International Workshop on Molecular Excited States (MolEx2025)

Organized by

Molecular Modeling Group, Faculty of Chemistry
Nicolaus Copernicus University in Torun, Poland

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Molecular Excited States 2025 Workshop
Faculty of Chemistry, NCU Torun, Poland
Program Schedule

9 June, Monday

08:30 – 09:00	Registration
09:00 – 09:20	Opening Remarks
09:20 – 10:30	**Class 1: Dr. Dariusz Kędziera, NCU Torun, Poland**
10:30 – 11:00	Coffee Break
11:00 – 13:00	**Tutorial 1: Dr. Iulia-Emilia Brumboiu, NCU Torun, Poland**
13:00 – 14:30	Lunch Break
14:30 – 16:30	**Tutorial 2: Dr. Marta Gałyńska, NCU Torun, Poland**
16:30	Social Event

10 June, Tuesday

09:00 – 10:30	**Class 2: Prof. Mario Barbatti, Aix-Marseille University, France**
10:30 – 11:00	Coffee Break
11:00 – 13:00	**Tutorial 3: Dr. Josene M. Toldo, ENS Lyon, France**
13:00 – 14:30	Lunch Break
14:30 – 16:30	**Lectures:**
	14:30 – 15:15: Prof. Katharina Boguslawski, NCU Torun, Poland
	15:15 – 16:00: Dr. Grzegorz Kowzan, NCU Torun, Poland
	16:00 – 16:30: Dr. Patryk Rybczyński, NCU Torun, Poland
16:30	Old Town Tour

11 June, Wednesday

09:00 – 10:30	**Class 3: Prof. Mario Barbatti, Aix-Marseille University, France**
10:30 – 11:00	Coffee Break
11:00 – 13:00	**Tutorial 4: Dr. Josene M. Toldo, ENS Lyon, France**
13:00 – 14:30	Lunch Break
14:30 – 16:30	**Tutorial 5: Dr. Josene M. Toldo, ENS Lyon, France**
16:30	Conference Dinner

12 June, Thursday

09:00 – 10:30	**Class 4: Prof. Artur Nenov, University of Bologna, Italy**
10:30 – 11:00	Coffee Break
11:00 – 13:00	**Tutorial 6: Prof. Artur Nenov, University of Bologna, Italy**
13:00 – 14:30	Lunch Break
14:30 – 16:30	**Tutorial 7: Prof. Artur Nenov, University of Bologna, Italy**
16:30	Free

13 June, Friday

09:00 – 10:30	**Class 5: Prof. Pavlo Dral, Xiamen University, China**
10:30 – 11:00	Coffee Break
11:00 – 13:00	**Tutorial 8: Mikolaj Martyka, University of Warsaw, Poland**
13:00 – 14:30	Lunch Break
14:30 – 16:30	**Tutorial 9: Jakub Martinka, Heyrovsky Institute of Physical Chemistry, Czech Republic**
16:30	Closing

Serial Number of Poster Presenters

Poster-1	**Juliana de Abrantes**
Poster-2	**Youssef Badawy**
Poster-3	**Juliana Cuéllar-Zuquin**
Poster-4	**Karolina Kapusta**
Poster-5	**Jakub Martinka**
Poster-6	**Dilara Balci**
Poster-7	**Maneesh Pyla**
Poster-8	**Shambhavi Verma**
Poster-9	**Xin-Yu Tong**
Poster-10	**Mariana Yoshinaga**
Poster-11	**Mikolaj Gruba**
Poster-12	**Magdalena Lesiczka**
Poster-13	**Dawid Falkowski**
Poster-14	**Natalia Wiszowska**
Poster-15	**Dominika Tabor**
Poster-16	**Joanna Zams**
Poster-17	**Erik Vitols**
Poster-18	**Bittu Lama**
Poster-19	**Tomasz Gryber**
Poster-20	**Dr. Prashant Kumar**
Poster-21	**Jonas Weiser**
Poster-22	**Gabriel Lalou**
Poster-23	**Luca Cascone**
Poster-24	**Filippo Brunetti**
Poster-24	**Pedro Lara**
Poster-26	**Kanyarat Ruengboon**
Poster-27	**Manuel Martinovic**
Poster-28	**Krishnandu Dey**
Poster-29	**Chaiyaporn Lakmuang**
Poster-30	**Luo Sheng**

ABSTRACTS

P-1: Excited-State Relaxation in DNA Tetramers: A TD-DFT Investigation

Juliana G. de Abrantes, Josene Toldo, Mario Barbatti and Marco Sacchi

The photophysics of DNA oligomers is crucial for understanding UV-induced damage mechanisms. The relaxation pathways that nucleobases may undertake are highly dependent on the method and size of the system under investigation [1]. Previous studies primarily focused on monomers and dimers, but the relaxation pathways in larger DNA fragments remain underexplored. This work investigates the post photoexcitation relaxation of the heteropolymer CGGC and homopolymer CGCG (Figure 1) using time-dependent density functional theory (TD-DFT) combined with surface hopping. The relaxation from the excited state can take multiple competing pathways, and our goal is to statistically determine which mechanisms are most relevant. The heteropolymer has been reported to undergo proton transfer (PT) more frequently [2], while the homopolymer should favour the formation of cyclobutane pyrimidine dimer (CPD)[3]. Previous computational studies have often displayed some bias toward these specific outcomes, such as including only stacked thymines in the QM region of a quantum mechanics/molecular mechanics (QM/MM) model or relying on semiempirical methods that might not adequately describe charge distribution. In contrast, our current TD-DFT investigation, conducted without solvent inclusion, aims to establish an unbiased baseline for the core excited-state dynamics and photodamage pathways in these sequences.

In the future, we will extend this investigation by incorporating a QM/MM framework to explicitly account for solvent and DNA backbone interactions. This approach is essential to provide a more realistic description of energy dissipation and nonadiabatic relaxation, potentially altering the dominant relaxation mechanisms and offering deeper insights into the sequence-dependent photochemistry of DNA.

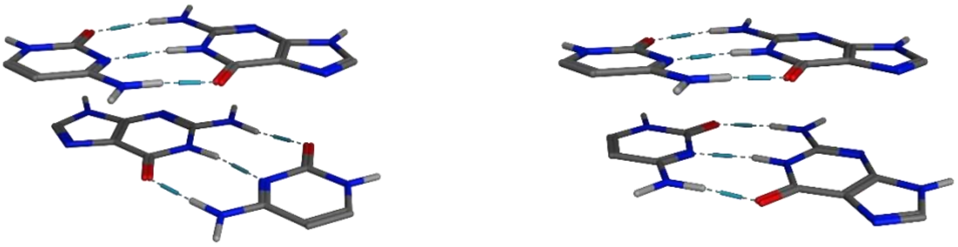

Fig 1: Hetero (left) and homopolymer (right) of guanine-cytosine base pairs.

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P-2: Exploring Electronic Structure in Thermally Activated Delayed Fluorescence Emitters Using Wavefunction-based Descriptors

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Thermally activated delayed fluorescence (TADF) systems, including multi-resonance (MR) and inverted singlet-triplet gap (INVEST) emitters, show great potential for applications such as organic light-emitting diodes due to their high emission efficiency. In this study, we investigate two important aspects of MR/INVEST emitters: their electronic structure and excited-state rate constants. First, we study the relationship between the electronic structure of MR/INVEST emitters and their energy gaps using wavefunction-based descriptors. These descriptors, originally proposed for ionic states, measure the distribution of charges in atomic centers based on the transition density matrix. Here, we directly analyze the transition density matrix connecting the singlet and triplet excited states involved in TADF. Our findings reveal a correlation between the wavefunction descriptor and the energy gap, with smaller (more negative) gaps corresponding to higher descriptor values. The descriptors also distinguish excited states involved in TADF within the triplet manifold. Then, we identified the potential deactivation pathways using vibronic calculations. We calculated excited-state decay rate constants, including fluorescence, direct and reverse intersystem crossing (RISC), where we assess the importance of Herzberg-Teller effects and broadening functions, among other parameters. Optimized structures and Hessians are obtained at (TDA)-DFT/CAM-B3LYP, and excitation energies are calculated using SCS-CC2 and ADC(2) to ensure accurate energy values for rate calculations and energy gaps. Overall, the calculated RISC rate constants align well with experimental values, typically within one order of magnitude, with the Herzberg-Teller correction playing a dominant role.

