Theoretical Chemistry Team

HEAD:
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GROUP MEMBERS:
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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 chiral-optical 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 chiral-optical 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:**