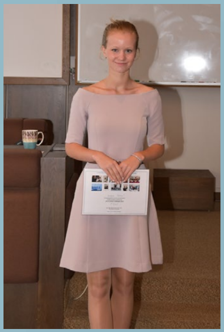
STUDENT SEMINAR 2026



May 13-14, 2026

J.Heyrovský Institute
of Physical Chemistry

KLÁŠTER
HEJNICE
vzdělávací, konferenční a poutní dům

Seminář studentů
Heyrovského ústavu 2026

Sborník příspěvků

ze studentské konference konané
13. – 14. května 2026
v konferenčním centru v klášteře v Hejnicích

Seminar of Students
of Heyrovsky Institute 2026

Collection of abstracts

of all lectures given at the student conference
held on 13-14 May 2026
in Conference centre in Hejnice Monastry

Seminář studentů Heyrovského ústavu 2026
Sborník příspěvků ze studentské konference
konané 13 - 14. května 2026
v konferenčním centru v klášteře v Hejnicích

Kolektiv autorů
Sestavila: Ing. Květa Stejskalová, CSc.
Vydává: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 00 Praha 8, Česká republika
Tisk: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 00 Praha 8
Vydání: první
Místo a rok vydání: Praha, 2026
Publikace neprošla jazykovou úpravou

List of presented students and postdocs (24)
Seznam prezentujících studentů a postdoků (24)

Bachelor and diploma students (3)
Diplomanti a zájemci z řad bakalářů

Bičák Vojtěch *(VŠCHT Praha, diplomant, školitel: A. Liška)*

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

Vítek Petr *(VŠCHT Praha, bakalářské studium, školitel: Š. Vajda)*

High school student in project Open Science AS CR (2)
Středoškolští stážisté v projektu Otevřená věda AV ČR (2)

Ševčík Michal *(Gymnázium Karviná, stážista v projektu Otevřená věda AVČR lektorky K. Stejskalové; prezentace středoškolské stáže z oboru analytické chemie z Univerzity Pardubice)*

Vícha Tadeáš *(BiGY Žďár nad Sázavou, stážista v projektu Otevřená věda AVČR lektorky K. Stejskalové; prezentace ročníkové práce v oboru didaktiky chemie)*

PhD Students (17):
Studenti DSP studia

Burattini Davide *(školitel J. Sýkora)*

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

Dostálková Lucie *(školitelka R. Sokolová)*

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

Hanušová Michaela *(školitel M. Velický)*

Hodaš Matúš *(školitelka Š. Jungwirth Pokorná)*

Ivakh Sofiia *(školitel B. Josypčuk)*

Johanovská Zuzana *(školitel M. Hof)*

Labzova Olexandra *(školitel T. Navrátil)*

Poolamanna Ashwathi *(školitel Š. Timr)*

Pradhan Krishna *(školitel R. Šachl)*

Saha Samrat *(školitel P. Nag)*

Samanta Madhav *(školitel Š. Timr)*

Sharma Muskan *(školitel M.Srnec)*

Soe Chan Thar *(školitel M. Velický)*

Šimek Jan *(školitel R. Šachl)*

Truong An Nguyen *(školitel Š. Timr)*

Postdocs (2)
Postdoci

Pirker Luka, Ph.D. *(Dep. of electrochemical materials)*

Sahu Satyam, Ph.D. *(Dep. of electrochemical materials)*

Referees:

Michal Horáček
Kinga Mlékodaj
Matěj Velický

SEMINÁŘ STUDENTŮ HEYROVSKÉHO ÚSTAVU 2026

PROGRAM 1. dne konference – středa 13. května 2026

Odjezd autobusu z parkoviště před ústavem v 10:00 hodin.

Předpokládaný příjezd do Konferenčního centra v klášteře v Hejnicích do 12 hodin.

Ubytování od 12 hodin (recepce), po té následuje oběd od 13 hodin v restauraci.

