.chem.uw.edu.pl* and *psiom.chem.uw.edu.pl/j_sadlej.html*

CURRENT RESEARCH ACTIVITIES:

MPK: Theory and modeling of Nuclear Magnetic Resonance and chiralooptical spectroscopic parameters:

- relativistic effects in NMR spectra;
- polarized-luminescence calculations;
- chiral recognition by molecular spectroscopy.

JC: Quantum-chemical spectroscopic calculations for molecules and supra-molecular complexes:

- circular- and axial-dichroism optical spectra, applications and methods development,
- high-quality vibrational spectra calculations,
- intermolecular interactions,
- noble-gas molecular systems,

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- quantum chemistry software development (DALTON, Dalton Project)

JJ: Theoretical photochemistry studies aided with nonadiabatic molecular dynamics simulations:
- fundamental photochemical processes (excited state proton transfer, photostability of proto-biological molecular systems),
- modern materials for photovoltaics (hybrid perovskites, highly-polarized molecular wires)
- molecular photoswitching (biased photoswitching of diarylethenes, complex molecular photo-devices)
- nonadiabatic molecular dynamics methods development for modeling processes in highly-excited electronic states.

SELECTED PUBLICATIONS:

1. J.M.H. Olsen, S. Reine, O. Vahtras et al., Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems, J. Chem. Phys. 152 (2020) 214115 (JCP Special Topic on Electronic Structure Software).
2. J. Cukras, J.M.E. Ahokas, J. Lundell, Vibrational spectrum of HXeSH revisited: Combined computational and experimental study, Chem. Phys. Lett. 741 (2020) 137083.
3. A. Królikowska, J. Cukras, M. Witkowski, D. Tymecka, A. Hernik-Magoń, A. Misicka, W. Dzwolak, SERS and DFT Study of Noble-Metal-Anchored Cys-Trp/Trp-Cys Dipeptides: Influence of Main-Chain Direction and Terminal Modifications, J. Phys. Chem. C. 124 (2020) 7097–7116.
4. K. Jakubowska, M. Pecul, Nuclear Magnetic Resonance parameters of mercury atom and water molecule complex: Relativistic calculations, Chem. Phys. Lett. 736 (2019) 136775.
5. J. Jankowska, A.L. Sobolewski, Efficient Separation of Photogenerated Charges in a Ferroelectric Molecular Wire: Nonadiabatic Dynamics Study on 3, 5-Dicyano-1, 7-dimethylopyrrolo [3, 2-f] indole Trimer, ChemPhotoChem. 3 (2019) 187-192.
6. J. Jankowska, O.V. Prezhdo, Real-Time Atomistic Dynamics of Energy Flow in an STM Setup: Revealing the Mechanism of Current-Induced Molecular Emission, J. Phys. Chem. Lett. 9 (2018) 3591-3597.
7. K. Jakubowska, M. Pecul, M. Jaszuński, Spin-spin coupling constants in HC=CXH3 molecules; X=C, Si, Ge, Sn and Pb, Theor. Chem. Acc. 137 (2018) 41.
8. J. Jankowska, M. Barbatti, J. Sadlej, A.L. Sobolewski, Tailoring the Schiff base photoswitching–a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer, Phys. Chem. Chem. Phys. 19 (2017) 5318-5325.
9. J. Cukras, J. Kauczor, P. Norman, A. Rizzo, G.L.J.A. Rikken, S. Coriani, A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion, Phys. Chem. Chem. Phys. 18 (2016) 13267–13279.
10. M. Kamiński, J. Cukras, M. Pecul, A. Rizzo, S. Coriani, A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption, Phys. Chem. Chem. Phys. 29 (2015) 19079–19086.