

Computational Spectroscopy Research Group

@ 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

Students (2025/26):

Ph.D. candidates: 1
M.Sc. students: 3
B.Sc. students: 2

GENERAL RESEARCH SCOPE

Theoretical Spectroscopy
Light-Driven Processes in Molecules and Materials
Machine Learning Models for Theoretical Chemistry
Noble-Gas Chemistry
Molecular Circular Dichroism

RESEARCH PUBLICATIONS (2025/26)

- Martyka M., Tong X.-Y., Jankowska J., Dral P. O., **OMNI-P2x: a universal neural network potential for excited-state simulations**, *Nature Communications*, Accepted
- Martyka M., Jankowska J., Lischka H., Dral P. O., **Gradients not needed: ML-driven propagation of nonadiabatic molecular dynamics without reference gradients**, *Chemical Science*, 2026, Advance Article
- Szycha K., Danowski W., Jankowska J., **Unidirectional molecular rotary motor with remotely-switchable rotation direction**, *Science Advances*, 2025, 11, eadt8008.
- Sheng J., Van Beek C. L. F., Stindt C. N., Danowski W., Jankowska J., Crespi S., Pooler D. R. S., Hilbers M. F., Buma W. J., Feringa B. L., **General strategy for boosting the performance of speed-tunable rotary molecular motors with visible light**, *Science Advances*, 2025, 11, eadr9326.
- Deresz K. A., Mikhailov A., Jankowska J., Donà L., Civalleri B., Krówczyński A., Kamiński R., Schaniel D., Jarzemska K. N., **Experimental Evidence for the Solid-State Nitrite-Ligand Photoisomerization Mechanism in Nickel(II) Square-Planar Complexes**, *ACS Omega*, 2025, 10, 51940.
- Martyka M., Zhang L., Ge F., Hou Y.-F., Jankowska J., Barbatti M., Dral P. O., **Charting electronic-state manifolds across molecules with multi-state learning and gap-driven dynamics via efficient and robust active learning**, *npj Computational Materials*, 2025, 11, 132.
- Accomasso D., Jankowska J., **Quantum-Classical Simulations Reveal the Photoisomerization Mechanism of a Prototypical First-Generation Molecular Motor**, *Chemistry – A European Journal*, 2025, 31, e202403768.
- Szycha K., Martyka M., Jankowska J., **Theoretical Insights into Ultrafast Separation of Photogenerated Charges in a Push-Pull Polarized Molecular Triad**, *ChemPhysChem*, 2025, 26, e202400671.
- Martyka M., Jankowska J., **Polarized molecular wires for efficient photo-generation of free electric charge carriers**, *Physical Chemistry Chemical Physics*, 2025, 27, 5631.
- Jędrzejewski K., Misztal O., Cukras J., Pupel K., Borowski Ł.S., Pałys B., **Investigation of spectro-electrochemical processes of JC-1 cyanine dye combined with gold nanoparticles, an important indicator of mitochondrial membrane potential: theoretical and EC-SERS studies**, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2025, 345, 126801
- Cukras J., Skóra G., Kamiński J., Bouř P., Misztal O., Tarnowski A., Coriani S., **Magneto-Chiral Dichroism and Other Dichroic Spectra of [3]-to [8] Helicenes**, *The Journal of Physical Chemistry A: Forty Years of Response Function Theory (Special issue)*, 2025, 129, 11538

