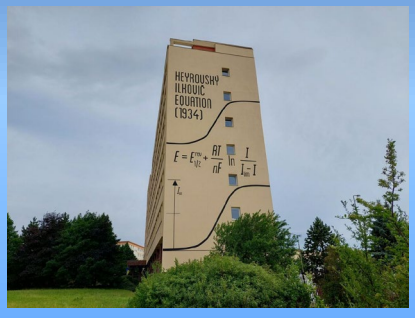
SEMINÁŘ STUDENTŮ ÚFCH JH 2025



Ústav Heyrovského v Praze

21.5. 2025

Seminář studentů 2025

Sborník příspěvků

ze studentské konference konané
21. května 2025
v ÚFCH J. Heyrovského v Praze

Student Seminar 2025

Collection of abstracts

of all lectures given at the student conference
held on 21 May 2025
in Heyrovský Institute in Prague

Seminář studentů 2025
Sborník příspěvků ze studentské konference
konané 21. května 2025
v ÚFCH J. Heyrovského v Praze

Kolektiv autorů
Sestavila: Květa Stejskalová
Vydává: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 00 Praha 8, Česká republika
Vydání: první, v elektronickém formátu
Místo a rok vydání: Praha, 2025

List of presented students (24)
Seznam prezentujících studentů (24)

Bachelor and diploma students (7)
Diplomanti a zájemci z řad bakalářů

Beneš Marek *(VŠCHT Praha, magisterské studium, školitelka R. Sokolová)*

Fárníková Karolina *(VŠCHT Praha, magisterské studium, školitelka: E. Krupičková Pluhařová)*

Gabaj David (Daniel *(VŠCHT Praha, bakalářské studium, školitelky: L.Šimková a K. Salvadori*

Mendicute Irene Echezarreta *(studentka v programu ERASMUS, školitelé K. Paldusová a M. Cebecauer)*

Myšák Daniel *(VŠCHT Praha, magisterské studium, školitelka: E. Krupičková Pluhařová)*

Vítek Petr *(VŠCHT Praha, bakalářské studium, školitel: S. Valtera)*

Šimková Paulína *(Přf UK Praha, magisterské studium, školitelka: E. Krupičková Pluhařová)*

PhD Students (17):
Studenti DSP studia

Bukhari Seyd Adeel Mahmood *(školitel O. Frank)*

Campoy Daniela G. B. *(školitel J. Sýkora)*

Čech Petr *(školitelé Z. Vlčková a O. Frank)*

González Navarro José Alfredo *(školitel M. Cebecauer)*

Hansen Niklas *(školitelka V. Petráková)*

Jindra Martin *(školitel O. Frank)*

Johanovská Zuzana *(školitel M. Hof)*

Martinka Jakub *(školitel J. Pittner)*

Nguyen Truong An *(školitel Š. Timr)*

Poolamanna Ashwathi *(školitel Š. Timr)*

Saha Samrat *(školitel P. Nag)*

Sahu Satyam *(školitel M. Velický)*

Samanta Madhav *(školitel Š. Timr)*

Simkovičová Karolina *(školitel Š. Vajda)*

Smeliková Valerie *(školitel M. Kalbáč)*

Šimek Jan *(školitel R. Šachl)*

Valtera Stanislav *(školitel Š. Vajda)*

Referees:

Alan Liška
Edyta Tabor
Štěpán Timr

SEMINÁŘ STUDENTŮ 2025

PROGRAM– středa 21. května 2025

STUDENT SEMINAR 2025

PROGRAM - Wednesday May 21, 2025

	Předseda-jící/ ***chairman***	*Přednášející/* ***lecturer***	*Název/* ***prezentation title***
9:00-9:10	**Zahájení konference „Seminář studentů 2025“** *Opening of Annual conference "Seminar of Students 2025"*		
9:10-9:25	**Valerie Smeliková**	Karolina Fárníková *(VŠCHT Praha, školitelka E. Krupičková Pluhařová)*	MOLECULAR MODELLING OF CATALYSTS FOR CO_2 REDUCTION
9:25-9:40		David Gabaj *(VŠCHT Praha, školitelky: L.Šimková a K. Salvadori)*	(SPEKTRO) ELEKTROCHEMICKÁ STUDIE DIFENYLIZOBENZOFURANŮ, NADĚJNÝCH KANDIDÁTŮ PRO ZVÝŠENÍ ÚČINNOSTI SOLÁRNÍCH ČLÁNKŮ
9:40-9:55		Daniel Myšák *(VŠCHT Praha, školitelka E. Krupičková Pluhařová)*	COMPUTATIONAL MODELLING OF GLUTAMATE DEHYDROGENASE IN CROWDED ENVIRONMENT WITH FOCUS ON THE ACTIVE SITE
9:55-10:10		Marek Beneš *(VŠCHT Praha, školitelka R. Sokolová)*	DEVELOPMENT OF METHODOLOGY FOR FLUORESCENCE SPECTROELECTROCHEMISTRY MEASUREMENTS
10:10-10:45	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** ***(Coffee break in lobby)***		
10:45-11:00	**Jakub Martinka**	Paulína Šimková *(Přf UK Praha, školitelka E. Krupičková Pluhařová)*	MOLECULAR DYNAMICS SIMULATION OF DEXTRAN INTERACTIONS WITH BIOLOGICALLY RELEVANT MOLECULES
11:00-11:15		Petr Čech *(školitelé Z. Vlčková a O. Frank)*	(SPECTRO)ELECTROCHEMISTRY IN CHAOTROPIC PERCHLORATE WATER-IN-SALT ELECTROLYTES
11:15-11:30		Petr Vítek*(VŠCHT Praha, školitel S. Valtera)*	ATOM BY ATOM BUILT ATOMICALLY PRECISE CuPd PENTAMER CLUSTERS FOR CYCLOHEXENE DEHYDROGENATION
11:30-11:45		Ashwathi Poolamanna *(školitel Š. Timr)*	SUBSTRATE BINDING IN ENZYME CLUSTERS: EFFECTS OF CROWDERS AND TRANSIENT INTERACTIONS
11:45-12:00		Stanislav Valtera *(školitel Š. Vajda)*	SELECTIVE OXIDATIVE DEHYDROGENATION OF CYCLOHEXENE OVER Cu_3Pd_2 CLUSTERS FOR H_2 GENERATION
12:00-13:00	**OBĚD VE VESTIBULU** ***(Lunch in lobby)***		
13:00-13:15		Madhav Samanta *(školitel Š. Timr)*	CROWDERS ALTER ACCESSIBILITY OF ADENYLATE KINASE CONFORMATIONAL SPACE