SEMINAR OF STUDENTS OF HEYROVSKY INSTITUTE 2026

PROGRAM - Wednesday May 13, 2026

Departure from the parking place
in front of the Heyrovsky Institute building at 10:00 a.m.
Check-in begins at 12:00 (at the reception desk),
followed by lunch starting at 1:00 p.m. at the restaurant

13:00 -14:00	**OBĚD** *Lunch at the restaurant* (podává se v restauraci)		
14:00-14:15	*Zahájení konference „Seminář Studentů ÚFCH JH 2026“* *Opening of the Annual conference* *„Seminar of Students of JHI 2026“*		
SEKCE AMULET: ***Prezentace 6 mladých vědců zapojených do projektu AMULET*** **AMULET SECTION:** ***The presentations of 6 young scientists participating in the AMULET project***			
Čas	*Předsedají-cí/Chairman*	*Přednášející/ Lecturer*	*Název příspěvku/ Title of the prezentation*
14:15-14:30	***Michaela Hanušová***	GONZÁLES Navarro José Alfredo (doctorand)	MULTIFACETED SUPER-RESOLUTION IMAGING TO REVEAL DYNAMIC NANOSCALE ORGANISATION OF ADHESION MOLECULES IN THE IMMUNE SYNAPSE
14:30-14:45		SAHA Samrat (doctorand)	STUDY OF ELECTRON AND ION-INDUCED DISSOCIATION OF IRON TETRACARBONYL ACROLEIN
14:45-15:00		JOHANOVSKÁ Zuzana (doctorand)	MICROMANIPULATIONS IN MEMBRANE STUDIES
15:00-15:15	**PŘESTÁVKA -** *Break*		
15:15-15:30	***Satyam Sahu***	HODOŠ Matúš (doctorand)	PROBING TRANSMEMBRANE PROTEIN NANO-ENVIROMENT USING FRET-GP
15:30-15:45		ŠIMEK Jan (doctorand)	LIPID NANOPARTICLE ENDOSOMAL ESCAPE: INSIGHTS FROM VESICLE-BASED MODEL SYSTEMS

15:45-16:00	***Satyam Sahu***	PIRKER Luka, Ph.D. *(postdoc)*	CORRELATION BETWEEN DEFECTS AND THE OPTICAL AND ELECTRICAL PROPERTIES INDUCED BY HELIUM IONS IN MoS_2
16:00-16:30	**PŘESTÁVKA NA KÁVU -** *Coffe break*		
16:30-17:45	*Pokračují prezentace dalších studentů Heyrovského ústavu* *Presentations by other students from the Heyrovský Institute are continuing*		
16:30-16:45	***Zuzana Johanovská***	MYŠÁK Daniel *(graduate student)*	COMPUTATIONAL MODELLING OF GLUTAMATE DEHYDROGENASE IN CROWDED ENVIRONMENT WITH FOCUS ON THE ACTIVE SITE
16:45-17:00		BIČÁK Vojtěch *(graduate student)*	ELECTROCHEMISTRY OF TAMOXIFEN
17:00-17:15		VÍTEK Petr *(undergraduate)*	ATOMICALLY PRECISE CuPd PENTAMER CLUSTERS FOR CATALYTIC DEHYDROGENATION OF CYCLOHEXENE
17:15-17:30		ŠEVČÍK Michal (*high school internship*)	„ZELENĚJŠÍ“ ROZPOUŠTĚDLA PRO PULZNÍ VOLTAMETRICKOU ANALÝZU PESTICIDU FOLPETU NA UHLÍKOVÝCH PRACOVNÍCH ELEKTRODÁCH
17:30-17:45		VÍCHA Tadeáš (*high school internship*)	DIDAKTICKÁ PRAXE V CHEMII A JEJÍ APLIKACE VE ŠKOLNÍ VÝUCE
17:45 **18:00**	*Ukončení prvního dne konference - End of the first day of the conference* **VEČEŘE v RESTAURACI - začátek v 18:00** *Dinner at the restaurant - 18:00*		