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P-3: Revealing the Impact of Active Space Selection in DNA Photochemistry

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Conical intersections (CIs) play a key role in the ultrafast deactivation of DNA/RNA nucleobases after UV excitation, mediating the efficient funneling down of excited-state population and converting it into thermal energy. These processes are essential for understanding DNA photostability and damage, making the accurate description of CIs crucial for simulating these phenomena. This study investigates the CIs between the lowest electronic states of various DNA/RNA nucleobases using high-level quantum chemistry methods to better understand their role in photoinduced processes.[4]

We use Cholesky decomposition-based Complete Active Space Self-Consistent Field (CASSCF) calculations, and characterize the CIs of all canonical DNA/RNA nucleobases: uracil, thymine, cytosine, adenine, and guanine. Different active spaces were explored for each nucleobase and CI type to assess the effect of the retained electron correlation on CI topographies. The research also examined the influence of basis set size, comparing double-ζ and triple-ζ contractions, to gauge the impact of computational cost on the accuracy of CI descriptions.

The results show CI topographies are highly sensitive to the amount of electron correlation included in the model, displaying significant variations when changing active space size. Interestingly, structural changes in the optimized geometries were minimal, suggesting that CI topographies are primarily influenced by the accurate description of the electronic states involved, rather than by geometry optimization procedures.

In conclusion, the study emphasizes the critical role of choosing an appropriate active space for accurately modeling conical intersections in DNA/RNA nucleobases, highlighting how variations in active space impact these calculations. The findings provide valuable insights into the influence of electron correlation on photoreactions, not only in the context of DNA but also in other fields, such as material science, where light-matter interactions are crucial.

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P-4: Modelling Excited State Dynamics of Organic Materials in the Condensed Phase

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Understanding the excited state dynamics in organic crystals is crucial for technological applications such as organic electronic devices, photovoltaic cells, and organic light-emitting diodes. In the condensed phase, organic luminescence can often be quenched due to the presence of intermolecular interactions. Occasionally, however, aggregation can enhance emission by stopping non-radiative energy dissipation pathways, leading to polymorph-dependent luminescence. [1] This can be due to the presence of hydrogen bonds, which play a significant role in processes such as excited-state intramolecular proton transfers (ESIPT). [2]

More work is needed to understand the competition of photochemical processes occurring, such as ESIPT and charge transfer (CT). Moreover, the complexity of molecular aggregates poses challenges such as increased computational cost, as well as the interactions between surrounding monomers. [3] Mutai *et al.* showed polymorph-dependent luminescence in an ESIPT chromophore, 2-(2'-hydroxyphenyl)imidazo[1,2-a]pyridine (HPIP), highlighting the importance of crystal packing and its effects on photophysical processes such as ESIPT. [4]

Potential energy surfaces (PESs) of the organic monomer HPIP in the condensed phase were calculated for both polymorphs and were modelled with Fromage, which uses the ONIOM scheme to model the organic crystal environment. [5] The PESs showed differences in excited-state tautomer stabilization based on the crystal environment. Preliminary results with trajectory surface hopping in the condensed phase modelled with point charge embedding show differences in ESIPT times between monomers of different polymorphs. We plan that our investigation will provide more insight into the photophysical processes that occur in molecular aggregates by excited-state dynamic modelling.

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P-5: A Descriptor Is All You Need: Accurate Machine Learning of Nonadiabatic Coupling Vectors

Jakub Martinka[1,2], Lina Zhang[3], Yi-Fan Hou[3], Mikołaj Martyka[4], Jiri Pittner[1], Mario Barbatti[5,6], Pavlo Dral[3,7,8]

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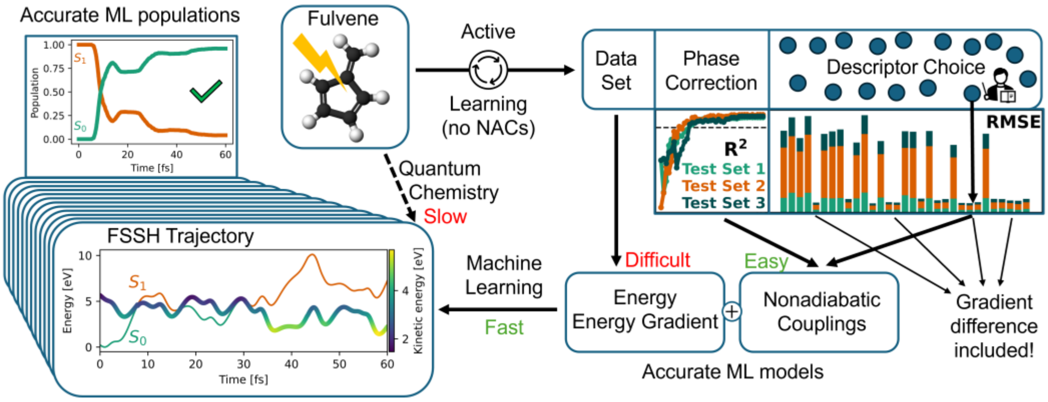
Nonadiabatic couplings (NACs) play a crucial role in modeling photochemical and photophysical processes with methods such as the widely used fewest-switches surface hopping (FSSH). There is therefore a strong incentive to machine learn NACs for accelerating simulations. However, this is challenging due to NACs' vectorial, double-valued character and the singularity near a conical intersection seam. For the first time, we design NAC-specific descriptors based on our domain expertise and show that they allow learning NACs with never-before-reported accuracy of R^2 exceeding 0.99. The key to success is also our new ML phase-correction procedure. We demonstrate the efficiency and robustness of our approach on a prototypical example of fully ML-driven FSSH simulations of fulvene targeting the SA-2-CASSCF(6,6) electronic structure level. This ML-FSSH dynamics leads to an accurate description of S_1 decay while reducing error bars by allowing the execution of a large ensemble of trajectories. Our implementations are available in open-source MLatom.



P-6: LOV Photoreceptor Engineering: From Mechanistic Simulations to Machine Learning

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Computational spectroscopy, particularly quantum mechanics/molecular mechanics (QM/MM) methods, has become an indispensable tool for investigating the photophysical and photochemical properties of protein-based chromophores. These techniques provide critical insights into electronic structure, excited-state dynamics, and reaction mechanisms, thereby enhancing our understanding of light-activated processes in photoreceptors. Our research focuses on the spectral engineering of light, oxygen, voltage (LOV) domain-based fluorescent proteins, integrating computational and experimental approaches. Using QM/MM simulations and spectroscopic measurements, we analyzed the iLOV-Q489K variant, identifying key excited-state properties that contribute to fluorescence tuning.[1]. Structural and mechanistic analyses of flavin-binding fluorescent proteins allowed us to pinpoint residues responsible for spectral shifts, enabling rational fluorescence engineering.[2] We also investigated the structural and photophysical properties of LOV-based fluorescent proteins in various crystalline and solution environments. By applying time-resolved spectroscopy and X-ray crystallography, we investigated how chromophore-protein interactions govern fluorescence quantum yield and photostability. Our findings highlight the role of hydrogen bonding networks and conformational flexibility in tuning LOV photoreceptor function.[3] A major breakthrough in our work was the reengineering of proton transfer (pT) pathways in the naturally non-photoreducible iLOV protein [4]. Through a single amino-acid substitution (Q489D), we enabled efficient photoreduction, demonstrating an intrinsic electron transfer (eT) pathway. Using site-directed mutagenesis, UV/Vis and transient absorption spectroscopy, and electron paramagnetic resonance (EPR), we provided strong evidence that conserved Tyr and Trp residues facilitate flavin photoreduction. This suggests that photoreduction capability is evolutionarily embedded in all LOV domains, while pT pathways modulate the stability of the neutral semiquinone radical. Furthermore, leveraging our machine learning-assisted spectral engineering,[5] we successfully designed LOV domain variants with fine-tuned dark recovery kinetics, expanding their functional range for optogenetic applications[6]. This integration of computational and experimental methodologies enhances our ability to manipulate LOV photoreceptors for advanced bioimaging and optogenetics.

