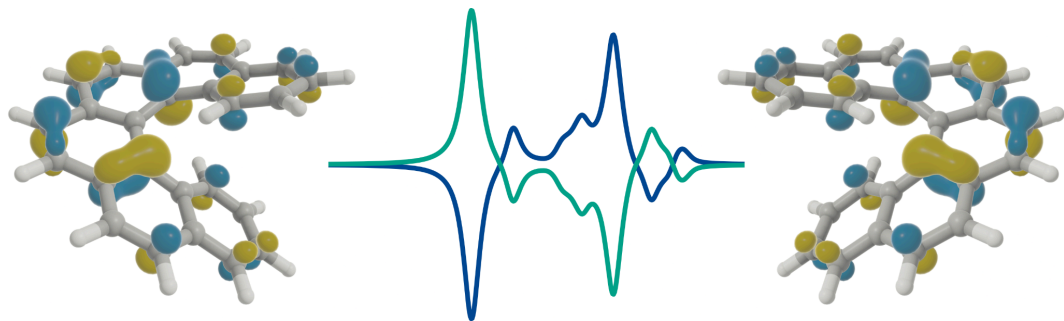




CCEC 2026 – Workshop program

14 – 18 September 2026,
Nicolaus Copernicus University in Toruń



FUNDACJA
ALEKSANDRA
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NICOLAUS COPERNICUS
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IN TORUŃ

Monday 14 September

09.00 - 09.15: Welcome and introduction (IEB)

09.15 - 10.30: Basis sets and DFT (PN)

10.30 - 11.00: Coffee break

11.00 - 12.30: Density functional theory (continued, PN)

12.30 - 14.00: Lunch break

14.00 - 15.30: Environment: QM/MM and CPCM (PN, IEB)

15.30 - 16.00: Coffee break

16.00 - 17.00: Density analysis: charges, dipole moments, bond orbitals, and more (ML)

Tuesday 15 September

09.00 - 10.30: Thermochemistry: reaction energies (MA)

10.30 - 11.00: Coffee break

11.00 - 12.30: Thermochemistry: conformers (MA)

12.30 - 14.00: Lunch break

14.00 - 15.30: Electrochemistry (MA)

15.30 - 16.00: Coffee break

16.00 - 17.00: Molecular properties and stability (MA)

17.30 - 20.00: POSTER Session and DINNER

Wednesday 16 September

09.00 - 10.30: Coordinates, potential energy surfaces (IEB)

10.30 - 11.00: Coffee break

11.00 - 12.30: Optimization and TS search (IEB)

12.30 - 14.00: Lunch break

14.00 - 15.30: Vibrational analysis & normal modes (IEB)

15.30 - 16.00: Coffee break

16.00 - 17.00: Zero-point vibrational energy, enthalpy, and Gibbs free energy (MA)

Thursday 17 September

09.00 - 10.30: UV/vis spectroscopy and CD (ML)

10.30 - 11.00: Coffee break

11.00 - 12.30: Visualization & excited state analysis (ML)

12.30 - 14.00: Lunch break

14.00 - 15.30: Infrared and Raman spectroscopy (IEB)

15.30 - 19.00: Free time / **16.00 - 18.00:** Scientific session

19.00 WORKSHOP DINNER in the old town

Friday 18 September

09.00 - 10.30: Work on your own computational workflow

10.30 - 11.00: Coffee break

11.00 - 12.30: Workflow (continued)

12.30 - 14.00: Lunch break

14.00 - 16.00: Workflow (continued)

Summary and farewell (+feedback questionnaires, IEB)

Workflow topics – from reaction to spectra

1. For a selected reaction in solution (PCM solvation), find the TS, reaction rates and concentration changes, as well as the related spectral changes in the UV/vis absorption spectrum (led by MA).
2. For a selected racemization reaction, determine the expected spectral changes in the circular dichroism (CD) spectrum. Based on a given CD spectrum, identify the concentrations of S and R enantiomers (led by ML).