PROGRAM 2. dne konference - čtvrtek 14.5.2026

PROGRAM - Thursday May 14, 2026

Čas	*Předseda-jící/ Chairman*	*Přednášející/ Lecturer*	*Název příspěvku/ Title of the prezentation*
8:55	*Zahájení druhého dne konference* *Opening of the second day of the conference*		
9.00-9:15	***Truong*** ***An Nguyen***	ČECH Petr (doctorand)	BORON-DOPED DIAMOND ELECTRODES IN HIGHLY CONCENTRATED CHAOTROPIC ELECTROLYTES: A (SPECTRO)-ELECTROCHEMICAL STUDY
9:15-9:30		SAMANTA Madhav (doctorand)	SLOW DANCING IN A CROWDED ROOM: EFFECT OF MACROMOLECULAR CROWDING ON DYNAMICS OF ADK
9:30-9:45		DOSTÁLKOVÁ Lucie (doctorand)	UNRAVELING THE OXIDATION MECHANISM OF THE TOPICAL DRUG TAPINAROF WITH A MULTIDISCIPLINARY APPROACH
9:45-10:00		SHARMA Muskan (doctorand)	H-ATOM ABSTRACTION SELECTIVITY IN PROZAC DERIVATIVES: INSIGHTS FROM THE OFF-DIAGONAL THERMODYNAMICS CONTROLLED THROUGH THE MODULAR DESIGN OF OXIDANTS
10:00-10:30	**PŘESTÁVKA NA KÁVU** *Coffee break*		
10:30-10:45	***Pirker*** ***Luka***	HANUŠOVÁ Michaela (doctorand)	INVESTIGATING INTERLAYER DECOUPLING IN EXFOLIATED TMDCS ON METAL SUBSTRATES
10:45-11:00		BURATTINI Davide (doctorand)	SPECTROSCOPIC READOUT OF WATER PERMITTIVITY WITHIN PROTEINS LUMEN
11:00-11:15		POOLAMANNA Ashwathi (doctorand)	SUBSTRATE BINDING IN ENZYME CLUSTERS: EFFECTS OF CROWDERS AND TRANSIENT INTERACTIONS
11:15-11:30		PRADHAN Krishna (doctorand)	SIMULATION AND EXPERIMENTAL STUDIES OF TRANSPORT OF CELL-PENETRATING PEPTIDES ACROSS BIOLOGICAL MEMBRANES
11:45-13:00	**PŘESTÁVKA NA OBĚD** *(podává se v restauraci od 11:45)* *Lunch at the restaurant 11:45-13:00*		
13:00-13:15	***Gonzales*** ***Alfredo***	IVAKH Sofiia (doctorand)	PORTABLE VOLTAMMETRIC PLATFORM FOR THE SENSITIVE DETECTION OF SALINOMYCIN USING SILVER AMALGAM SCREEN-PRINTED ELECTRODES
13:15-13:30		SOE Chan Thar (doctorand)	SEQUENTIAL GOLD-ASSISTED EXFOLIATION FOR ULTRACLEAN TMDC HETEROSTRUCTURES WITH STRONG INTERLAYER COUPLING

13:30-13:45	***Gonzales*** ***Alfredo***	TRUONG An Nguyen (doctorand)	MECHANISTIC INSIGHTS INTO ALLOSTERIC REGULATION OF HUMAN PHOSPHOFRUCTOKINASE-1
13:45-14:00		LABZOVA Olexandra (doctorand)	VOLTAMMETRIC DETERMINATION OF TRAZODONE IN URINE USING BORON-DOPED DIAMOND ELECTRODE AFTER HOLLOW-FIBER MICROEXTRACTION
14:00-14:15		SAHU Satyam, Ph.D.¨ *(postdoc)*	WHEN PHONONS TALK TO EACH OTHER
14:15-14:45	**PŘESTÁVKA NA KÁVU** *Coffee break*		
14:45-15:00	**14:45 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ SOUTĚŽNÍ KONFERENCE A JEJÍ UKONČENÍ** *Closing ceremony - Results announcement (in conference hall)*		
15:15	**Odjezd do Prahy -** *autobusem z parkoviště u kláštera* ***v 15:15*** ***Departure from the parking place (in front of the monastery) - 3:15 p.m.***		

