Theoretical Chemistry Team

@ Laboratory of Spectroscopy and Intermolecular Interactions (PSiOM)

PEOPLE

http://tct.chem.uw.edu.pl/

Permanent staff
prof. dr hab. Magdalena Pecul-Kudelska
Head of the team
dr Janusz Cukras
dr Joanna Jankowska

Postdoctoral scholars
dr Davide Accomasso *(Polonez Bis Fellow)*

In academic year 2023/24:
Ph.D. candidates: 2
M.Sc. students: 3
B.Sc. students: 1

GENERAL RESEARCH SCOPE

- Theoretical spectroscopy
- Light-driven processes in molecules and materials
- Noble-gas chemistry

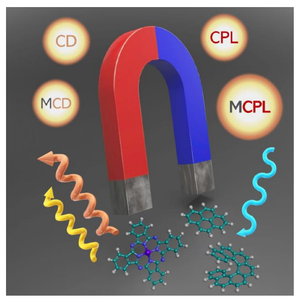
SELECTED ONGOING PROJECTS

#1 Comparison of magnetic circular dichroism and magnetic-field induced circular luminescence of aromatic rings

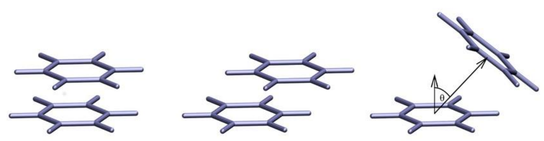
Mikołaj Piekarek (M.Sc.), and Magdalena Pecul-Kudelska

The goal of the project is to calculate MCPL spectra of a series of aromatic molecules in order to establish a relationship between the MCPL spectrum and molecular structure. The calculations are being carried out for:

a) benzene, naphatelene, anthracene and pyrene. The aim is to check whether the chosen method reproduces the order of magnitude of the experimentally recorded MCD/MCPL and how the number of the coupled pi bonds (or aromatic rings) influences the MCPL intensity,



b) b) the benzene dimer. The aim is to check the influence of stacking interactions on the MCPL spectra.



The A and B terms contributing to magnetic circular dichroism (MCD) or magnetic-field induced circular luminescence (MCPL) can be calculated as double and single residues of a quadratic response function, respectively, and this approach (employing use damped and resonant response theory) is used in the project. The electronic structure is modelled by means of time-dependent density functional theory. Basis sets are based on the aug-cc-pVXZ family augmented by the diffuse functions.

#2 Magnetic spectroscopies

Mikołaj Piekarek (M.Sc.), Maksymilian Mucha (B.Sc.), Oliwier Misztal, Jakub Szewczyk (B.Sc.), Grzegorz Skóra (M.Sc.), Łukasz Rybski, Marek Tolsdorf, and Janusz Cukras

- Magneto-chiral dichroism – novel spectroscopy from fundamental light-matter interaction
- Connection to homochirality of life and abiogenesis
- Proteinogenic amino acids and bio-relevant molecular systems
- Enantioselective photoreactions
- Framework of the damped response-theory
- Python coding and supercomputers
- The goal: to develop new type of spectroscopy and find new signal-to-structure correlations

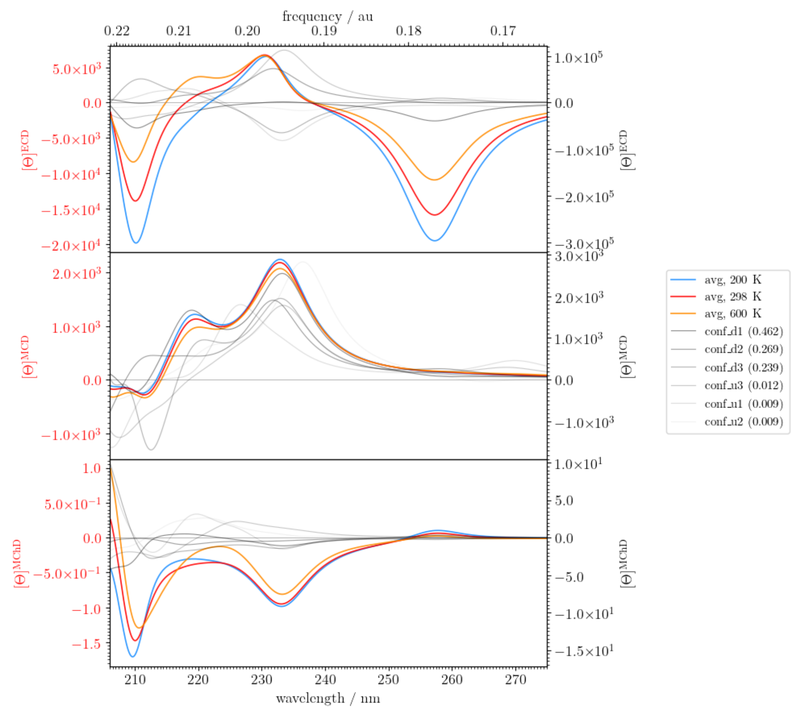


Figure 2.1: Three dichroic spectra (in terms of ellipticities) of the carvone molecule including conformational analysis.