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P-7: Exploring electronic resonances in pyridine: Insights from Orbital Stabilization Techniques

Maneesh Pyla and Spiridoula Matsika

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Understanding low-energy electron attachment to cyclic conjugated molecules, such as the nucleobases, may provide valuable insights into radiation-induced damage of genetic information carriers, such as DNA. Pyridine, a molecule structurally similar to pyrimidine nucleobases, serves as a useful model for investigating how such molecules interact with low-energy electrons. Our study was focused on forming negative ion resonances in pyridine due to low-energy electrons below the ionization threshold (≈10 eV). Our primary objective was to identify and characterize the π resonances in pyridine using high-level electronic structure theory combined with orbital stabilization techniques (OSM). For this, we implemented and applied both quadratic and cubic generalized Padé approximant (GPA) methods to calculate the resonance parameters, energies, and lifetimes in pyridine using OSM and compared the results with previous theoretical and experimental values. In our study, we identified a total of eight resonances, four with $^2B_1$ symmetry and four with $^2A_2$. Notably, one of the $^2B_1$ and two of the $^2A_2$ resonances were previously unreported in experimental studies, highlighting significant new findings from our research. The two lowest energy resonances are identified as one-particle shape resonances, while the others are mixed or primarily core-excited (two-particle one-hole) resonances, which are generated by attaching an electron to an excited state of the neutral. We found that multi-reference perturbation theory offered the most accurate description of these resonances, particularly for states with mixed character. Additionally, analyzing resonance decay channels through the calculation of Dyson orbitals provided deeper insights into the nature of these resonances.

References:

Pyla, M., & Matsika, S. (2024). Exploring electronic resonances in pyridine: Insights from orbital stabilization techniques. *The Journal of Chemical Physics*, *161*(15).

P-8: Bridging Classical and Quantum Dynamics: A Stable and Generalizable Approach for Nonadiabatic Transitions

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Simulating excited-state molecular dynamics requires accurate modeling of nonadiabatic transitions, where nuclei evolve on multiple electronic States. Among mixed quantum-classical approaches, fewest switches surface hopping (FSSH) remains widely used due to its simplicity and efficiency. However, challenges such as incomplete decoherence treatment, frustrated hops, and velocity reversals can sometimes lead to inconsistencies in state populations and nuclear motion. Also, the independent trajectory approximation, which assumes that nuclear motion follows a single classical path without collective quantum effects, comes up like generally non intuitive formalism.

To improve upon this, recent developments have introduced coupled-trajectory methods, which allow information exchange between trajectories to better conserve coherence, and multiple spawning approaches, which enhance wavefunction representation by dynamically creating new basis states in regions of strong nonadiabatic coupling.

In this work, we aim to propose a method that would be an extension of these trajectory-based techniques, integrating their strengths to create a more stable and accurate framework for nonadiabatic dynamics. Our approach aims to provide a systematic and mathematically rigorous treatment of decoherence, ensuring stability while remaining applicable to wide molecular systems. By bridging the gap between classical trajectory-based and fully quantum mechanical methods, this approach will offer a promising tool for studying excited-state dynamics in both gas-phase and condensed-phase environments, making it a viable choice for real systems.

P-9: Theoretical Study of Donor-Acceptor Alternating Fused Compounds and Outlook for Machine Learning Interatomic Potentials for Excited States

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Quantum mechanics (QM)-based excited-state simulations provide meaningful insight into the fundamental nature of electronic excitation and are a powerful tool in designing photocatalysts and photo-materials. For example, we used QM methods to elucidate the nature of the electronic excitations in the DACs, namely, hyper-conjugated molecules composed of alternating naphthalene diimide (NDI) and thiophene units[1]. These molecules have attracted much attention due to their unique photophysical properties. In these simulations, we used MLatom[2-5] to perform the TD-DFT analysis based on the ground-state geometries optimized with an AI-enhanced QM method (UAIQM[6, 7]). The TD-DFT results show that thiophene units act as donors and NDI units act as acceptors during the molecular excitation, and the simulation of the UV-vis spectra (Figure 1) shows that with the expansion of conjugated units, the UV-vis absorption spectra of DACs are only slightly red-shifted. The electronic-hole plot analysis shows that during the excitations, the electronic effect is the charge transfer from thiophene units to NDI units (major) and local excitation on NDI and thiophene units (minor). The theoretical investigation of the optical and electronic properties of DACs could potentially contribute to the rational design of novel photochemical and electrochemical materials.

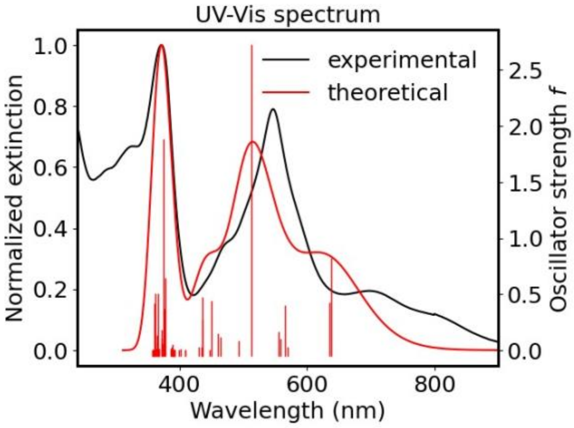

Figure 1. Selected UV-vis spectrum obtained with MLatom (the theoretical spectrum is shifted by 56.24 nm and shown with a bandwidth of 0.25)

However, the computational cost of high-accuracy QM methods is expensive, which hinders the design of materials with desired photophysical and photochemical properties. Machine learning interatomic potentials (MLIPs) provide a data-driven approach to predict chemical properties with a force-field cost, with an accuracy comparable to the reference QM methods they were trained on. While MLIPs are developing rapidly for molecular ground-state properties predictions, the research on MLIP for excited-state properties prediction has been slower due to the complexity of the excited-state electronic density. To lay a solid foundation for excited-state MLIP, we collected datasets containing molecular excitation information, on which we trained the multi-State ANI (MS-ANI[8]) neural network as implemented in MLatom[2-5]. The results show that it is potentially possible to create the foundational excited-state MLIPs[9, 10].

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P-10: Evaluation of Flavonoid-Based Candidates as Photosensitizers in Photodynamic Therapy: Photophysical and Photochemical Analysis

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Photodynamic therapy (PDT) involves the excitation of a photosensitizer (PS) by light, promoting its transition from the ground state (S_0) to excited singlet states. Intersystem crossing may allow population of triplet states, where interactions with molecular oxygen ($^3O_2$) can generate reactive oxygen species. This process follows either a Type I mechanism (electron transfer) or a Type II mechanism (energy transfer leading to singlet oxygen ($^1O_2$) production).

A promising application of PDT is in agriculture, where microbial contamination leads to significant economic losses and health risks. Antimicrobial PDT has demonstrated effectiveness against pesticide-resistant microbial strains without negatively affecting plant growth or food safety.[1] Natural PSs offer advantages over conventional pesticides, as their degradation products can be metabolized by plants, reducing environmental impact.