MULTIFACETED SUPER-RESOLUTION IMAGING TO REVEAL DYNAMIC NANOSCALE ORGANISATION OF ADHESION MOLECULES IN THE IMMUNE SYNAPSE

José Alfredo González Navarro

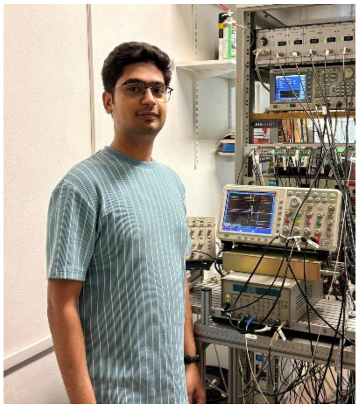
Mgr. Cebecauer Marek, Ph.D

The immune synapse (IS) is a morphological structure formed between T cells and target cells holding antigen. It coordinates signalling and adhesion for T-cell activation. The nanoscale 3D organisation of adhesion molecules in the IS remains poorly understood. We used multifaceted approach for sample preparation combined with several microscopy techniques and quantitative data analysis to uncover spatial arrangement of adhesion proteins from the first contact until maturation of the IS. We integrated immunofluorescence confocal microscopy, single-molecule localisation microscopy (SMLM, ~20 nm localisation precision), and two-colour STED microscopy (~80 nm resolution) to interrogate adhesion molecules at distinct spatial scales. Confocal microscopy of human primary T cells forming contact with superantigen-primed monocyte-derived macrophages enabled 3D morphometric analysis and quantitation of protein polarisation using semi-automated CellProfiler workflows. SMLM provided nanoscale distribution of LFA-1, ICAM-1, CD2, and CD58 proteins for cluster analysis with SR-Tesseler algorithm [1, 2]. Two-colour 3D STED with high-resolution z-line scanning was employed to directly visualise LFA-1–ICAM-1 and CD2–CD58 interactions within the synaptic interface. Our results demonstrate that early cell-cell contacts are mediated by membrane protrusions enriched in adhesion molecules. Upon cell contact, adhesion molecules reorganize within the synaptic interface, suggesting important role of the membrane topography and nanoscale protein organisation in the synapse initiation. In summary, this work demonstrates how integrating advanced sample preparation with high-resolution imaging techniques and quantitative data analysis enables detailed characterisation of dynamic molecular organisation in complex multicellular structures.

References:

[1] Franke, C., Chum, T., Kvíčalová, Z., Glatzová, D., Gentsch, G.J., Rodriguez, A., Helmerich, D.A., Herdly, L., Mavila, H., Frank, O., Brdička, T., van de Linde, S., Cebecauer, M. Communications Biology. 2022, 5, 218.

[2] Levet, F., Hosy, E., Kechkar, A., Butler, C., Beghin, A., Choquet, D., Sibarita, J.-B. Nature Methods. 2015, 12, 1065–1071.



STUDY OF ELECTRON AND ION-INDUCED DISSOCIATION OF IRON TETRACARBONYL ACROLEIN

Samrat Saha, MSc.

Dr. Pamir Nag, Ph.D.

