Theoretical Chemistry Team

@ Division of Physical Chemistry and Radiochemistry

PEOPLE

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

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

In academic year 2024/25:
Ph.D. candidates: 2
M.Sc. students: 2
B.Sc. students: 1

GENERAL RESEARCH SCOPE

- Theoretical Spectroscopy
- Light-Driven Processes in Molecules and Materials
- Noble-gas chemistry
- Machine Learning models for Theoretical Chemistry
- Molecular circular dichroism

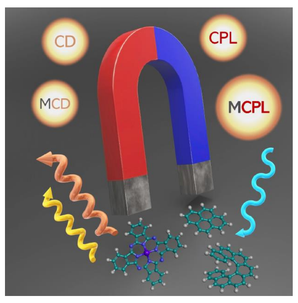
SELECTED ONGOING PROJECTS

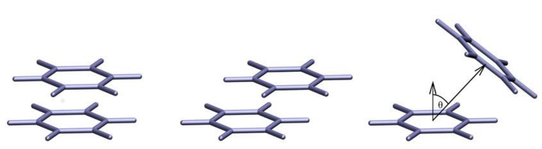
#1 Comparison of magnetic circular dichroism and magnetic-field induced circular luminescence of aromatic rings

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:

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





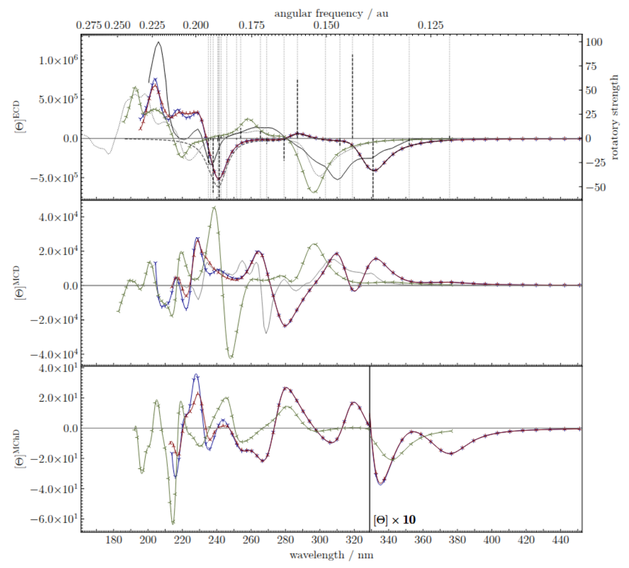
The A and B terms contributing to magnetic circular dichroism (MCD) or magnetic-field induced circular luminescence (MCPL) can be calculated as double and single residues of a quadratic response function, respectively, and this approach (employing use damped and resonant response theory) is used in the 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.

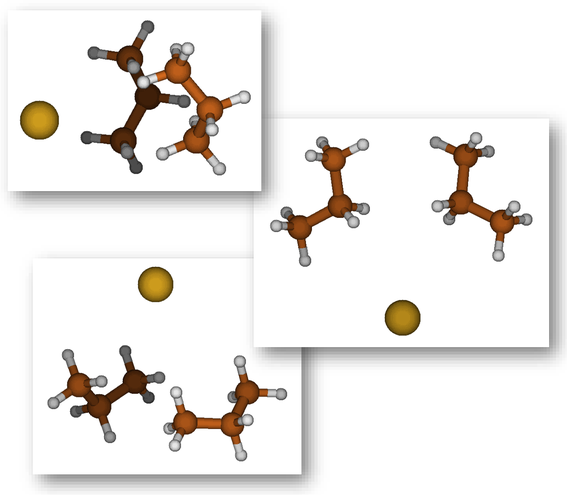
#2 Magnetic spectroscopies

Mikołaj Piekarek (M.Sc.), Oliwier Misztal, Jakub Szewczyk (B.Sc.), Grzegorz Skóra (M.Sc.), Emilia Cieślik, Jędrzej Pawłowski, and Janusz Cukras

Dichroic spectroscopies and chirality

- ECD, MCD and Magneto-chiral dichroism (MChD) – novel spectroscopy from fundamental light-matter interaction
- Connection to homochirality of life and abiogenesis
- 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





Xe atom interaction with aliphatic chains

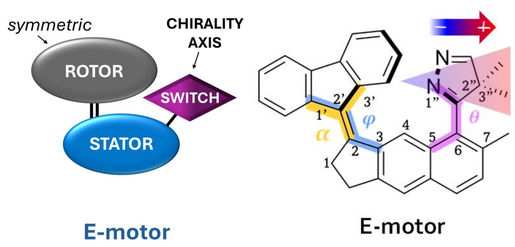
- Xenon in a great anesthetic but mechanism of its action is unknown
- one of the hypothesis: modulating the action of the neuron by influencing the lipids in cellular membranes
- the presented complexes have intermolecular interaction energy lower than –3 kcal/mol