Flavonoids (Fig. 1), a class of natural pigments, have gained significant interest due to their therapeutic potential. Recent studies suggest that the generation of triplet states enables flavonoids to act as key photosensitizers in photochemical processes.[2]

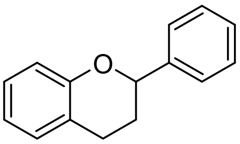

Figure 1. Molecular structure of the basic flavonoid backbone

This study uses computational chemistry to evaluate flavonoid derivative compounds as potential photosensitizers for antimicrobial PDT. Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) were employed to analyze spectroscopic and photophysical properties, as well as the thermodynamic feasibility of charge and energy transfer reactions between the excited-state photosensitizers and molecular oxygen, providing insights into their potential as effective photosensitizers.

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P-11: Possible Interstellar Benzonitrile Formation via Photoinduced Charge Transfer

Mikołaj Gurba, Rafał Szabla

Benzonitrile has been proposed as a precursor in the interstellar formation of polycyclic aromatic hydrocarbons (PAHs). Its presence in the interstellar medium was first detected in 2018 [1], and a possible formation pathway involving ice grains containing benzene and acetonitrile (ACN) was subsequently proposed [2]. This reaction is triggered by the irradiation of these ices with Lyman-alpha photons, but the exact chemical mechanism remains unclear.

We investigated this mechanism using ADC(2), TDDFT, and CASPT2 methods. Our results suggest that the direct formation of a benzonitrile precursor is possible via a photoinduced charge transfer process. Excitation of the benzene-ACN complex with Lyman-alpha photons provides sufficient energy to transfer an electron from benzene to acetonitrile. The resulting excited state can relax to the ground state through a minimum energy crossing point, leading to a [2+2] cycloaddition reaction. The cyclic product of this reaction can be further excited and relaxed to the ground state, yielding at least three different products, one of which serves as a precursor to benzonitrile.

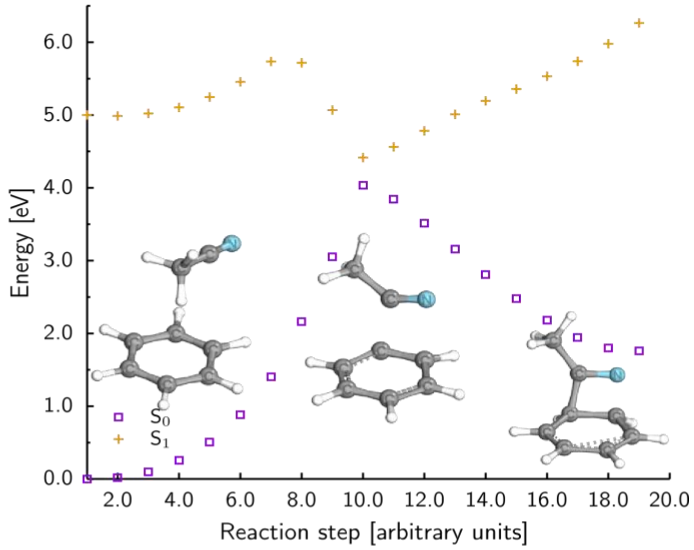

Figure 1. Benzene and ACN cycloaddition reaction pathway.

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P-12: Spiropyran to Merocyanine Conversion

Magdalena Lesiczka

Photochromism is the phenomenon of changing the optical properties of a compound when exposed to light. In this project, we study such compounds, focusing on spiropyrans and merocyanines. The project is aimed at discovering interesting features, such as various colors, among others, which could be used in construction, color-changing eyeglass lenses, or as photoswitches.

The results of the optimization of structures and simulation of NitroBIPS spectra using various functionals are presented. Calculations were carried out using the TD-DFT method and ORCA software to predict the position and intensity of absorption bands. The calculation time for different functionals was analyzed, showing that the PBE0-D3BJ provides the shortest calculation time with sufficient accuracy. The computation results for the CCC and TCC isomers of NitroBIPS show similarity with the experimental data for the PBE0-DH and PBE0D3BJ functionals. A comparison of free Gibbs energies and the absorption spectra of the CCC, TCC, CCT and TTC isomers calculated using the Vertical Gradient (VG) and Adiabatic Hessian After a Step (AHAS) methods showed that the CCT and TTC forms give results closest to the experimental spectrum.

The work provides important information on the selection of suitable methods for the simulation of NitroBIPS spectra, which may be important for future research on this compound. Calculations confirmed the agreement of theoretical and experimental results, which is crucial for future research on NitroBIPS. To verify which of the above two isomers is in solution, thermodynamics calculations are recommended.

P-13: Computationally supported SSbD design of Solid Oxide Electrolyzer Cell anodes: Integrating Quantum Mechanical calculations with Machine Learning methods

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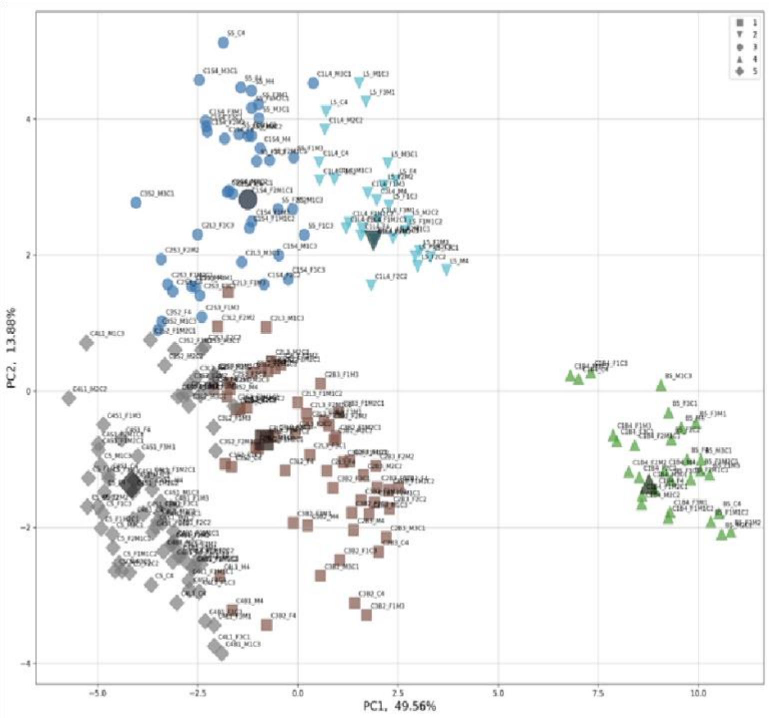
Solid Oxide Electrolyzer Cells (SOEC) systems represent a promising alternative to traditional energy sources in the energy transition process. These systems are capable of both producing and generating hydrogen in a reversible cycle. Unfortunately, there is still lack of knowledge how to use more efficient SOEC systems. The research employed a computational approach to propose designs for SOEC anode components that are free of lanthanum (REE metal), thereby aligning with the principles of SSBD (*Safe and Sustainability by Design)* approach. For the first time, we introduce a combined quantum mechanical and machine learning approach to support the SOEC design process. This approach eliminates the need for expensive and resource-intensive experimental studies and significantly reduces the number of structures required for experimental validation.

As part of the research, molecular models were developed for 240 structures that could potentially serve as anode configurations for SOEC cells. The doped Brownmillerite systems are represented by a fragment consisting of 29 atoms (20 oxygen atoms, with 5 in octahedral center positions and 4 in tetrahedral center positions).

Calculations for 240 potential SOEC structures were performed using the Gaussian16 computational chemistry software package, applying density functional theory (DFT) at the MN15/LANL2DZ/6-31G level. From these calculations, a set of quantum mechanical descriptors was obtained. Based on these descriptors, machine learning analysis was applied to characterize and group similar samples according to the QM-derived descriptors. Five groups were identified, and using the k-means method, the most promising representatives were selected for further experimental evaluation.