We recently studied electron beam-induced dissociation of iron tetracarbonyl acrolein, $Fe(CO)_4(CH_2{=}CHCHO)$, a potential FEBID (Focused Electron Beam Induced Deposition) precursors molecule [1]. We probed the formation of anionic fragments resulting from dissociative electron attachment (DEA) via low-energy (0 to 12 eV) electron beam interactions, as well as the formation of cationic fragments due to dissociative ionisation at an incident electron energy of 70 eV.

We utilized two complementary experimental setups: a trochoidal electron monochromator with a quadrupole mass spectrometer (TEM-QMS) [2] to study the DEA process, and the CLUster Beam (CLUB) [3] apparatus to study both DEA and dissociative ionisation. Furthermore, Density Functional Theory (DFT) calculations were performed to determine reaction thresholds and elucidate the various reaction channels. Understanding these fragmentation patterns is highly relevant for understanding FEBID efficiency and quality, as secondary low-energy electrons via DEA process can cause incomplete dissociation leading to broadening of the deposited region as well as contamination.

Importantly, we observed that during dissociative ionisation, the most prominent channel is the formation of bare Fe^+ ions, whereas the production of bare Fe^- via the DEA process is weak [1]. With the higher mass resolution ($M/\Delta M = 4000$) of the CLUB setup, we were able to separate the Fe and acrolein ions.

References:

1. S. Das et al., J. Phys. B: At. Mol. Opt. Phys. **59** 035201(2026)
2. J. Langer et al., Eur. Phys. J. D, **72**, 112 (2018)
3. M. Fárník et al., Phys. Chem. Chem. Phys., **23**, 3194(2021).

MICROMANIPULATIONS IN MEMBRANE STUDIES

Mgr. Zuzana Johanovská

supervisors:
prof. Martin Hof, Dr. rer. nat., DSc.
Doc. RNDr. Radek Šachl, Ph.D.

Micromanipulation techniques offer relatively new and not yet fully explored possibilities for biomembrane research, as they enable the direct modification of the mechanical properties of cell membranes or giant unilamellar vesicles (GUVs), which serve as model systems for cellular membranes.

This approach allows us to expand the range of studies, including protein–membrane interactions, membrane organization, and the material characterization of membranes with different compositions. It allows to address research questions concerning mechanical aspects, which are commonly present in vivo but only rarely investigated in vitro.

The presentation will showcase a range of original results, demonstrating the broad applicability of this method, recently implemented at the Heyrovský Institute.

References:

Dimova R., Marques C.M. (**2020**), The Giant vesicle book, CRC Press, Boca Raton, ISBN 1498752179

Vinklarek I. et al (**2019**), Experimental Evidence of the Existence of Interleaflet Coupled Nanodomains: An MC-FRET Study, J. Phys. Chem. Lett., 10, 2024−2030

Shi, Z. & Baumgart, T. (**2015**), Membrane tension and peripheral protein density mediate membrane shape transitions. Nat. Commun. 6, 5974

Wang, H., Zhou, F., Guo, Y. et al. (**2022**), Micropipette-based biomechanical nanotools on living cells. Eur Biophys J 51, 119–133

Supported by: The Charles University Grant Agency (GA UK)

PROBING TRANSMEMBRANE PROTEIN NANO-ENVIROMENT USING FRET-GP

Mgr. Matúš Hodoš

Mgr. Šárka Jungwirth Pokorná, Ph.D.

Transmembrane proteins (TMPs) embedded in lipid bilayer facilitates crucial processes in cells including communication and material exchange. Increasing evidence show that TMPs' function is affected by the lipid packing of the membrane in their close proximity (TMP nano-environment).[1]

To probe the TMP nano-environment, we combine Förster resonance energy transfer (FRET) and generalized polarization (GP) approach. As the FRET is efficient in distances up to ~10 nm, we can selectively excite the probe in the close proximity of TMP. Combined with the ratiometric fluorescence readout (GP) we obtain the information about lipid packing only from TMP nano-environment. By establishing and validating the FRET-GP approach for live cell application, we aim to provide the insights into the transmembrane protein regulation by their lipid nano-environment in physiologically relevant conditions. This will eventually help to understand the lipid role in pathology.