13:15-13:30	**Karolina Simkovičová**	Niklas Hansen *(školitelka V. Petráková)*	HIGH-YIELD ASSEMBLY OF PLASMON-COUPLED NANODIAMOND SYSTEMS VIA DNA ORIGAMI FOR TUNABLE LIGHT EMISSION
13.30-13:45		Samrat Saha *(školitel P. Nag)*	ELECTRON COLLISION WITH LIQUID MICRO-JET: QUANTIFYING SOLVATED ELECTRONS
13:45-14:00		Jakub Martinka *(školitel J. Pittner)*	MACHINE LEARNING ACCELERATED SIMULATIONS OF PHOTOCHEMICAL PROCESSES
14:00-14:15		Jan Šimek *(školitel R. Šachl)*	LIPID SCRAMBLING PATHWAYS IN THE SEC61 TRANSLOCON COMPLEX
14:15-14:30	**PŘESTÁVKA** ***(Break)***		
14:30-14:45	**Niklas Hansen**	Valerie Smeliková *(školitel M. Kalbáč)*	TREATMENT OF MOS_2 MONOLAYERS BY ATOMIC DEUTERIUM
14:45-15:00		Martin Jindra *(školitel O. Frank)*	RAMAN SPECTROELECTROCHEMISTRY OF GRAPHENE ELECTRODES
15:00-15:15		Seyed A. M. Bukhari *(školitel O. Frank)*	RESTORING PHOTOLUMINESCENCE IN METAL-EXFOLIATED, LARGE AREA MOLYBDENUM DISULFIDE
15:15-15:30		Zuzana Johanovská *(školitel M. Hof)*	INTRODUCE METHOD, WE HAVE NOT USED HERE BEFORE, THEY SAID. IT WILL BE FUN, THEY SAID.
15:30-15:45		Satyam Sahu *(školitel M. Velický)*	EXPLORING RESONANCE RAMAN SCATTERING AND STIMULATED RAMAN SCATTERING EFFECTS IN CrSBr
15:45-16:15	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** ***(Coffee break in lobby)***		
16:15-16:30	**Zuzana Johanovská**	José Alfredo González Navarro *(školitel M. Cebecauer)*	DISTRIBUTION OF ADHESION MOLECULES IN THE IMMUNOLOGICAL SYNAPSE
16:30-16:45		Karolina Simkovičová *(školitel Š. Vajda)*	INSIGHTS INTO PARTICLE-SUPPORT INTERACTIONS AND THEIR ROLE IN CO_2 HYDROGENATION CATALYSIS
16:45-17:00		D. G. Blanco - Campoy *(školitel J. Sýkora)*	TUNING PEG BASED MOLECULES FOR CUSHIONING SUPPORTED LIPID BILAYERS MONITORED BY GRAPHENE INDUCED ENERGY TRANSFER
17:00-17:15		Truong An Nguyen *(školitel Š. Timr)*	MECHANISTIC INSIGHTS INTO ALLOSTERIC REGULATION OF HUMAN PHOSPHOFRUCTOKINASE-1 BY MOLECULAR DYNAMICS SIMULATIONS
17:15-17:30		Irene Echezarreta Mendicute *(školitelé K. Paldusová a M. Cebecauer)*	NEUTROPHIL RESPONSE TO MULTIPLE STIMULI
17:30-17:45	**UZAVŘENÍ KONFERENCE** - ***V SÁLE RUDOLFA BRDIČKY*** ***Closing ceremony (in Brdička Hall)***		

MOLECULAR MODELLING OF CATALYSTS FOR CO_2 REDUCTION

Bc. Karolína Fárníková

Mgr. Ing. Eva Krupičková Pluhařová, Ph.D.

Reduction of the total emissions of carbon dioxide is a pressing societal challenge. Cutting its production as well as the capture and subsequent conversion of CO_2 into valuable chemicals will most likely contribute to its solution [1,2]. One of the promising approaches for CO_2 conversion is electrochemical reduction, which needs to be catalyzed to increase efficiency and selectivity.

This research deals with molecular modelling of cobalt porphyrin catalysts in solutions of various electrolytes. Using quantum-chemical calculations, ab initio and classical molecular dynamics, we investigated the catalytic cycle and the influence of the composition of the solution on its course. First, we focused on the energetics of the various reaction steps and how they are influenced by the present alkali-metal cations. We saw, that the cations aid in the reduction of the system, but prevent the protonation due to Coulombic interactions. Next we analyzed the behavior of the various reaction intermediates in aqueous solution of alkali-metal cations. The obtained results will contribute to a better understanding of the entire environmentally relevant process.

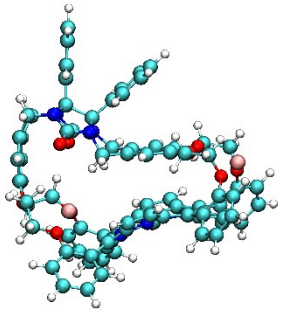


Fig. 1: Deformed structure of the cobaltoporphyrin cage catalyst with two K^+ cations

References:

[1] Yu, K. M.; Curcic, I.; Gabriel, J.; Tsang, S. C., Recent advances in CO2 capture and utilization. ChemSusChem 2008, 1 (11), 893–899.

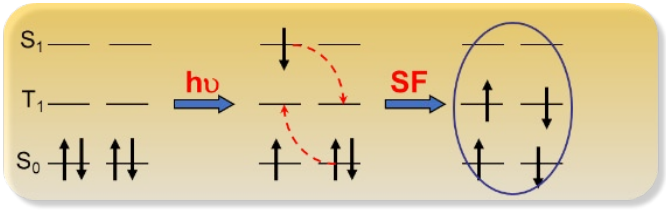
[2] Sun, S.; Sun, H.; Williams, P. T.; Wu, C., Recent advances in integrated CO2 capture and utilization: a review. Sustainable Energy Fuels 2021, 5, 4546–4559.

(SPEKTRO) ELEKTROCHEMICKÁ STUDIE DIFENYLIZOBENZOFURANŮ, NADĚJNÝCH KANDIDÁTŮ PRO ZVÝŠENÍ ÚČINNOSTI SOLÁRNÍCH ČLÁNKŮ

David Gabaj

Mgr. Ludmila Šimková, Ph.D.
Ing. Karolína Salvadori, Ph.D.

Organický fotovoltaický článek je založený na absorpci světla chromoforem. Tento děj vede k excitaci singletového elektronu, který svojí deexcitací do tripletového stavu část energie ztratí. Tuto disipovanou energii lze zužitkovat pomocí procesu singletového štěpení, díky kterému je možné vygenerovat 2 elektrony místo jednoho [1,2], a tak zvýšit efektivitu přeměny elektromagnetického záření v elektrický proud.



Požadavky singletového štěpení splňuje molekula 1,3-difenylisobenzofuran (DPIBF) [3]. Molekuly DPIBF jsou hojně používány u Dielsových-Alderových reakcí [4] nebo jako standardní reagenty pro stanovení singletového kyslíku. Mohou však sloužit i jako chromofory. Pro jejich využití v solárním článku jsou klíčové jejich optické a redoxní vlastnosti. V této práci jsme se zaměřili na detailní vyhodnocení a porovnání vlastností DPIBF a jeho vybraných dimerními analogů. Vedle klasických elektrochemických (DC-polarografie, CV a RDE) a optických (UV-vis-NIR) metod byla použita i jejich kombinace. Mechanismus přenosu prvního elektronu byl podpořen *in-situ* EPR spektroskopií. V neposlední řadě byla studována stabilita zkoumaných molekul (pomocí UV-vis, NMR a MS).