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Acknowledgments

The study was conducted under funding that has been received from the European Union’s Horizon Europe research and innovation programme via the NOUVEAU project Grant ID: 101058784 and support from the Polish Ministry of Science and Higher Education within the programme “Doktorat Wdrożeniowy 2023” Grant ID DWD/7/0321/2023.

P-14: Excess electron binding energy nearing 15 eV in polynuclear antimony fluoride anions: structural evolution from molecules to nanoscale clusters

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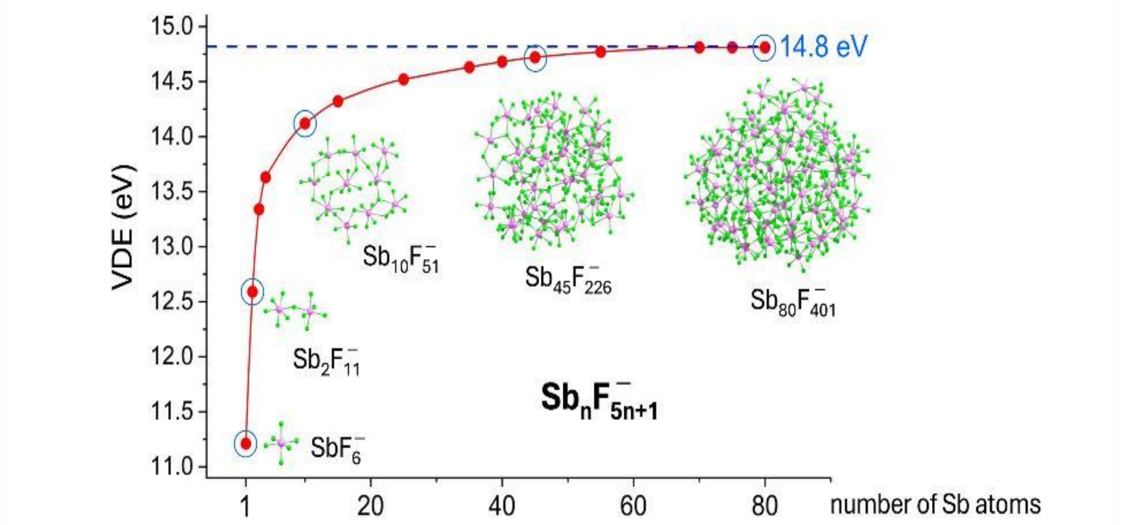
The excess electron binding energies of $(Sb_nF5_{n+1})-$ (n = 2–80) polynuclear superhalogen anions were investigated using a density-functional tight-binding method (GFNn-xTB), allowing for the analysis of nanoscale systems with nearly 500 atoms. The molecular structures generated by this approach were validated, and the predicted binding energies were calibrated by comparing them with results from an ab initio method (DFT). This enabled an assessment of the electronic stability of anions containing up to 80 antimony atoms. The study also discusses the saturation of excess electron binding energies for anions with n ≥ 65 and reports the highest recorded binding energy for a molecular anion, nearing 15 eV.



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P-15: Understanding photophysical features of a coumarin derivative via quantum chemical calculations

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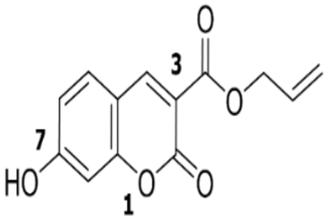

Fig. 1. Examined coumarin derivative.

Organic luminescent materials showing such fascinating photophysical properties as dual fluorescence (*DF*) produced by a single excitation and room-temperature phosphorescence (*RTP*) [1] have been gaining increasing attention due to broad applications in optoelectronics and bioimaging. In this context, coumarin derivatives emerge as especially promising because of their photostability, high quantum yield, and ability to tune their properties through structural modifications. Importantly, to ensure a deep understanding of structure-properties relationships in such systems theoretical studies via quantum-chemical calculations appear indispensable. Recently, a coumarin derivative with an electron-withdrawing ester and electron-donating hydroxyl groups at positions 3 and 7, respectively (Fig. 1), have been synthesized and its photophysical properties have been experimentally studied, showing occurrence of *DF* in methanol [2] and possibly *RTP* upon immobilization in a polymer matrix [3]. The goal of the presented work is to develop a reliable theoretical model to explain observed emission properties of the system.

The performed calculations included geometry optimizations in the ground S_0 and excited S_1 and T_1 states ((time-dependent) density functional theory (DFT)) with solvent (methanol) effects modelled via a polarizable continuum model. Additionally, a wavefunction-based correlation method at the coupled cluster (CC) level was used to asses emission energies. The possible intersystem crossing (ISC) mechanism was evaluated via computed spin-orbit coupling (SOC) interactions between S_1 and low-energy triplet excited states.

Fluorescence emission energies computed for different conformers do not change much with a change in the ester' spatial arrangement and correspond well with a higher-energy signal in the experimental spectrum, especially at the CCSD level of theory. *DF* effect cannot be thus explained based on the co-existence of various rotameric structures; ongoing studies consider aggregation and explicit solvent effects to explain this phenomenon. Interestingly, while ester' arrangement does not affect much fluorescence energy, the obtained SOC values indicate its strong impact on ISC efficiency.

Acknowledgements. We gratefully acknowledge the Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within the computational grant no. PLG/2024/017662.

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P-16: Photocatalytic CO2 reduction – theoretical study on a Cu(I) photosensitizer

Joanna Zams

Rising atmospheric CO_2 levels are considered one of the major reasons for the quick progression of global warming. Therefore, combating high CO_2 concentration via different pathways is currently one of the main research purposes of many groups. Photoactivated CO_2 reduction is one of the possible pathways towards achieving that goal. The photocatalytic system typically consists of a photosensitizer, a catalyst, and an electron donor. One of the main challenges of this approach is designing a photosensitizer that is both effective and can be prospectively used in an upscaled process. Heteroleptic copper(I) complexes Cu(I)(N^N)(P^P) have emerged as promising alternatives. They have been synthesized and their photocatalytic properties have been confirmed. However, in order to elucidate the molecular mechanism of the photoreduction reaction, an in-depth understanding of the complex's excited states' character and their time evolution is crucial, which may be achieved only through the use of computational chemistry methods. Due to the size of the complexes in question, the computational methods that may be employed are nearly limited to DFT-based methods. However, DFT and its time-dependent variant famously struggle with cases with large regions of π-electron delocalization and significant charge transfer character, both of which are present in the Cu(I) complexes. Additional difficulty in conducting such research is the scarcity of available experimental data.

Therefore, the aim of my research was to establish a computational scheme which on the one hand will allow one to reliably describe the excited states of the Cu(I)-based complexes in terms of energetics and structural changes upon excitation, and which on the other hand will be computationally cost-effective to enable extensive studies of such large systems. The chosen method is then put to the test by comparing the obtained results with the experimental ground state and transient absorption spectra.

P-17: RIXS: How well does Time-Dependent Density Functional Theory Perform?