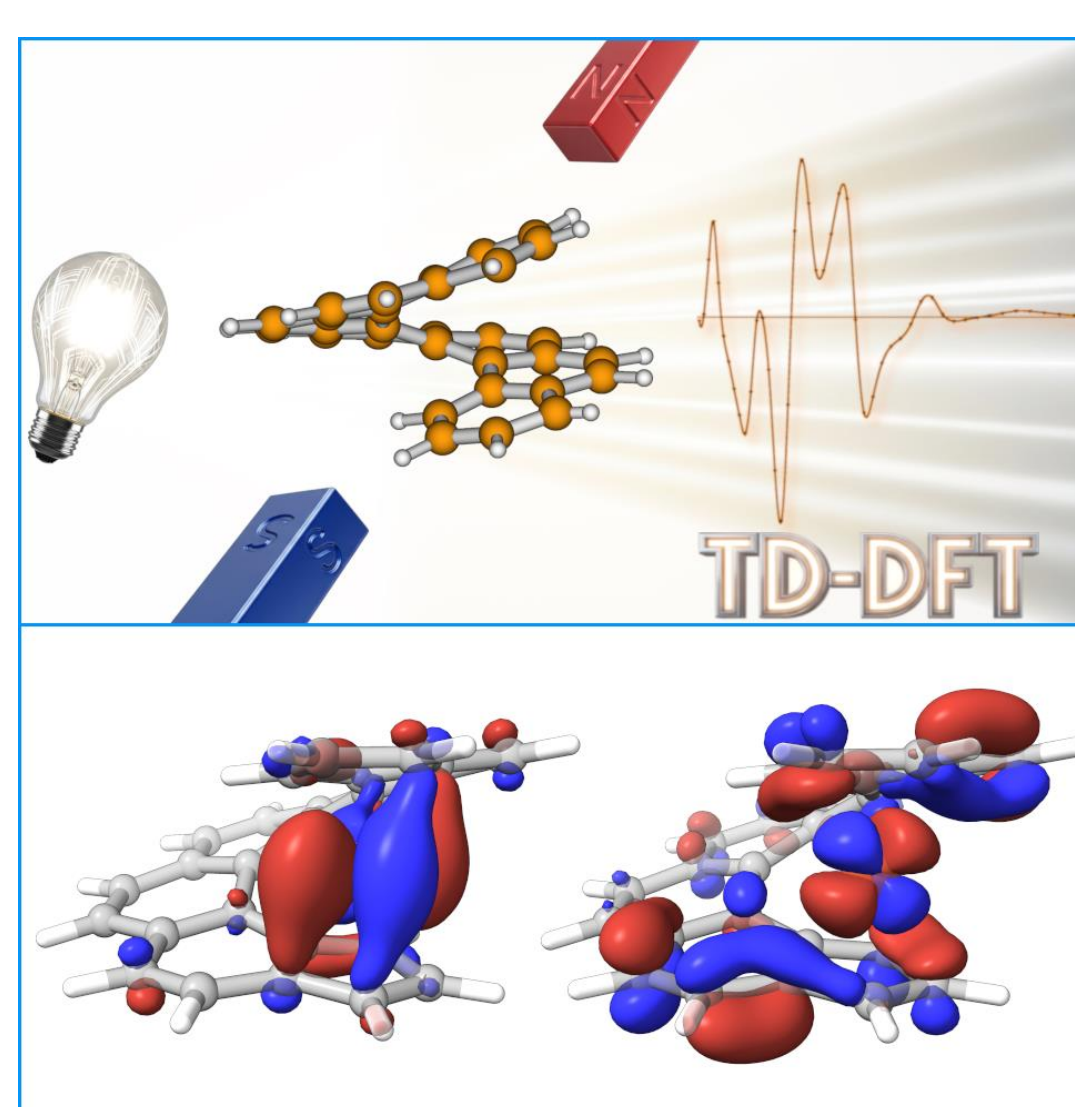
SELECTED ONGOING PROJECTS

#1 Magneto-Chiral Dichroism of Molecular Architectures: In Search of Strong Signals

CSRG members: Michał Andrzejewski, Jakub Szewczyk, Janusz Cukras

Magneto-Chiral Dichroism (MChD) is a fundamental, non-reciprocal chiroptical effect. It manifests as a difference in absorption depending on whether light propagates parallel or antiparallel to an external magnetic field. Due to typically weak signals, MChD remains experimentally elusive.

This project utilizes TD-DFT damped response theory to identify molecules exhibiting strong MChD. By investigating strongly chiral systems like carbo[n]helicenes and helical metallocenophanes, we demonstrate how structural parameters systematically amplify the MChD response. Moreover, we explore how the central metal atom in metallocenophanes influences the resulting dichroic spectra. Ultimately, this research aims to establish a computational framework for understanding complex chiroptical properties and aims to guide future experimental measurements.