Poděkování
Tato práce vznikla za podpory grantu GA ČR 21-23261S a institucionální podpory RVO: 61388955.

Literatura
[1] Smith, M. B.; Michl, J. *Annu. Rev. Phys. Chem*. **2013**, *64*, 361-386.
[2] Smith, M. B.; Michl, J. *Chem. Rev.* **2010**, *110*, 6891-6936.
[3] Michl, J. *Chemické listy* **2016**, *110*, 365-370.
[4] Howard J. A., Mendenhall G. D. Can. J. *Chem.* **1975**, *53*, 2199-2201.

COMPUTATIONAL MODELLING OF GLUTAMATE DEHYDROGENASE IN CROWDED ENVIRONMENT WITH FOCUS ON THE ACTIVE SITE

Daniel Myšák

Krupičková Pluhařová Eva, Mgr. Ing., Ph.D.

Living organisms regulate their life functions by biocatalyst called enzymes. Enzyme's activity is very sensitive to its surrounding which allows the cells to quickly react and change metabolism. Cell's interior contains large variety of macromolecules, thus it is crowded. However, most of the in vitro experiments are made in simple aqueous buffer. That is why we focus on the influence of the crowded environment.

Using all-atom classical molecular dynamics, we simulated Glutamate dehydrogenase (GDH), an important enzyme at a metabolic branching point in all living organisms [1]. Our model systems contained a bovine GDH trimer (Fig. 1) under various conditions (pH, molecular crowding agents such as glucose or dextran) [2]. We observed that the active site residues and substrates in the active site (Glutamate, Norvaline) are flexible. Interestingly, under certain conditions substrates spontaneously left the active site in two directions. Thus, by applying external force on the substrate we developed a protocol of pulling in a well-defined way. The results were discussed in the context of our previous simulations and available experimental data. These observations may help in explaining how enzymes behave in the crowded cellular environment and how such conditions affect substrate binding.

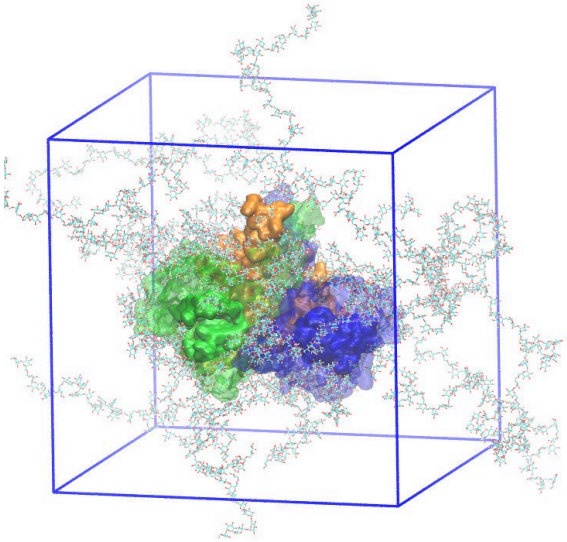


Figure 1: Simulation box with GDH trimer and displayed dextrans from the solvent.

References:

1. Smith, H.Q., et al., *Glutamate Dehydrogenase, a Complex Enzyme at a Crucial Metabolic Branch Point.* Neurochem Res, 2019. **44**(1): p. 117-132.
2. Lay, W.K., M.S. Miller, and A.H. Elcock, *Reparameterization of Solute-Solute Interactions for Amino Acid-Sugar Systems Using Isopiestic Osmotic Pressure Molecular Dynamics Simulations.* J Chem Theory Comput, 2017. **13**(5): p. 1874-1882.

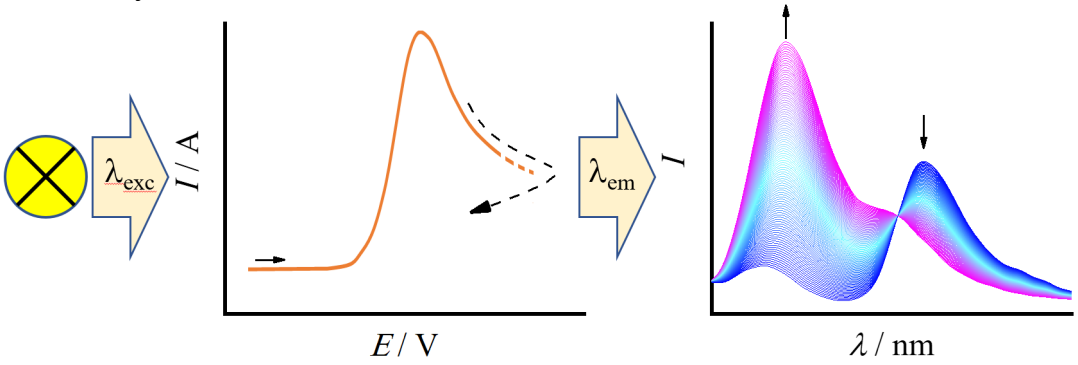
DEVELOPMENT OF METHODOLOGY FOR FLUORESCENCE SPECTROELECTROCHEMISTRY MEASUREMENTS

Bc. Marek Beneš

doc. RNDr. Romana Sokolová, PhD.

Spectroelectrochemical techniques contribute significantly to the understanding of the spectroscopic properties of substances in the oxidized or reduced state. The in-situ combination of electrochemical and spectroscopic methods is important for determining the mechanism of reduction or oxidation of organic compounds and for characterization of obtained products. The techniques are essential in the study of molecules that respond to an applied potential by changing their spectral properties (colour change, etc.) such as organic dyes, some bioactive substances or compounds used in material chemistry as components of LCD or OLED panels.

The aim of this work was to extend the already established techniques of spectroelectrochemistry in the ultraviolet, visible and infrared regions by monitoring fluorescence (FL) during the electrochemical process (the principle is shown in the figure below). So far, three different experimental setups for *in-situ* FL-spectroelectrochemical experiments have been constructed and tested. The substances eosin Y and methylene blue were used to verify the applicability and functionality of the methodology and experimental setups, and their fluorescence behavior during reductive transformations was successfully described.



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Slanina, T.; Oberschmid, T. *ChemCatChem* **2018**, *10*, 4182-4190.
Gemünde, A.; Gail, J.; Janek, J.; Holtmann, D. *Biosensors and Bioelectronics: X* **2023**, *14*, 100378.