POSTER ABSTRACTS

P1. Theoretical Prediction of the Singlet-Triplet Energy Gap in Thermally Activated Delayed Fluorescence Emitters

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Thermally activated delayed fluorescence (TADF) is a mechanism that allows organic molecules to harvest both singlet and triplet excitons, and thus to reach a theoretical 100% exciton utilisation in organic light-emitting diodes (OLEDs). The key requirement for an efficient TADF emitter is a small singlet-triplet energy gap (ΔEST), which enables fast reverse intersystem crossing (RISC) from the triplet to the singlet state. Besides high external quantum efficiency, a small ΔEST is also decisive for the operational stability of the device: the accelerated RISC shortens the triplet exciton lifetime, thereby reducing degradation from triplet-triplet and triplet-polaron annihilation, resulting in a longer TADF OLED lifetime [3]. A reliable theoretical estimation of ΔEST is therefore highly desirable, as it reduces the experimental effort needed to identify promising candidates [1,2].

Here we report a theoretical study of ΔEST for a series of donor-acceptor emitters. The calculations were performed using the time-dependent density functional theory (TD-DFT) correction scheme proposed by Huang et al. for charge-transfer compounds [1]. In this approach, the optimal Hartree-Fock exchange percentage in the exchange-correlation functional is linked to the charge-transfer amount (q) of a given excitation through the relation $\text{OHF} = 42q$, which makes it possible to

reproduce the zero-zero transition energies of the first singlet and first triplet states and to distinguish their locally excited and charge-transfer character. The theoretical results obtained are compared with experimental data to evaluate the accuracy of the adopted methodology for this class of emitters.

References:

1. S. Huang, Q. Zhang, Y. Shiota, T. Nakagawa, K. Kuwabara, K. Yoshizawa, C. Adachi, Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds, *J. Chem. Theory Comput.* 9 (2013) 3872–3877.
2. H. Xie, Z. Huang, N. Li, T. Hua, J. Miao, C. Yang, Rational molecular design of TADF emitters towards highly efficient yellow electroluminescence with a nearly 30% external quantum efficiency and low roll-off, *J. Mater. Chem. C* 10 (2022) 11239–11245.
3. S. K. Jeon, H. L. Lee, K. S. Yook, J. Y. Lee, Recent Progress of the Lifetime of Organic Light-Emitting Diodes Based on Thermally Activated Delayed Fluorescent Material, *Adv. Mater.* 31 (2019) 1803524.

P2. Local Chemical Environment in Cu₃N and Pd-doped Cu₃N Nanoparticles: Insights from Spectroscopy

Igor Sawicki¹, Iulia Emilia Brumboiu¹, Igor Di Marco¹, Tadeusz Muzioł², Robert Szczęsny²

¹Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Poland

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Copper nitride (Cu₃N) nanoparticles have a variety of possible applications in fields like photovoltaics, energy storage, electronics, or catalysis [1, 2]. Doping with Pd can be used to tune their electronic and optical properties [1, 2, 3] to optimize them for specific applications. When doping Cu₃N with Pd, the Pd atom can assume the position at the body center of the Cu₃N primitive cell, but can also replace Cu at the face center position, or, ultimately, form a Cu-Pd alloy. In this joint experiment-theory study, we use density functional theory (DFT) as implemented in GPAW [4] to model Pd-doped Cu₃N lattices. In addition, we use DFT within an excited core-hole (XCH), multiple scattering approach as implemented in FDMNES [5] to calculate their N K-edge and Cu L-edge X-ray absorption spectra. By modeling several lattice structures of perfect and defective Cu₃N and Cu₃PdN crystals with defects including Pd substitution, Pd-Cu switches, and N or Pd vacancies, we are able to reproduce the trends observed experimentally when comparing pristine Cu₃N to Pd-doped nanoparticles. In particular, both the measured N K-edge and Cu L-edge X-ray absorption spectra of the Pd-doped system can be qualitatively reproduced by a Cu₃PdN lattice with Pd and N vacancies.