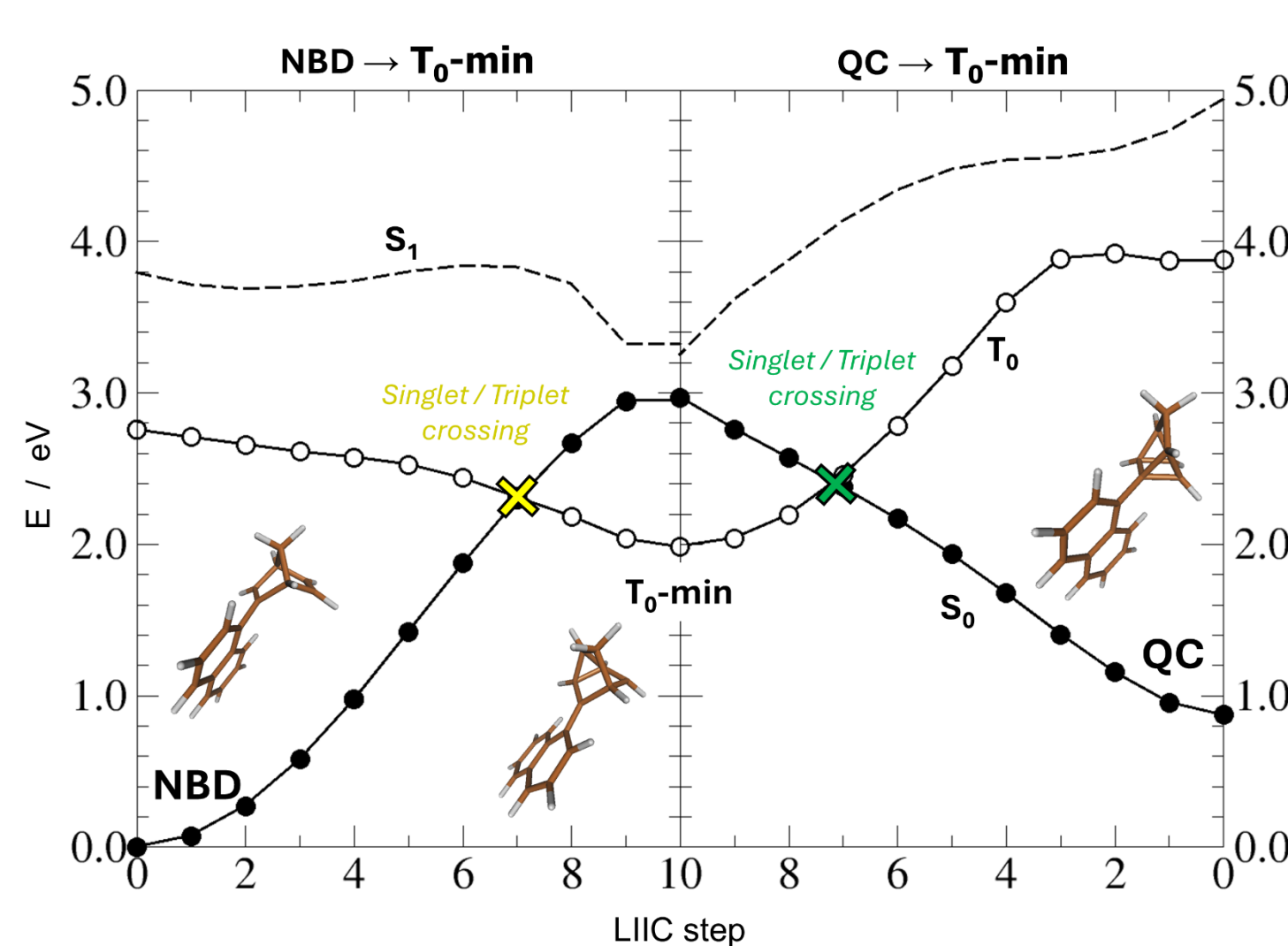


#2 Design and characterization of Molecular Solar Thermal (MOST) systems operating under visible-light conditions

CSRG members: Maria Piątek, Joanna Jankowska

MOST systems are an emerging class of materials that enable the storage of solar energy in the form of chemical bonds and its later release as heat. This is achieved using molecular photoswitches – compounds that undergo reversible structural changes upon light absorption. To date, the most widely studied MOST systems are modified norbornadienes and azobenzene derivatives, yet new exciting heterocyclic MOST candidates also emerge.