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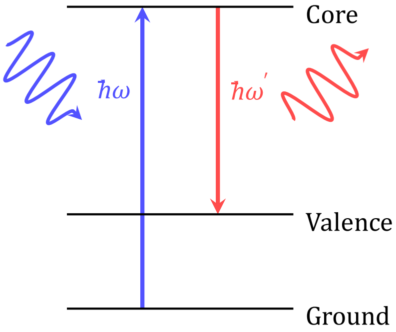

Resonant inelastic X-ray scattering (RIXS) stands as one of the most information-rich spectroscopic techniques, uniquely capable of probing excited states through their dependence on momentum, energy, and polarization. Recent advances, particularly through the use of X-ray free electron lasers (XFELs), have pushed the experimental limits of RIXS, achieving unprecedented spectral resolution [1]. However, the inherent difficulty in interpreting RIXS signals underlines the critical need for both accurate and efficient spectral calculations to facilitate their understanding. While hierarchical methods such as the algebraic diagrammatic construction (ADC) scheme for the polarization propagator have shown promising results in the calculation of RIXS spectra [2], these methods suffer from high computational costs. To enable fast and efficient RIXS calculations, we have evaluated and benchmarked the performance of linear response time-dependent density functional theory (LR-TDDFT) approaches on a set of organic molecules. Using ADC at the ADC(2), ADC(2)-x, and ADC(3/2) levels of theory as references, two LR-TDDFT approaches have been investigated: subspace-restricted LR-TDDFT [3], which uses a subset of occupied and virtual orbitals, and the two-shot LR-TDDFT approach [4], where the core- and valence-excited states are calculated separately. In this work, we benchmark a range of density functionals – including hybrid, range-separated, and tailored range-separated variants – to establish a foundation for applying LR-TDDFT to RIXS spectral calculations. Our benchmark enables computational approaches to keep pace with experimental advancements and provides a framework for reliable predictions – paving the way for future applications of LR-TDDFT in RIXS studies.

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P-18: Photoinduced Excited-State Relaxation Mechanism in Para-Amino Derivatives of GFP Chromophore

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Photoinduced *cis-trans* switching behaviour of Green Fluorescent Protein (GFP) chromophore and its derivatives plays a pivotal role in the myriads of photochemical dynamics and has emerged as of great interest in various applications. These light-controlled switching behaviour of GFP-like chromophores, which toggle between fluorescent 'on-state' and a nonfluorescent 'off-state' is governed by the rotation of exocyclic methine bridged single and double bonds within the chromophore. Here, based on the *ab initio* electronic structure approaches in conjunction with Tully's Fewest Switches surface hopping dynamics, we investigated the ultrafast photoinduced *cis-trans* isomerization phenomenon in the para-amino derivative of GFP chromophore. Upon excitation into the Franck-Condon region, the chromophore relaxes to ground-state (S_0) via various photochemical pathways, which involve S_1/S_0 internal conversion. The amino group possesses "coherent photoinduced ICT" effects, which pull down the Z/E photoisomerization barriers, facilitating the tortional motion of exocyclic methine-bridged bonds and thereby enabling efficient S_1/S_0 relaxation processes. Thus, this work is about the effect of the para-amino group in conjugation during cis-trans ultrafast photoisomerization phenomena. The findings can be useful in enhancing our understanding of excited-state dynamics and help to establish correlations between structure and dynamics.

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P-19: Proton Transfer from Deprotonated 8-oxoguanine to Adenine: A Theoretical Study

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According to the RNA world theory, life originates from RNA molecules capable of self-replication.[1] Such early molecules had to be capable of conducting basic biochemical reactions. While there are proofs for RNA being able to carry out some of them, for redox reactions, there is still little evidence. One of the most frequently proposed candidates for the ancestor of redox cofactor is 8-oxoguanine (8OG). Similarities between the chemistry of 8OG and flavin/dihydroflavin systems have been reported.[2] This system is a part of modern redox cofactor – flavine adenine dinucleotide (FAD/$FADH_2$). Experimental studies show that 8OG is capable of repairing thymine dimers[3] and that the repair rate increases in slightly basic solutions, which suggests that the deprotonated form of 8OG may be responsible for the reaction.[4] In this work, the alleged precursor of FADH2, dinucleotide of 8OG- and adenine (O-AD), is modeled with a complex of both nucleobases(O-A). Some calculations were performed for a model with methyl groups attached to N9 atoms to retrieve part of the steric effects. A S1/S0 conical intersection (CI) was detected, in which a proton transfer occurred from the N7 atom of 8OG- to the C8 atom of adenine. A LIIC reaction path from the optimized ground state to the CI was obtained. Calculations were performed at the SOS-MP2[5]/cc-pVDZ level for the ground state and at the SOSADC(2)/cc-pVDZ level for the excited state. CI was found as a crossing point of PESs calculated at the mentioned levels by using the algorithm proposed by Levine et al.[6]. It minimizes the energy function with a penalty function. Its major advantage is calculating CIs without a need for nonadiabatic coupling vectors. Calculations were benchmarked against MRSF-TDDFT[7]/cc-pVDZ level with a modern DTCAM-VEE[8] functional optimized for vertical excitation energies and D3 dispersion correction.

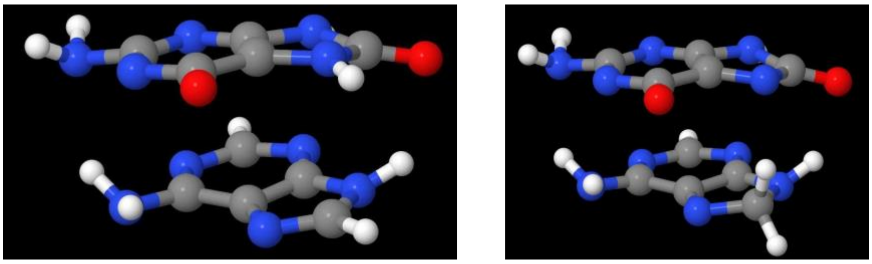

Figure 1: O-A complex: ground state (left), conical intersection (right)

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P-20: Deciphering the Mechanisms Behind Efficient Doublet Emission in Radical-Based Light-Emitting Diodes

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The emission in radical-based organic light-emitting diodes (OLEDs) originates from a spin doublet state rather than singlet or triplet excitons. In these OLEDs, the emission process is spin-allowed, circumventing the limitations imposed by triplet excitons.[1] However, some radicals typically exhibit low optical absorption and photoluminescence yields while others very emissive through the lowest first excited doublet state (D_1), making it crucial to understand the underlying mechanisms of how D_1 state is reached from the doublet ground-state (D_0) and establish design principles to enhance the absorption and luminescence yields of radical emitters.[2] To the best of our knowledge, no simulations of the complete pathway from D_0 to D_1 have been conducted. In this study, we investigate three commonly used radical emitter molecules: TTM-1Cz, TTM-3NCz, and TTM-3PCz. These molecules share a common core structure of tris(2,4,6-trichlorophenyl) methyl (TTM) and contain varying carbazole (Cz) moieties. We compute the rates of several competitive pathways contributing to the formation of the D_1. The pathways analyzed include: i) D_1 formation via radical-anion generation, ii) D_1 formation via radical-cation generation, iii) D_1 formation via charge-charge annihilation, and iv) D_1 formation via higher-lying doublet or quartet states.[3] This in-depth analysis of competitive pathways provides critical insights for designing next-generation radical emitters with improved efficiency and performance.

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P-21: Theoretical Insights into Spin-State Interconversion in Carbazole-Containing TADF Emitters

Jonas Weiser and Christian Wiebeler

This study presents a comprehensive theoretical and computational investigation of spin-state interconversion mechanisms in carbazole-containing thermally activated delayed fluorescence (TADF) emitters, focusing on the role of spin-orbit coupling (SOC) in facilitating reverse intersystem crossing (RISC).[1] We systematically analyzed three cyanoarene-based TADF emitters – 3CzClIPN, 4CzIPN, and 5CzBN – with varying singlet-triplet energy gaps (ΔE_{ST}). Efficient RISC requires ΔE_{ST} to be within the range of thermal energy at room temperature, but the exact mechanism of the spin flip process is still under debate.[2,3] Our computational approach identified points of contact between the excited-state potential energy surfaces (PES) of these molecules, including minimum energy crossing points (MECPs) and conical intersections (CIs), to uncover the spin flip dynamics without requiring explicit excited-state molecular dynamics simulations.