#3 Theoretical design and characterization of molecular systems for clean energy generation

Kamil Szychta (B.Sc.), Mikołaj Martyka (M.Sc.), and Joanna Jankowska

- **Proton-Coupled Electron Transfer (PCET)** is often a key, first step in solar-driven hydrogen production.
- By means of computational chemistry, we study details of the **PCET mechanism** in small and medium-size **organic systems.**
- The goal is to **determine structural factors** which enhance the **efficiency and rate** of the PCET process.

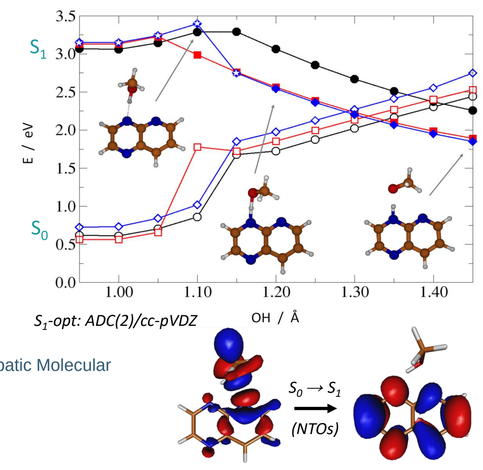
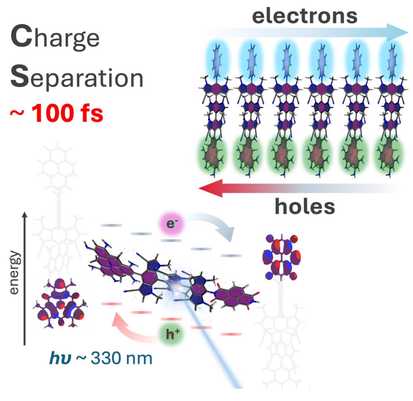


Photo-Oxidation of Methanol in Complexes with Pyrido[2,3-b]pyrazine: a Nonadiabatic Molecular Dynamics Study, J. Jankowska, A.L. Sobolewski, PCCP 2024, 26, 5296-5302



- **Polarized Covalent Organic Frameworks (COF-Pol):** our proposed concept of a **new material for photovoltaics**
- By means of quantum chemistry and nonadiabatic molecular dynamics (NAMD) we investigate the **photo-generation and separation of charges**.
- The goal is to **design efficient molecular units** that could be used in COF-Pol materials.

Ultrafast Separation of Photogenerated Charges in a Donor-Polarized Molecular Wire-Acceptor Triad
K. Szychta, M. Martyka, and J. Jankowska, *manuscript in preparation*

#4 Unravelling and optimizing the photoisomerization dynamics of light-driven molecular rotary motors

Davide Accomasso, Kamil Szychta (B.Sc.), and Joanna Jankowska

- **Light-driven rotary motors (LDRMs)** are molecules capable of converting **light** energy into unidirectional intramolecular **rotary motion**.
- The **rotary movement** is achieved through four consecutive steps (Figure 4.1): two **photoisomerization reactions** of the central double bond (steps 1 and 3) and two thermal helix inversions (steps 2 and 4).

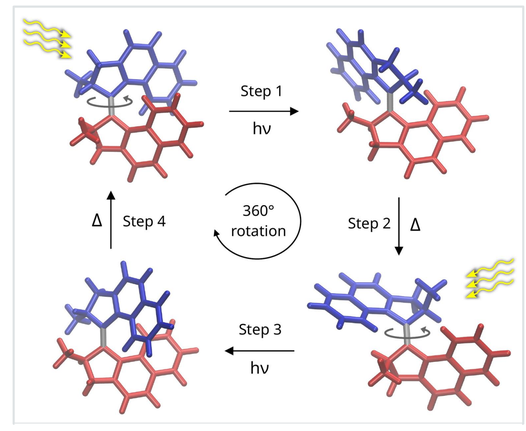


Figure 4.1: Photocycle of unidirectional rotation in a LDRM.

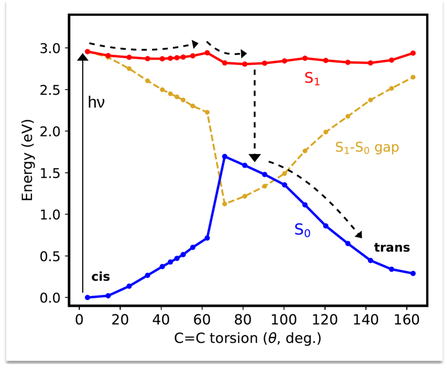


Figure 4.2: Potential energy profiles of the S_1 and S_0 states of a LDRM along the torsion around the central C=C bond.

- In this project, we intend to study the elusive **photoisomerization reactions** of **LDRMs** by performing **quantum chemical calculations** (Figure 4.2) and **excited-state dynamics simulations**.
- The knowledge acquired from our simulations will be exploited to propose new **LDRMs** with **improved photoisomerization efficiency**.

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