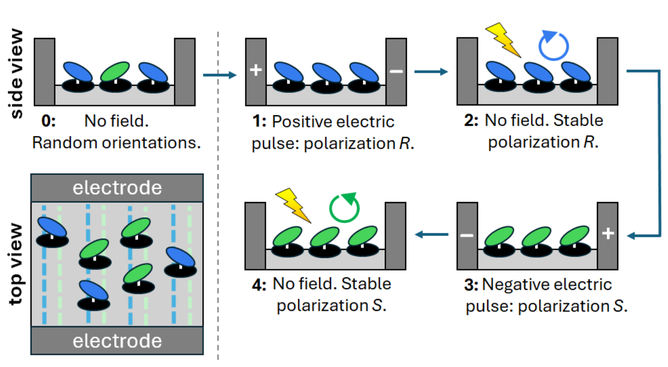
#3 Unidirectional molecular rotary motor with remotely-switchable rotation direction

Kamil Szychta (B.Sc.) and Joanna Jankowska

ChemRxiv
(DOI: 10.26434/chemrxiv-2024-vmxdz)

Light-driven rotary motors convert light energy into unidirectional nanoscale motion, with chirality determining the rotation direction but typically requiring chemical modification to change. We propose a new motor architecture, the E-motor, where rotation direction can be switched in situ using an external electric-field pulse without altering the chemical structure.





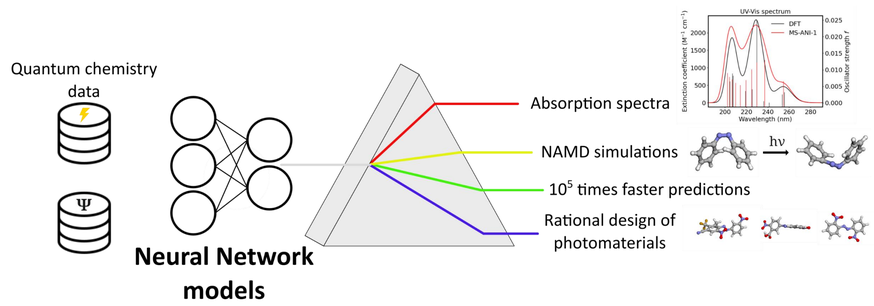
Quantum-chemical calculations and nonadiabatic molecular dynamics simulations on a tailored system (PFCN) demonstrate that chirality—and thus rotation direction—depends on the orientation of a polar switching unit controlled by the field.

#4 Developing machine learning methods for excited states' simulations

Mikołaj Martyka (M.Sc.) and Joanna Jankowska

Martyka et al., ChemRxiv
(DOI: 10.26434/chemrxiv-2024-dtc1w)

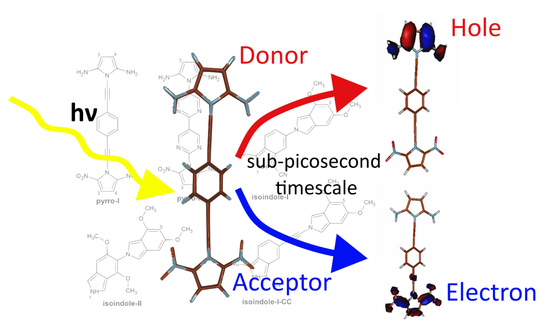
We develop deep neural networks machine learning models for simulating electronic excited states of molecules and their photodynamics. Our latest achievement is a physics informed multi-state model, which can make predictions with state-of-the-art accuracy for multiple electronic states, across chemical space. Coupled with an efficient active learning protocol, it can learn photodynamics of molecular systems with unprecedented speed. Now, we are extending this approach to a universal model that delivers out-of-the-box electronic spectra predictions at TD-DFT accuracy while reducing computational costs by a factor of 10^5.



#5 Polarized molecular wires for efficient photo-generation of free electric charge carriers

Mikołaj Martyka (M.Sc.) and Joanna Jankowska

We have designed and investigated properties of five all-organic polarized molecular wires (**PMWs**) for photovoltaic applications. Our systems, based on polarized pyrrole and isoindole moieties, exhibit efficient and ultrafast charge separation upon light absorption. We analyze their charge-carrier separation mechanisms and efficiencies through quantum-chemical calculations and nonadiabatic molecular dynamics simulations. Importantly, the proposed **PMWs** can be easily integrated into larger molecular frameworks, which enhances their potential for photovoltaic use.



Phys. Chem. Chem. Phys., 2024, Accepted Manuscript