We found that SOC-mediated RISC in these molecules proceeds via a higher-energy triplet state (T_2) as an intermediate, rather than directly between the T_1 and S_1 states. Consequently, RISC is not directly dependent on ΔE_{ST}, but instead on the activation energy $E_{act.}$, the energy difference between the equilibrium T_1 state and the T_2-S_1 MECP. The calculated SOC values at the MECPs are significantly higher than the corresponding 1 hyperfine coupling constants, confirming SOC as the dominant mechanism.

Experimental temperature-dependent magnetic field effect (MFE) measurements[1] align well with our computational predictions, revealing activation energies consistent with the T_1-T_2-S_1 pathway. These findings highlight the importance of considering higher triplet states in the design of efficient TADF materials and provide a robust framework for understanding spin dynamics in organic emitters. This work advances the theoretical understanding of spin-state interconversion and offers insights for optimizing TADF-based OLEDs.

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P-22: Theoretical study of resonant core-hole spectroscopy of metalloporphyrins and metallophthalocyanines

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We studied the free base Phthalocyanine molecule, H2Pc, and metallophthalocyanines with various metals in the gas phase. Various computational methods to simulate valence photoelectron spectra, X-ray absorption (XAS), and Resonant Auger spectra were tested, compared, and optimized to obtain a systematic framework.

P-23: Theoretical study of Photoinduced Proton Coupled Electron Transfer in Peptides

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Photoinduced Proton Coupled Electron Transfer (PCET[1,2]) reactions constitute an important class of reactions of biological[3] and technologic[4] relevance. They are increasingly recognized in areas such as synthetic chemistry and photocatalysis as well as in energy transformation reactions in natural and artificial systems.[5] From a mechanistic point of view, these reactions can be distinguished by the degree of synchronicity and directionality by which both the proton and the electron are transferred following photoexcitation. Theoretical and computational methods can contribute to the molecular interpretation of the PCET mechanism and of spectroscopic data.

We report a theoretical and computational study of photoinduced PCET reactions in oligopeptides. We have studied the mechanism ruling the PCET reactions in a tripeptide model system in aqueous solution, consisting of tryptophan (W), proline (P), and tyrosine (Y). The kinetics and the thermodynamics of PCET reactions in solution depend on a fine interplay of the electronic and the nuclear motion, as well as of solute-solvent interactions, which represent crucial features in standard electronic methods to properly describe the electronic density along the proton transfer coordinate and the resulting potential energy surface.[6-8]

To account for the conformational flexibility of the tripeptide, molecular dynamics simulations were performed in explicit aqueous solvent. This allowed for the exploration of the conformational space and the identification of the most populated peptide conformers.

The next step consisted into simulating PCET reactions in photoinduced reactive species — i.e., tryptophan oxidized state (radical cation). The reaction pathway was analyzed by simulating various potential scenarios through a computational study of the excited and ionized states of the WPY peptide. A comparison is presented and discussed between results from Time-Dependent DFT (TD-DFT) calculations and time-resolved spectroscopic data. In detail, we investigated the effects of solvent models on the electronic absorption spectra and employed TD-DFT to identify the electronic states involved in the UV–Visible region. The TD-DFT results are used to simulate the steady-state and transient UV–Visible spectra of neutral and ionized WPY peptide. By combining theoretical predictions with experimental data, we aimed to enhance the understanding of the reaction at an atomistic and molecular level, providing new insights beyond experimental observation.

This study can contribute to a better understanding of the PCET reaction as well as to the interpretation of spectroscopic time-resolved data[9], that suggest an ultrafast kinetics of the PCET process.

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P-24: Multiscale Modelling of DSB-Derivative Photothermal Transducers Forming Membrane Channels

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The controlled transport of ions and molecules across lipid bilayers via specific channels is a crucial mechanism for living cells. In the context of phototherapy, modulating the activity of membrane channels by light irradiation in a safe and controlled way is a promising route towards developing new therapeutic strategies beyond optogenetics. Dicyano-distyryl-benzene (DSB) derivatives serve as effective 2 photon-absorption photothermal transducers and have the unique ability to self-assemble within lipid membranes, potentially forming water or ion channels.

The goal is to gain a better understanding of the self-assembly mechanisms and channel formation of DSB derivatives. For this purpose, a multiscale modelling approach is employed. Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) calculations are used to investigate the photophysical properties of both individual dyes and their aggregates, with a focus on the first two excited states. Molecular Dynamics (MD) simulations further explore the conformational space of DSB derivatives in solution and inside the lipid membranes, assessing the influence of the environment and giving insight into the dynamics of the aggregation mechanism. The computational findings are then compared with experimental data to validate the methodologies used.

P-25: Exploring the Photostability of DNA: Computational Insights into the Electronic Properties of Purine Derivatives

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Photostability of DNA, defined as its ability to resist chemical changes induced by UV-light absorption, is crucial for life on Earth. Understanding the factors that contribute to it is an important area of research. The systematic study of the photophysics of nucleobase derivatives can shed light on the factors that govern the excited-state deactivation of these systems. The intrinsic photostability of DNA's nucleobases arises from their unique excited potential energy surface topography, where ultrafast internal conversion funnels efficiently redirect the excited population back to the ground state. This mechanism minimizes excited-state lifetimes, luminescence, and intersystem crossing processes. By exploring the impact of the substitution pattern in the photophysics of purine and pyrimidine derivatives, it is possible to elucidate the factors that underpin the photophysical superiority of canonical nucleobases over other heterocycles.

The topography of potential energy landscapes can be explored using computational techniques such as multiconfigurational methods and Density Functional Theory. To gain a deeper understanding of the structural and electronic factors that govern the photostability of purine nucleobase derivatives, we have identified and analyzed key features, including stationary points, inter-state surface crossings, and minimum energy paths in a selected set of purine derivatives. These insights contribute to a better understanding of the electronic properties of DNA components, which could be crucial for advancing the study of their photophysical behavior and stability.

P-26: Understanding Organic Cocrystals for Room Temperature Phosphorescence

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Organic co-crystals provide a versatile platform for designing efficient room temperature phosphorescent (RTP) materials. Despite the increasing number of reported organic co-crystals with RTP, the role of intermolecular interactions in enhancing phosphorescence remains poorly understood. Various strategies, including crystallisation, H-aggregation, and the heavy atom effect, have been employed to extend excited-state lifetimes [1]. Recently, Abe et al. utilised these strategies to modulate RTP in co-crystals of 1,4-diiodotetrafluorobenzene (DITFB) with polycyclic aromatic hydrocarbons (PAHs) such as phenanthrene (Phen), pyrene (Pyr), and chrysene (Chry) [2] (Figure 1).

To investigate how intermolecular interactions and crystal packing influence excited-state mechanisms, we examined the electronic transitions and the effects of spin-orbit coupling in these co-crystals. Our calculations reveal that DITFB-PAH co-crystals exhibit a high population of the triplet manifold near the first singlet excited state (S_1), enhancing intersystem crossing (ISC) and subsequently improving RTP efficiency. Additionally, the calculated phosphorescence emission energies align well with experimental observations. These findings offer valuable insights into controlling photophysical properties in these systems through specific intermolecular interactions, guiding the rational design of organic materials for diverse applications.

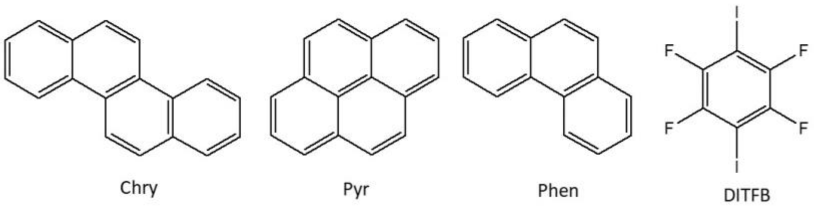

Figure 1: Components of the co-crystals with RTP under study

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P-27: Understanding Photoinduced Molecular Reactions Through Interpretation of Ultrafast Spectroscopy

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The demand for advanced materials in fields such as solar energy, photocatalysis, and biological imaging is driving increased interest in understanding light-matter interactions. Simulating excited-state dynamics is crucial for predicting how molecules respond to light, enabling the development of new functional materials.