References:

1. A. Ścigala, E. Szłyk, L. Dobrzańska , D. H. Gregory, and R. Szczęsny, *Coord. Chem. Rev.* 436 213791 (2021).
2. M. Parvizian, A. Duràn Balsa, R. Pokratath, C. Kalha, S. Lee, D. Van den Eynden, M. Ibáñez, A. Regoutz, and J. De Roo, *Angew. Chem. Int. Ed.* 61, e202207013 (2022).
3. A. L. Ji, N. P. Lu, L. Gao, W. B. Zhang, L. G. Liao, and Z. X. Cao, *J. Appl. Phys.* 113, 043705 (2013)
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5. O. Bunău, A. Y. Ramos and Y. Joly, *Int. Tables Crystallogr. I*, ch. 6.6., 752–757 (2024).

P3. Reverse Water-Gas-Shift Reaction (CO₂ to CO) Mediated by an Ir-PCP Pincer Complex Under Mild Conditions

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The catalytic transformation of CO₂ into value-added chemicals represents a central goal in sustainable chemistry. The reduction of CO₂ to CO is of particular industrial relevance, as CO is a major feedstock in syngas-based chemical production. In homogeneous catalysis, however, transition metal pincer complexes have predominantly been explored for the reversible hydrogenation of CO₂ to formate as part of hydrogen storage strategies. In these systems, even traces of CO must be avoided as they poison downstream fuel cell catalysts. Consequently, catalyst development has largely focused on selective formate production while suppressing CO generation.

In contrast to this, we explore a complementary approach in which CO formation is the targeted outcome. We investigate the reactivity of an Ir(III)-trihydride complex bearing a neutral PCP pincer ligand featuring a central NHC donor. Upon exposure to CO₂ at atmospheric pressure, an Ir-formato is initially observed. However, the formato species converts into a cationic Ir(I)-carbonyl complex in the presence of Na[BarF₄], as

confirmed by NMR spectroscopy and single-crystal XRD. Rather than regarding the carbonyl formation as a detrimental side reaction, we interpret this as a key step that enables the reverse water-gas shift reaction, in which CO_2 is reduced with H_2 to CO and H_2O . Mechanistically, the observed CO -complex formation is proposed to proceed via an “abnormal insertion” of CO_2 into a metal-hydride bond, yielding a hydroxycarbonyl intermediate (M-COOH), which then reacts further to give the CO complex. In contrast, the initial formate complex arises from reversible “normal CO_2 insertion”, as shown in Fig. 1. [1].

Importantly, upon addition of KOtBu and H_2 to the CO complex under atmospheric pressure, the starting Ir(III) -trihydride is regenerated at 60°C under release of CO . This closes a complete stepwise stoichiometric cycle for CO_2 reduction to CO (see Fig. 1). The ability to generate CO from recycled CO_2 under such mild conditions thus highlights a homogeneous system for CO production that contrasts with conventional high-temperature heterogeneous steam reforming.

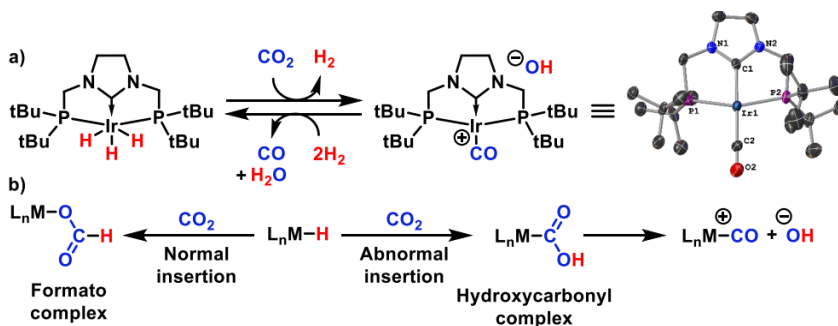


Figure 1. a) Suggested stepwise cycle of the reverse-water-gas-shift reaction mediated by an Ir-PCP complex, b) Normal and abnormal insertion of CO_2 into a metal-hydrogen bond.