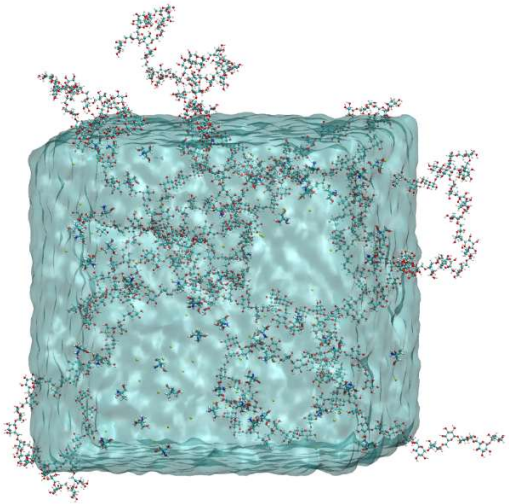
MOLECULAR DYNAMICS SIMULATION OF DEXTRAN INTERACTIONS WITH BIOLOGICALLY RELEVANT MOLECULES

Bc. Paulína Šimková

Mgr. Ing. Eva Krupičková Pluhařová, Ph.D.

The cellular interior is densely packed with organelles and macromolecules, creating a crowded environment that significantly affects the kinetics, thermodynamics, and function of biomolecular processes. Despite this, most biochemical experiments are still performed in dilute aqueous buffers, lacking crowded environment. Hence, macromolecular crowding agents are employed to mimic these conditions. [1]

In this study, we employed all-atom molecular dynamics simulations to investigate the interactions between dextran, a commonly used synthetic crowder, and tris(hydroxymethyl)aminomethane (TRIS), a widely used buffering agent in biochemical assays. Our results provide molecular-level insights into how buffer molecules interact with crowding agents, emphasizing the potential role of solvent composition and pH conditions in modulating crowding effects. This work contributes to a more accurate interpretation of in vitro studies and highlights the need to consider crowding-buffer interactions in experimental design.



References:

[1] T. P. Silverstein and K. Slade, “Effects of Macromolecular Crowding on Biochemical Systems”, *Journal of chemical education*, vol. 96, no. 11, 2019, doi: 10.1021/acs.jchemed.9b00399.

(SPECTRO)ELECTROCHEMISTRY IN CHAOTROPIC PERCHLORATE WATER-IN-SALT ELECTROLYTES

Ing. Petr Čech

Mgr. Otakar Frank, Ph.D.
Ing. Zuzana Vlčková, Ph.D.

Chaotropic water-in-salt electrolytes are a promising route towards green energy storage. Their high salt concentration and low charge density (chaotropy) disrupt the hydrogen bond network and therefore broaden the electrochemical stability window (ESW). In addition, the increased number of anions in the cation solvation sheath facilitates the formation of a solid electrolyte interphase layer (SEI) at the anode through the reaction of inorganic anions prior to any hydrogen evolution. The SEI enables the transport of active ions and is crucial for further stability of the electrode-electrolyte interface [1], [2].

To examine the compatibility of anode materials with WiSE systems, this study investigates boron- and phosphorus-doped diamonds as possible anode materials in comparison to glassy carbon electrodes. ESWs were evaluated using linear sweep voltammetry, while macro- and micro-scale in-situ Raman spectroelectrochemistry measurements were conducted to explore electrode-electrolyte interfacial reactions [3].

References:

[1] Z. A. Zafar *et al.*, 'Chaotropic anion based "water-in-salt" electrolyte realizes a high voltage Zn–graphite dual-ion battery', *J. Mater. Chem. A*, vol. 10, no. 4, pp. 2064–2074, 2022, doi: 10.1039/D1TA10122F.

[2] H. Gao *et al.*, 'Recent advances in "water in salt" electrolytes for aqueous rechargeable monovalent-ion (Li+, Na+, K+) batteries', *Journal of Energy Chemistry*, vol. 69, pp. 84–99, Jun. 2022, doi: 10.1016/j.jechem.2021.12.025.

[3] Z. V. Živcová *et al.*, 'Electrochemistry and in situ Raman spectroelectrochemistry of low and high quality boron doped diamond layers in aqueous electrolyte solution', *Electrochimica Acta*, vol. 87, pp. 518–525, Jan. 2013, doi: 0.1016/j.electacta.2012.09.031.

ATOM BY ATOM BUILT ATOMICALLY PRECISE CuPd PENTAMER CLUSTERS FOR CYCLOHEXENE DEHYDROGENATION

Petr Vítek

Ing. Stanislav Valtera

The subnanometer size of the clusters grants them different properties compared to bulk materials, owing to pronounced quantum effects at this scale. Most metal atoms are undercoordinated, making even minor changes in their composition [1] or size [2] significantly more impactful than in the bulk material. In addition, support influences the clusters through the cluster-support interaction by altering the electronic structure of the clusters [3], offering an additional parameter with which the catalytic properties can be fine-tuned.

During this study, atomically precise $Cu_{5-n}Pd_n$ ($0 \leq n \leq 5$) clusters, which were deposited on ultra-thin zirconia (ZrO_2) support, were tested during cyclohexene dehydrogenation. All clusters containing palladium showed catalytic activity, and their activity depends on the palladium content. Switching an atom of Cu for the Pd atom in the cluster Cu_5 had a significant effect on the catalytic properties, altering the activity while maintaining a high selectivity for the benzene formation. The results also revealed that under given reaction conditions, set for oxidative dehydrogenation (ODH), the reaction proceeds as a combination of oxidative and non-oxidative dehydrogenation (DH). The DH pathway is particularly relevant for hydrogen storage, as organic molecules can serve as liquid organic hydrogen carriers (LOHC), providing a viable option for energy-efficient hydrogen storage.

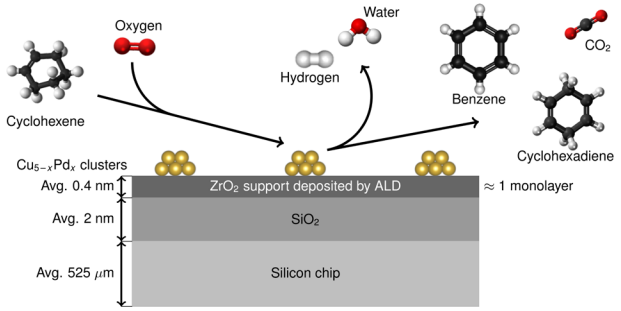


Figure 1: Schematic representation of the dehydrogenation of cyclohexene on the surface of the nanocatalyst.