Time-resolved valence-level photoemission is a well-established and powerful technique for studying molecular dynamics, typically conducted using laboratory lasers or free-electron lasers (FELs). However, for time-resolved X-ray photoemission spectroscopy (TRXPS), laboratory lasers generally lack the necessary flux; thus, experiments are typically performed at FELs. A key advantage of XPS at core levels is its ability to reveal chemical states and their quantitative populations, providing deeper insight into electronic structure and molecular behavior.

Building on our experience with TR-valence-level photoelectron spectroscopy simulations, we will provide computational support for recent C 1s, N 1s, and O 1s core-level spectroscopy studies on the excited-state dynamics of organic molecules performed at FELs. Specifically, we aim to investigate the electronic and nuclear relaxation dynamics of gas-phase uracil using time-resolved core-level photoelectron spectroscopy at carbon sites, offering a detailed understanding of its ultrafast response to light excitation.

P-28: Effects of electron-withdrawing and donating group substituents on diazirine: An excited state non-adiabatic molecular dynamics study.

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Photolysis of diazirine from an excited state proceeds via the conical intersection (CI) and avoided crossings. These crossings promote the formation of products in the ground electronic state. When two or more electronic states have nearly equal or equal energies, it results in coupling between the electronic states and nuclear motions, and hence the Born-Oppenheimer approximations break down at such junctions.[1] These couplings provide opportunities for the excited molecule to reach the ground state via the narrow-shaped channels in a radiationless manner. Such an overall process is called a non-adiabatic phenomenon.[2] In this study, the initial dynamics for diazirine and its substituted derivatives were started at n-π* excited state at the S_1 level, and predictably, the molecule hops back into the S_0 ground state after a certain period. Such a process occurs via a non-adiabatic mechanism, and the products yielded are molecular nitrogen and carbene. We have characterized four diazirine systems, those are 1) unsubstituted diazirine CH_2N_2 (DAZ), 2) fluoro-diazirine $CHFN_2$ (FDAZ), 3) methoxydiazirine $CH(OMe)N_2$ (MDAZ) and 4) fluoromethoxy-diazirine or push-pull diazirine $CF(OMe)N_2$ (PPDAZ).[3] These four systems have been chosen in such a way that they enable us to have a distinct comparative study among the substituents that have electron-withdrawing effect (EWG), i.e., fluorine, and electron-donating effect (EDG), i.e., methoxy, and effects of both the EWG and EDG, i.e., push-pull effect, on diazirine.[4]

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P-29: Mechanistic Study of the Conversion of Primary Alcohols and Butadiene to Branched Ketones Using Rhodium Catalyst

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The direct formation of ketones without premetalation is a key focus in catalysis research due to its simpler reaction process and fewer steps.[1] Here, we present a reaction mechanism of converting 3-methoxybenzyl alcohol and butadiene to (branched) isobutyl ketone using density functional theory.[2] The reaction consists of four main steps: (i) the oxidation of the alcohol reactant, generating a corresponding aldehyde and rhodium(I) hydride complex as an active catalyst, (ii) hydrogenation of butadiene to form the allyl rhodium(I) complex, (iii) the carbonyl addition from the allylic carbon to produce rhodium(I) alkoxide intermediate, and (iv) hydrogen transfer processes to generate the desired ketone product, which is liberated as the enolate form. The rate-determining states are in the carbonyl addition process (both intermediate and transition state) with the uphill energy of +37.6 kcal/mol. Generating a linear ketone requires much higher energy due to the lack of the π-bond to help stabilize transition states. Moreover, the positions of transferred hydrogens in our proposed catalytic cycle correspond to the deuterium labeling experiment, highlighting the hydrogen (auto)transfer process in this conversion of primary alcohol to branched ketones.

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P-30: Quantum Chemical Calculations for Iron-complexes for Ammonia Oxidation

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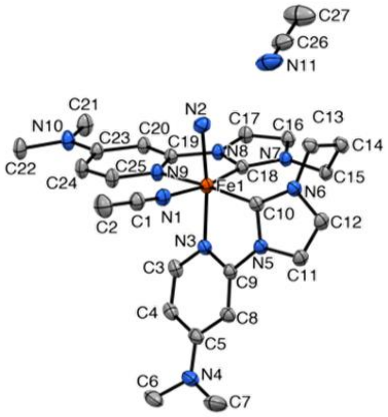
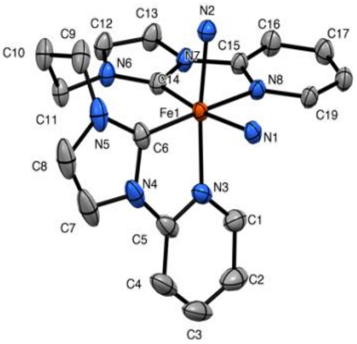
Ammonia oxidation (AO) is a key transformation in both energy conversion and nitrogen cycle management, offering a promising pathway for utilizing ammonia as a carbon-free energy carrier. molecular-level studies of AO are vital for developing efficient and selective electrocatalysts capable of operating under certain conditions, However, despite significant advances in transition metal catalysis, detailed mechanistic understanding of AO remains scarce, highlighting the need for complementary theoretical investigations[1].

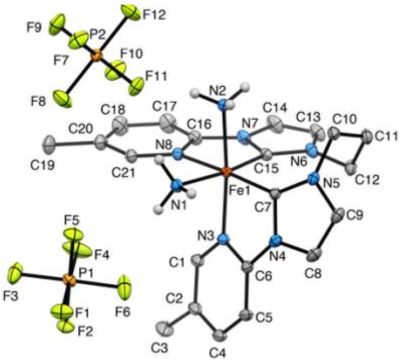
A series of iron complexes with varying redox potentials were synthesized and tested for their ability to catalyse ammonia oxidation; however, no catalytic activity was observed. In the present study, we carried out a comprehensive investigation of these compounds, comparing their reduction potentials and bond dissociation energies (BDEs) for hydrogen atom abstraction. Some selected complexes are shown below.



[^{NMe2}(NCCN)Fe(NH_3)($NCCH_3$)][PF_6]$_2$



[^{H}(NCCN)Fe (NH_3)$_2$][PF_6]$_2$



[^{Me}(NCCN)Fe(NH_3)$_2$][PF_6]

The redox potential values were systematically investigated by first analysing the spin-state splitting of the compounds. All complexes, both Fe(II) and Fe(III), were found to adopt low-spin configurations across all tested functionals. While it was initially challenging to obtain reliable reduction potential values due to solvent surface effects, the use of universal solvation model (SMD) model in combination with the DRACO approach yielded excellent agreement with experimental data.

The N–H bond dissociation energy (BDE) is a key factor in determining the viability of ammonia oxidation, We obtained BDE values in the range of 75-105 kcal/mol. Which is higher than benchmark value 77.1kcal/mol associated with known catalytically active systems[5],suggesting a possible limitation for these iron complexes.

In addition, our current results suggest that the Fe–C bonds in the complexes may represent a structural vulnerability. Further calculations are ongoing to validate this hypothesis.

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The hands-on tutorial sessions will be conducted using the **Bem2** supercomputer. The organizers gratefully acknowledge the support of the **Wroclaw Center for Networking and Supercomputing** (http://wcss.pl) for providing access to the necessary computational resources.

The organizers also extend their sincere thanks to the **Faculty of Chemistry, NCU Torun administration,** for their continued support and assistance in facilitating the event.