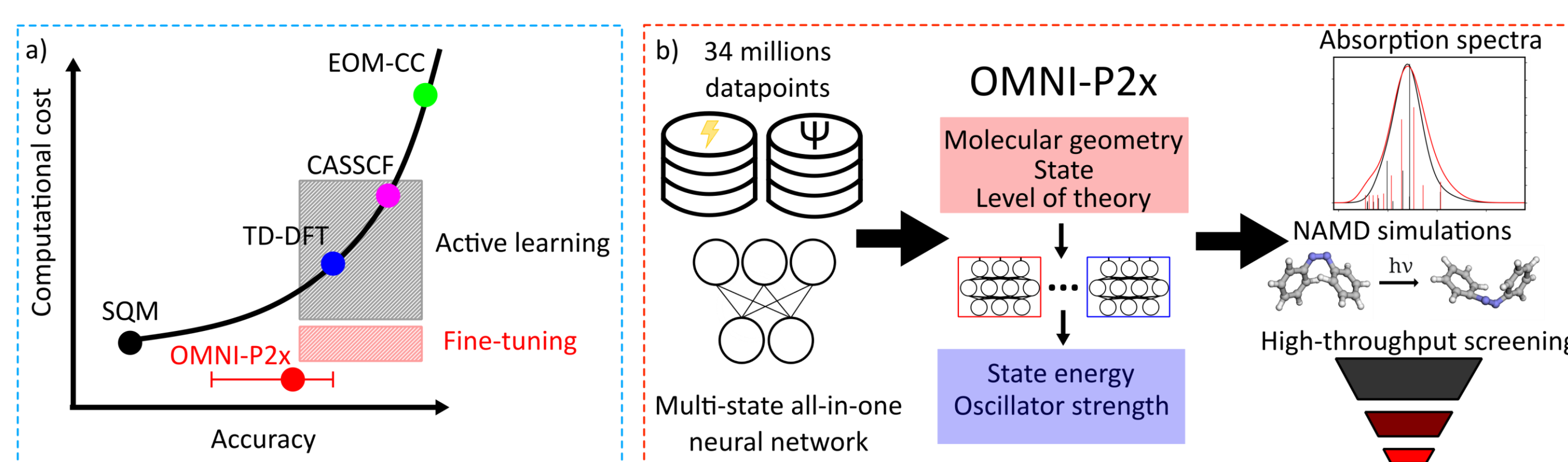
Our project aims to better understand the mechanisms governing the most promising MOST systems and to propose new molecules that overcome current efficiency limitations. We use molecular quantum chemical calculations at the DFT and *ab initio* level of theory to study the stability of key structures in ground and excited states, analyze potential energy surfaces of structural transformations, and evaluate optical and electronic properties.



#3 Machine learning for excited-state photodynamics

CSRG members: Mikołaj Martyka, Joanna Jankowska

Simulating how molecules respond to light demands millions of costly quantum-chemical calculations, restricting practical applicability. We develop neural network potentials that break through this limitation. A key component is a physics-informed multi-state model that can learn an arbitrary number of electronic states with near-perfect accuracy, paired with active learning that builds training data from scratch. These enabled **OMNI-P2x**: the first universal excited-state potential. Trained on 3 million molecules, it predicts UV/Vis spectra at TD-DFT quality while outperforming semiempirical methods in speed and accuracy, and serves as a powerful starting point for fine-tuning to higher levels of theory.