References

[1] A. Halder, M.-A. Ha, H. Zhai, B. Yang, M. J. Pellin, S. Seifert, A. N. Alexandrova, and S. Vajda. “Oxidative Dehydrogenation of Cyclohexane by Cu vs Pd Clusters: Selectivity Control by Specific Cluster Dynamics”. *ChemCatChem* 12.5 **2019.**

[2] S. Valtera, J. Jašík, M. Vaidulych, J. E. Olszówka, M. Zlámalová, H. Tarábková, L. Kavan, and Š. Vajda. “Atom by atom built subnanometer copper cluster catalyst for the highly selective oxidative dehydrogenation of cyclohexene”. *The Journal of Chemical Physics* 156.11 **2022.**

[3] J. Jašík, S. Valtera, M. Vaidulych, M. Bunian, Y. Lei, A. Halder, H. Tarábková, M. Jindra, L. Kavan, O. Frank, S. Bartling, and Š. Vajda. “Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu4 – *n*Pd*n* ($0 \leq n \leq 4$) tetramer clusters: the effect of cluster composition and support on performance”. *Faraday Discuss.* 242 **2023.**

Substrate Binding in Enzyme Clusters: Effects of Crowders and Transient Interactions

MSc. Ashwathi Poolamanna

Mgr. Štěpán Timr, Ph.D

In living cells, various enzymes have been found to assemble into transient structures that can appear and disassemble depending on external conditions. Such assemblies have been found in various pathways, including glycolysis, oxidative phosphorylation, purine synthesis, etc. However, the molecular mechanisms driving their formation and functional relevance remain poorly characterized.

In this study, we develop a highly coarse-grained computational model based on insights from all-atom molecular dynamics simulations to investigate how the presence of crowders, as well as transient interactions between enzyme assembly constituents—enzymes, substrates, and crowders—influence the active site occupancy.

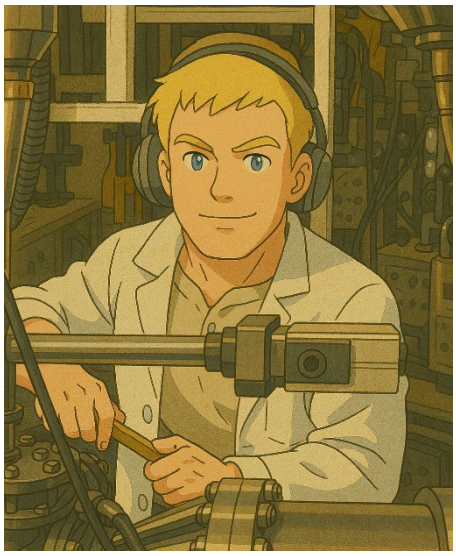
Our simulations allow us to identify the sets of conditions that lead to maximised or minimised substrate binding. These findings reveal how the properties of the crowded environment in enzyme assemblies govern the efficiency of metabolic pathways.

References:

Ranganathan, Srivastav, Junlang Liu, and Eugene Shakhnovich. "Enzymatic metabolons dramatically enhance metabolic fluxes of low-efficiency biochemical reactions." *Biophysical Journal* 122.23 (2023): 4555-4566.

Castellana, Michele, et al. "Enzyme clustering accelerates processing of intermediates through metabolic channeling." *Nature biotechnology* 32.10 (2014): 1011-1018.

Zhang, Youjun, and Alisdair R. Fernie. "Metabolons, enzyme–enzyme assemblies that mediate substrate channeling, and their roles in plant metabolism." *Plant Communications* 2.1 (2021).



SELECTIVE OXIDATIVE DEHYDROGENATION OF CYCLOHEXENE OVER Cu_3Pd_2 CLUSTERS FOR H_2 GENERATION

Ing. Stanislav Valtera

RNDr. Štefan Vajda, CSc. Dr.habil.

Recent advancements in nanocatalysis have highlighted the potential of bimetallic clusters to enhance catalytic performance. This study focuses on atomically precise Cu_3Pd_2 clusters were studied on ultra-thin ZrO_2 (deposited by ALD on a SiO_2 support) with two thicknesses, 4 Å and 10 Å, respectively. Additionally, the impact of pre-annealing the support in O_2 at 550 °C was investigated. It was found that clusters deposited on 4 Å ZrO_2 exhibited the highest activity, whereas annealing in O_2 led to significantly higher cluster stability, as evidenced by temperature programmed reaction (TPR) measurements.

In the next step, the effect of oxygen content in the working gas mixture (C_6H_{10}:O_2 with ratios of 1:10, 1:5, 1:1, 1:0.1, 1:0.02, and 1:0) was investigated, revealing a significant influence of O_2 concentration on the resulting reaction rates and the preferred reaction pathway. The latter is an important finding, demonstrating that even in the presence of oxygen, the reaction can proceed not only via the expected oxidative dehydrogenation (ODH) pathway but also through a non-oxidative dehydrogenation (DH) pathway. Moreover, the fraction of DH, producing pure hydrogen, was above 80% for a 1:1 ratio. Importantly, in the absence of oxygen, no reaction occurred. These findings are of great interest in the field of liquid organic hydrogen carriers - LOHCs, providing a more energy-efficient reaction pathway, where a small amount of O_2 can effectively decrease the reaction barrier and trigger the reaction at a lower temperature.

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CROWDERS ALTER ACCESSIBILITY OF ADENYLATE KINASE CONFORMATIONAL SPACE

MSc. Samanta Madhav

Mgr. Timr Štěpán Ph.D.

Enzymes in biological cells exist in crowded conditions, surrounded by membranes, proteins, sugars, and other biomolecules. These conditions are very different from the traditional in-vitro assays, which rely on studying the protein in an isolated manner. Crowders can alter enzyme activity in in a non-trivial way. Thus, it is essential to understand these effects.

We used all-atom molecular dynamic simulations (MD) to characterize the effects of various crowders on adenylate kinase (ADK) as a model enzyme. Previously observed experimental results indicate the role of the excluded volume effect in altering the opening and closing mechanism of ADK in the presence of a crowder. Our findings show that crowders interact intimately with the enzyme, limiting its accessibility to extreme conformations. They disrupt conformational changes by interacting with the active site, substrates, or essential residues. They also slow down local and global fluctuations of the LID and NMP domains, crucial for enzyme activity.

Our results suggest that a crowded milieu can affect enzyme activity by changing the conformational landscape and directly interacting with the substrate or residues of the active site. This work highlights the complex ways in which cellular crowding can affect enzyme function.

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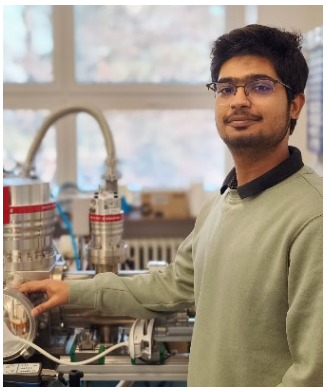
HIGH-YIELD ASSEMBLY OF PLASMON-COUPLED NANODIAMOND SYSTEMS VIA DNA ORIGAMI FOR TUNABLE LIGHT EMISSION

Niklas Hansen MSc.

Vladimíra Petráková, PhD

Spatial arrangement of optically active elements is a crucial factor in natural and engineered photonic systems. Color centers in nanodiamond offer a diverse portfolio of advantages in quantum sensing and information processing; however, precise and reproducible positioning, as well as coupling, into complex optical nanoarchitectures is challenging. DNA origami offers an elegant solution with the construction of fully addressable nanostructures, as previously demonstrated with precise positioning of various kinds of nanoparticles. Here, we present a robust method for covalent functionalization of fluorescent nanodiamonds, enabling the high-yield assembly of nanodiamonds and gold nanoparticles on DNA origami nanostructures. We reveal a distance dependent modulation of the color center emission with varying inter-particle space. Our findings further indicate selective plasmon-driven effects in regard to radiative and non-radiative processes. We overcome key limitations in current nanodiamond assembly strategies and provide insight into the modulation of nitrogen vacancy color centers via plasmonic coupling that advance to quantum photonic and sensing applications.