Funding: Swedish Research Council, Lund University

References:

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P4. Toward Dark Electronic Molecular States Visualisation

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Dark electronic molecular states do not interact with the light directly, but they can be detected indirectly thanks to their interaction with the bright states. These states may be probed by the surface-enhanced Raman scattering (SERS) and the wavelength-dependent excitation spectra.

In this research, the effect of adding nanoparticles on dark states of the platinum (II) octaethylporphyrin will be investigated (Fig. 1). Gold nanoparticles were synthesized with plasmon resonance matching the wavelength of phosphorescence of the molecule. Their effect on the electronic spectra will be tested.

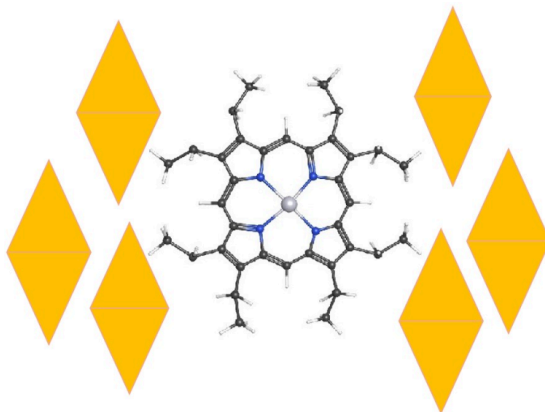


Fig. 1. Platinum (II) octaethylporphyrin with nanoparticles – visualisation.

P5. Controllable Spin Polarization and Spin-Filtering in Magnetized Borophosphene Nanoribbons under a Transverse Electric Field

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Borophosphene as a novel two-dimensional (2D) anisotropic Dirac material with its long spin coherence length and ultrahigh carrier velocity represents great potential for future spintronic technologies [1,2]. In the present paper, we investigate the spin-dependent transport properties of borophosphene nanoribbons (BPNRs) using non-equilibrium Green's function (NEGF) formalism combined with a tight-binding (TB) Hamiltonian. We systematically study the effect of local exchange fields, induced by the proximity effect of ferromagnetic (FM) and antiferromagnetic (AFM) insulating substrates, on the electronic structure and spin-dependent conductance of both zigzag and armchair BPNRs with different edge shapes. Our results demonstrate that BPNRs subjected to local FM exchange field at the ribbon edges can act as efficient, controllable spin filters with 100% spin polarization. Furthermore, we show that this proximity effect can induce half-metallic behavior in zigzag BPNRs, where the nanoribbon acts as a conductor for one spin channel and an insulator for the other [3]. Notably, this half-metallicity can be effectively tuned by an externally applied transverse electric field. Our findings highlight BPNRs

as highly tunable and promising candidates for developing spintronic device applications [4].

References:

1. Y. Zhang, J. Kang, F. Zheng, P. F. Gao, S. L. Zhang, and L. W. Wang, J. Phys. Chem. Lett. 10 (2019) 6656–6663.
2. Y. Zhang et al., Phys. Chem. Chem. Phys. 22 (2020) 20851–20857.
3. F. Norouzi, M. Farokhnezhad, M. Esmaeilzadeh, and B. Szafran, Phys. Rev. B 104 (2021) 1–10.
4. M. Farokhnezhad et al., J. Appl. Phys. 117 (2015).

P6. Tree-Based Machine Learning Model for Fluorescence Lifetime Prediction in Organic Compounds

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Fluorescence lifetime is a fundamental excited-state property describing the average time a fluorophore remains in the excited state before photon emission. It reflects the competition between radiative and non-radiative decay pathways and is therefore important for fluorescence lifetime imaging microscopy, sensing, optoelectronic materials and high-throughput fluorophore screening. However, experimental lifetime measurements require specialized instrumentation, while time-dependent density functional theory can be computationally demanding for large molecular libraries.