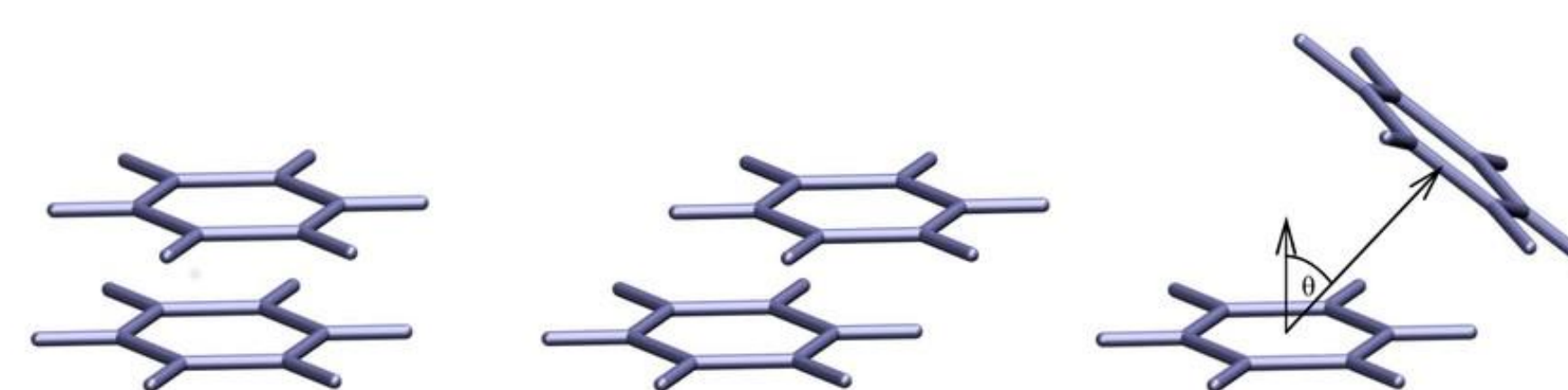
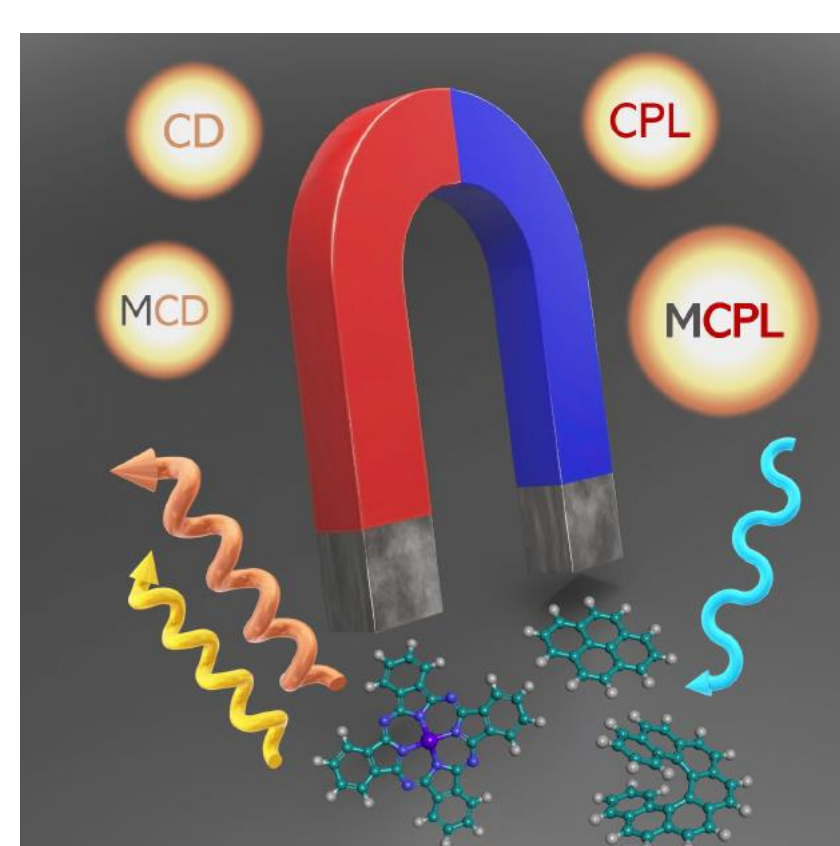


#4 Comparison of magnetic circular dichroism and magnetic-field induced circular luminescence of aromatic rings

CSRG members: Mikołaj Piekarek i 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, naphthalene, 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.