ELECTRON COLLISION WITH LIQUID MICRO-JET: QUANTIFYING SOLVATED ELECTRONS

Samrat Saha, MSc.

Dr. Pamir Nag, Ph.D.

When high-energy radiation, including charged particles, passes through matter and living cells, it transfers energy to the medium, leading to the generation of secondary electrons. Both primary radiation and low-energy secondary electrons (around <15 eV) can damage the living cells and also cause DNA-strand breaks. In radiation therapy, the primary impact is largely attributed to the secondary low-energy electrons generated by the primary radiation sources. Until now, most of the radiation induced studies on biologically important molecules were performed either on isolated gas phase, molecules on surfaces or in water cluster environments [1]. But it is impotant to study any biologically important molecules in their natural environment, i.e., in aqueous solvated phase.

Our research group recently developed a unique recirculating liquid micro-jet setup [2] to study the electron-induced chemical reactivity in the solvated phase. We can irradiate the liquid phase sample with an energy controlled electron beam ranging from 50 eV to 1 KeV. Unitll now, it was challenging to quantify the solvated electron. Currently we are using nitrate to nitrite ion reduction reaction, $\mathrm{NO_3^-} + 2\,\mathrm{e_{hyd}^-} + 2\,\mathrm{H^+} \rightarrow \mathrm{NO_2^-} + \mathrm{H_2O}$, to quantify the solvated electron dose in the liquid micro-jet.

We irradiated the sample with different incident electron energies and varying doses. We collected the irradiated samples and performed ex-situ chemical analysis, followed by fluorescence measurements using a spectrofluorometer to determine the dose. We plan to continue the experiments with biologically relevant molecules to study electron-induced processes in aqueous environments.

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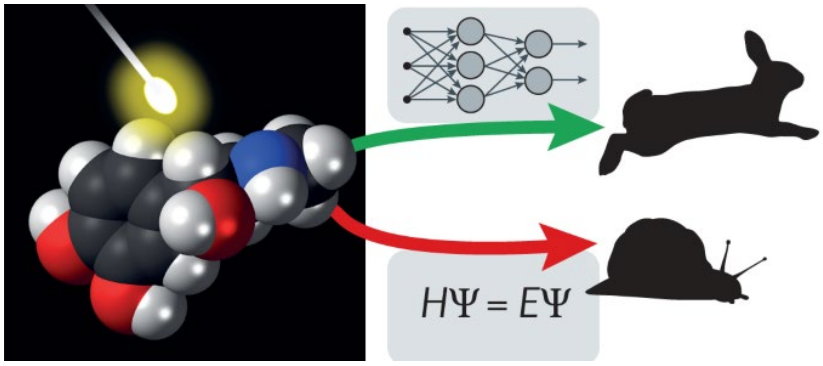
MACHINE LEARNING ACCELERATED SIMULATIONS OF PHOTOCHEMICAL PROCESSES

Mgr. Jakub Martinka

prof. Mgr. Jiří Pittner Dr. rer. nat., DSc.

Machine learning (ML) has significantly advanced computational chemistry, particularly in simulating molecules in their electronic ground state. However, applying ML to photochemical processes, where molecules are in excited states, remains challenging, with notable progress occurring only recently. A major difficulty lies in predicting nonadiabatic couplings (NACs), as they are vectorial, exhibit large values only at specific molecular geometries, and can be either positive or negative at the same geometry. We have developed an iterative procedure for learning NACs and demonstrate its performance on a prototypical photochemical system, fulvene. This approach overcomes the limitations of standard computational methods, extending both the accuracy and length of simulations.



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LIPID SCRAMBLING PATHWAYS IN THE SEC61 TRANSLOCON COMPLEX

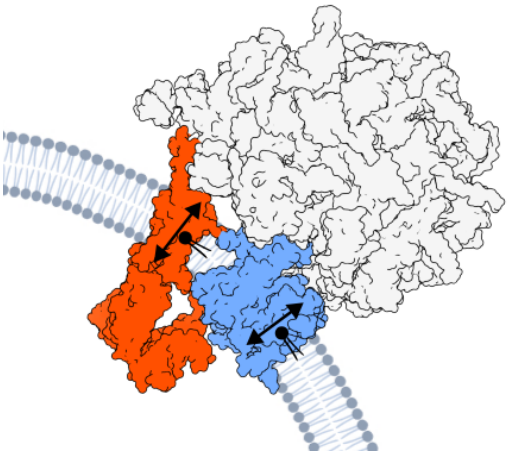
Mgr. Jan Šimek

Assoc. Prof. Radek Šachl

Cellular homeostasis depends on the efficient transport of metabolic products, including the translocation of newly synthesized phospholipids across the endoplasmic reticulum (ER) membrane. This process is mediated by scramblases, which function without energy consumption and translocate lipids through biophysical features such as membrane thinning and polar cavities.

We identified these features in the structure of the Sec61 translocation channel in complex with the translocon-associated protein (TRAP). After purifying this complex and reconstituting it into liposomes, we used complementary fluorescence assays to detect non-selective lipid scrambling activity by the reconstituted translocon complexes. Notably, this activity was unaffected by Sec61 inhibitors that block the lateral gate, suggesting the existence of an alternative scrambling pathway within the complex.

Molecular dynamics simulations revealed a lipid scrambling route through Sec61 and suggested a possible pathway within TRAP. The simulations confirmed that local membrane thinning enhances scrambling efficiency. Although the scrambling is non-selective, phosphatidylcholine is translocated more rapidly than phosphatidylethanolamine and phosphatidylserine. Since the Sec61 polar cavity is likely inaccessible under physiological conditions, we propose that TRAP functions as the physiologically relevant scramblase.



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TREATMENT OF MOS_2 MONOLAYERS BY ATOMIC DEUTERIUM

Ing. Valerie Smeliková

doc. RNDr. Ing. Martin Kalbáč Ph.D., DSc.

Two-dimensional (2D) materials, such as transition metal dichalcogenides (TMDs), exhibit exceptional physical and chemical properties due to their atomic-scale thickness [1]. In this work, we present molybdenum disulfide (MoS_2) as a representative TMD material, prepared via gold-assisted exfoliation under ultra-high vacuum (UHV) conditions. The samples were subsequently modified through low-temperature atomic deuterium adsorption followed by annealing. We demonstrate that this process enables a phase transition from the stable 2H phase to the metastable 1T phase. The presence of deuterium in monolayer was confirmed by thermal programmed desorption (TPD) in combination with a quadrupole mass spectrometer [2]. Structural and chemical changes in the MoS_2 monolayer were analyzed using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), and X-ray diffraction (XRD).