This study presents an interpretable tree-based machine learning framework for predicting fluorescence lifetimes of organic chromophores in solvent environments. The model was developed using chromophore-solvent data derived from the Deep4Chem database. Molecular structures were represented using RDKit descriptors, Morgan and MACCS fingerprints, three-dimensional geometry descriptors, predicted pKa values and engineered photophysical features, including absorption/emission descriptors, and chromophore-solvent interaction terms. A LightGBM regressor was selected because it provides efficient learning and strong interpretability for heterogeneous tabular molecular descriptors.

The optimized model was evaluated using cluster-stratified cross-validation and achieved a mean absolute error of 0.8324 $\pm$ 0.0617 ns and an R² value of 0.7523 $\pm$ 0.0317. External validation against TD-DFT benchmark systems and independent experimental data confirmed that the model captures global lifetime trends and can support rapid screening. SHAP analysis identified quantum yield, molecular geometry, emission-related descriptors, topological indices and local fragment motifs as key contributors, indicating that the model learns physically meaningful structure-property relationships. Overall, this workflow provides a fast and interpretable route for fluorescence lifetime prediction and fluorophore prioritization.

References:

1. Vovea, DC., Chiş, V. Tree-Based Machine Learning Model for Fluorescence Lifetime Prediction in Organic Compounds. *J Fluoresc* 36, 4121–4139 (2026).
<https://doi.org/10.1007/s10895-026-04839-9>

P7. Local Structural Modifications as a Strategy for Tuning the Photophysical Properties of BF₂-Carrying Dyes

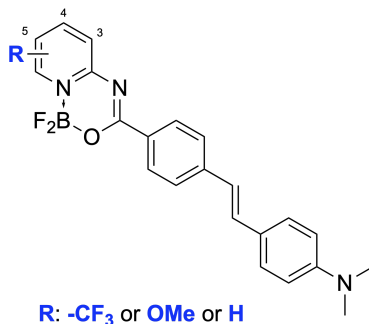
Anna Piec¹

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Organic fluorescent dyes are widely used in various fields, including bioimaging, where their applicability depends on several photophysical properties. High fluorescence quantum yield (FQY) and excitation within biological optical windows [1], particularly the first (700–1000 nm) and second (1000–1350 nm), are highly desirable [2]. Dyes exhibiting multiphoton absorption are especially attractive, as excitation at longer wavelengths can reduce light scattering and autofluorescence and enable deeper imaging. This introduces additional requirements, including two-photon absorption cross-section (σ 2PA) and the two-photon action cross-section (TPACS), defined as the product of σ 2PA and FQY [1].

To investigate the effect of local modifications of the electron-accepting unit, a series of seven fluorescent dyes with donor- π -acceptor (D- π -A) architecture was studied. Trifluoromethyl (R = CF₃) and methoxy (R = OMe) groups, representing electron-withdrawing and electron-donating substituents, respectively, were introduced at the 3-, 4-, and 5-positions of the pyridine ring, while the unsubstituted dye (R = H) served as a reference. The position and character of the substituent enabled tuning of the charge-transfer and photophysical properties within the tested core.

Photophysical measurements revealed a strong influence of mentioned modifications on the properties of dyes. The CF_3 substituent caused a bathochromic shift of absorption and emission bands, while the OMe derivatives showed only minor spectral changes compared with the unsubstituted, reference molecule. Moreover, the position of CF_3 group, within the pyridine ring, strongly affected the position of bands, while the fluorescence quantum yield (FQY) decreased from 1 for the 3- CF_3 derivative to 0.05 for the 4- CF_3 analogue. All dyes exhibited two-photon absorption within the first biological window. Five compounds showed TPACS values above 100 GM, including two above 400 GM. These results demonstrate that even small local modifications within the electron-accepting unit can significantly affect both one- and two-photon photophysical properties.



References:

1. A. Hajda, E.F. Petrusevich, R. Zaleśny, B. Ośmiałowski, J. Olesiak-Bańska, *Chem. Commun.* 2025, 61, 3990.
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