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RAMAN SPECTROELECTROCHEMISTRY OF GRAPHENE ELECTRODES

Ing. Martin Jindra

Mgr. Otakar Frank, Ph.D.

Raman spectroelectrochemistry is a powerful tool that offers detailed insights into electrochemical processes. In this presentation, we focus on the behaviour of graphene, a two-dimensional allotrope of carbon. Working with such materials requires tailored approaches to control critical parameters such as defect density and charge transfer localization. To address this need, we have developed the μ-droplet technique, which enables precise simultaneous electrochemical and spectroscopic studies on the microscale.

Using our setup, we are able to investigate the effect of defects on charge transfer in graphene, as well as examine how low density of states influences the charge distribution within the graphene layer. Furthermore, we can monitor phonon behaviour under high charge doping regimes—a range typically difficult to access with other techniques. In addition, our approach allows us to measure low-intensity Raman signals, which are otherwise completely attenuated using classical spectroelectrochemistry methods, e.g., in the antiStokes region, providing access to microscale thermometry.

Our work lays a solid foundation for future experiments with graphene-based nanostructures and other two-dimensional materials, such as TMDCs.

RESTORING PHOTOLUMINESCENCE IN METAL-EXFOLIATED, LARGE AREA MOLYBDENUM DISULFIDE

Adeel Bukhari

Mgr. Otakar Frank Ph.D.

Metal-mediated exfoliation has been increasingly adopted during the preparation of two-dimensional (2D) material-based devices to create large monolayers of these materials. Exfoliating a 2D material, like molybdenum disulfide (MoS_2), onto a fresh layer of Au can facilitate the production of single-crystal MoS_2 monolayers with lateral dimensions in the range of millimeters. This technique leverages the strong interaction between the MoS_2 and the Au surface; however, this comes at the cost of the photoluminescence (PL) of the MoS_2 being quenched due to the charge transfer from the hybridised semiconductor to the gold. Fabricating electrical contacts and gating on these systems is also not straightforward due to the continuous layer of Au underneath the monolayer.

Here we demonstrate how metal-assisted exfoliation can be used to produce large monolayers of MoS_2, which retain their ability to emit light, by treating the substrate with oxygen plasma. The intensity of this PL can be controlled by adjusting the thickness of the Au layer and the amount of time that it is exposed to the plasma. These Au surfaces can also be pre-patterned such that upon exfoliation, the flakes are already contacted and isolated, and ready for electrical measurements.

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INTRODUCE METHOD, WE HAVE NOT USED HERE BEFORE, THEY SAID. IT WILL BE FUN, THEY SAID.

Mgr. Zuzana Johanovská

Prof. Martin Hof

The research is driven by a pioneers, who are willing to search through the unexplored areas. For most PhD students, whole scientific world is one big jungle, so they have the best preconditions to fall into such unknown places, and became creative and adventurous against their own will.
In my talk, I plan to share my experience with the PhD project including techniques, which were not used at our group before and which had to be built (almost) from a scratch. Hopefully, it can be source of inspiration, (de)motivation and opportunity to share my hard earned knowledge about possible pitfalls and challenges with the implementation of new approach into current research. In the end, I will show the preliminary results, obtained thanks to all this effort and also indicate the future plans for other possible usage.

To get at least small idea what to expect, I will tell you, that methods I am talking about include optical tweezer and direct mechanical manipulation of few-micrometer samples.

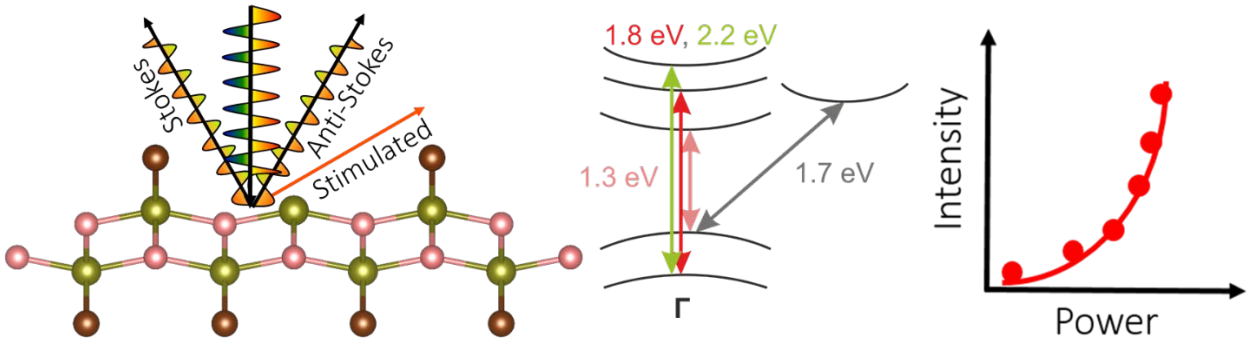
EXPLORING RESONANCE RAMAN SCATTERING AND STIMULATED RAMAN SCATTERING EFFECTS IN CrSBr

Satyam Sahu M.Sc.

Dr. Matěj Velický, Supervisor

Dr. Otakar Frank, Co-supervisor

CrSBr is an air-stable magnetic semiconductor and a van der Waals material with notable intrinsic properties, such as crystalline anisotropy, quasi-1D electronic behavior, and layer-dependent magnetism. In this seminar, I will discuss the origin of the emission peak near 1.7 eV observed in its photoluminescence spectrum and the excitation energy-dependent Raman spectroscopy. I will also discuss the observation of stimulated Raman scattering in CrSBr and $CrSBr_{(1-x)}Cl_x$ ($0 \leq x \leq 0.5$), highlighting the interplay between electronic and vibrational states in CrSBr and the Raman gain, which surpasses those reported in many three-dimensional systems. Additionally, I will comment on the unusually high anti-Stokes to Stokes intensity ratio in CrSBr, which varies with the laser power and crystal orientation. These findings underscore the unique vibrational and electronic interactions in these materials.



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DISTRIBUTION OF ADHESION MOLECULES IN THE IMMUNOLOGICAL SYNAPSE

M.Sc. José Alfredo González Navarro

Marek Cebecauer, PhD.

Adhesion molecules drive formation and stabilize immune synapses (IS) formed between T-cells and antigen-presenting cells (APCs) during immune response to pathogen or cancer cells. Adhesions molecules localize to the plasma membrane [1]. The two cell types are covered with diverse morphological structures, especially microvilli [2]. To date, nanoscale localization of adhesion molecules in or out of the microvilli, and their reorganization during the IS formation, is unknown. In this work, we determine the nanoscopic distribution of adhesion molecules at the surface of T-cells and APCs before and during the formation of the immune synapse. Using super-resolution microscopy, we show different organization of the studied adhesion molecules (CD2-CD58 and LFA-1 - ICAM1 pairs) with respect to the microvilli prior stimulation. Nevertheless, LFA-1 is predominantly localized in the membrane base of T-cells, whereas CD2 and ICAM1 are predominantly excluded from the tips of the microvilli. Using confocal microscopy, we captured high-resolution images of primary T-cells and APCs pulsed with antigens. During the IS formation, the CD2-CD58 reorganize and accumulates in outer ring of the IS, whereas LFA-1-ICAM1 receptor-ligand pair localizes in the central IS. Our study will continue with super-resolution microscopy approach to precisely localize both receptor-ligand pairs in the IS of activated cells. Our study highlights the importance of the nanoscale localization of adhesion molecules and how their localization in the microvilli may differ from other types of ligands.

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INSIGHTS INTO PARTICLE-SUPPORT INTERACTIONS AND THEIR ROLE IN CO_2 HYDROGENATION CATALYSIS

Mgr. Karolína Simkovičová

RNDr. Štefan Vajda, CSc. Dr.habil.

Developing efficient strategies for CO_2 utilization is crucial for sustainable energy production and emissions reduction. The conversion of carbon dioxide and hydrogen into valuable products such as methane, methanol, and longer-chain hydrocarbons offers a promising solution. However, the high stability of CO_2 presents a major challenge for efficient hydrogenation under mild conditions (atmospheric pressure and 350 °C). Designing highly selective and efficient catalysts is crucial to overcoming these limitations and steering the reaction toward desired products.

This presentation discusses the use of a copper/iron nanosized catalyst, which exhibits high surface area and high dispersion of active sites, promoting efficient CO_2 activation and the subsequent hydrogenation and hydrocarbon chain growth. The unique combination of Cu and Fe is taking advantage of copper's ability to activate hydrogen and promote hydrogen spillover and iron oxide's role in coupling of C1 units by the in-situ generated Fe_5C_2, enabling the formation of hydrocarbon chains [1].

Recent studies on copper-based catalysts reveal dynamic changes in surface structure and oxidation state under reaction conditions [2]. In this work, the catalysts were characterized using a variety of techniques, including X-ray, infrared, and Raman spectroscopy, temperature-programmed reduction, and N_2 sorption, both ex-situ and in-situ, to gain insights into the structural and electronic properties under reaction conditions.

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TUNING PEG BASED MOLECULES FOR CUSHIONING SUPPORTED LIPID BILAYERS MONITORED BY GRAPHENE INDUCED ENERGY TRANSFER

MSc. Daniela G. Blanco-Campoy
Mgr. Jan Sýkora, Ph.D.

In recent years, super-resolution microscopy techniques have undergone a great revolution in terms of spatial details. The enhance axial resolution is necessary for studying lipid bilayers, which are highly dynamic self-assembly with a typical thickness of about 5 nm. Graphene Induced Energy Transfer (GIET) is one of the approaches resolving axial distances of fluorescent emitters with nanometer resolution. This approach depends on graphene-induced fluorescence quenching, which reduces the lifetime in a distance-dependent manner. The GIET allows to discriminate between membrane organization in bottom and top leaflets.

Our research aims to design and build substrates suited for GIET investigations on Supported Lipid Bilayers (SLBs). We use a graphene monolayer on a glass support that is coated with cushions made of Perylene-bisimide-Polyethylene Glycol (PBI-PEG) for this purpose. We have tested a number of PEG polymers with varying lengths and elaborating methods to achieve the best SLB formation. We use for SLB characterization fluorescence techniques including Fluorescence Recovery After Photobleaching (FRAP) and Fluorescence Correlation Spectroscopy (FCS) to track lateral motility of labeled lipid and Fluorescence Lifetime Imaging (FLIM) to measure the thickness of the formed lipid system attached to the substrate by GIET and Atomic Force Microscopy (AFM) to confirm the correct SLB formation.
The system described herein have the potential to be used for a wide range of biophysical applications, including the study of asymmetric bilayer motility, lipid flip-flop between leaflets in a single bilayer, etc.

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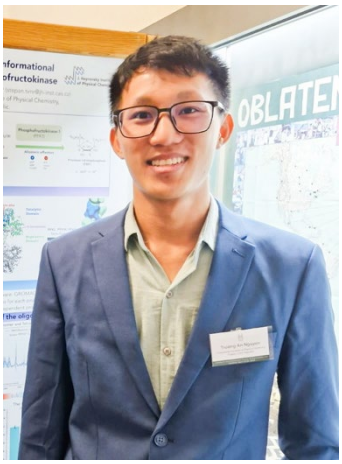

MECHANISTIC INSIGHTS INTO ALLOSTERIC REGULATION OF HUMAN PHOSPHOFRUCTOKINASE-1 BY MOLECULAR DYNAMICS SIMULATIONS

Truong An Nguyen

Mgr. Štěpán Timr Ph.D.

Phosphofructokinase-1 (PFK1) is a key enzyme in the glycolytic pathway, playing an important role in regulating this metabolic process based on the concentrations of ATP, ADP, and AMP. ATP acts as an inhibitor of the protein, while ADP and AMP serve as activators. To gain a better understanding of this allosteric regulation, we perform molecular dynamics simulations combined with replica exchange umbrella sampling, focusing on nucleotide binding to an experimentally determined activating site. This approach allows us to clarify how the different nucleotides interact with various residues in the activating site and compare the binding free energies. The results help us elucidate the factors contributing to the selectivity of the activating site, thus deepening our understanding of the mechanisms underlying the complex allosteric regulation of PFK1.

NEUTROPHIL RESPONSE TO MULTIPLE STIMULI

BSc. Irene Echezarreta Mendicute

Mgr. Katerina Paldusova
Mgr. Marek Cebecauer, Ph.D.

Neutrophils are the most abundant white blood cells serving as the first line defense against microbes. Apart from ingestion of pathogens and release of granules containing lytic proteins, neutrophils expel neutrophil extracellular traps (NETs) during the process of NETosis to capture and immobilise and/or kill microbes. NETs are web-like DNA structures decorated with protein assemblies with specific antimicrobial functions. NETosis has been examined in response to multiple stimuli, including bacteria (*Staphylococcus aureus)*, fungi (*Candida albicans)* and chemical compounds such as Phorbol 12-myristate 13-acetate (PMA). In this framework, our aim is to evaluate and compare the efficiency of NETosis induced by different stimuli. We are testing bacteria of different origin and physiological states with non-bacterial stimuli such as PMA, immune complexes and cholesterol crystals. Our team's preliminary work indicates that *S. aureus* exhibits greater potency in inducing NETosis than non-physiological PMA. Compared to PMA, neutrophils stimulated with *S. aureus* also result in more abundant NETs with different primary structure. Our next step is to investigate potential differences in the molecular structure of NETs in higher detail by using super-resolution imaging, specifically Single Molecule Localization Microscopy (SMLM).

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SEMINÁŘ STUDENTŮ ÚFCH JH 2025

Sál Rudolfa Brdičky a vestibul
Ústavu Heyrovského v Praze

21.5.2025