References:

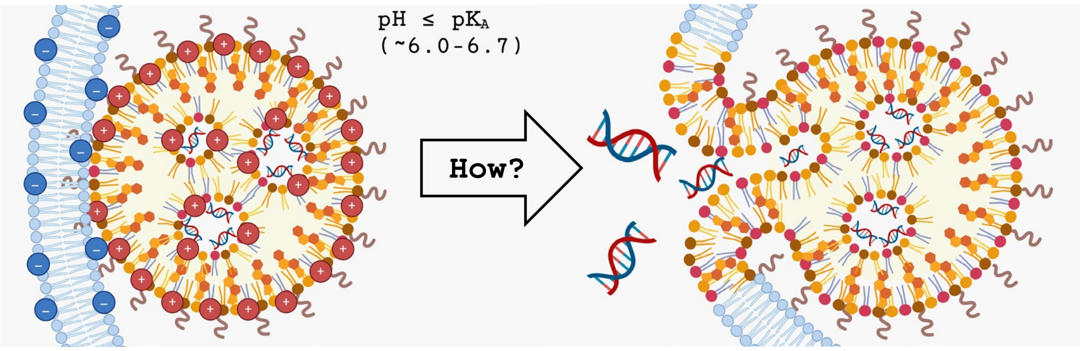
[1] Levental, I. et al. Nat. Rev. Mol. Cell Biol. 24, 107 (2023)

LIPID NANOPARTICLE ENDOSOMAL ESCAPE: INSIGHTS FROM VESICLE-BASED MODEL SYSTEMS

Mgr. Jan Šimek

Doc. RNDr. Radek Šachl, Ph.D.

Lipid nanoparticles (LNPs) have emerged as safe and versatile systems for the delivery of therapeutic RNA into human cells. [1] Successful delivery of siRNA or mRNA enables a broad range of gene therapy applications, including treatment of cancer, genetic disorders, and vaccination. [2] However, delivery efficiency remains a major challenge, as endosomal escape has been identified as a key bottleneck in the delivery process and its mechanism remains poorly understood. [3] Here, we study LNPs of different compositions under various pH conditions to identify links between formulation, chemical environment, and mechanisms of content release. Fusion of selected LNP formulations with liposomes mimicking endosomal membranes was examined using FRET-based assays, Laurdan Generalized Polarization, and Fluorescence Quenching, revealing strong dependencies on both pH and LNP composition. To directly address cargo delivery, LNPs loaded with fluorescently labeled DNA were imaged after delivery into Giant Unilamellar Vesicles (GUVs). Comparison of DOPE and DSPC as helper lipids revealed higher delivery efficiency for DOPE-containing LNPs, especially at pH 6.0. Fluorescence Correlation Spectroscopy (FCS) showed that delivered species often correspond to oligonucleotide-sized cargo, while in some cases larger objects—potentially intact LNPs—were detected within the GUV lumen, particularly at pH 5.0.



References:

[1] S. F. Dowdy, Nature biotechnology, 2017
[2] Y. Zong, Y. Lin, T. Wei, and Q. Cheng, Advanced Materials, 2023
[3] J. Gilleron et al. Nature biotechnology, 2013

CORRELATION BETWEEN DEFECTS AND THE OPTICAL AND ELECTRICAL PROPERTIES INDUCED BY HELIUM IONS IN MoS_2

Luka Pirker, Ph.D.

Research on two-dimensional materials is rapidly expanding because of their importance for fundamental science and technological applications. Their atomically thin structure makes them highly sensitive to external influences, creating opportunities to tune their properties through deformation, chemical doping, and controlled defect engineering [1,2]. Understanding defect-induced changes requires both precise defect creation and micro- and nanoscale characterization methods.

In this work, we study the electrical, optical, and structural properties of MoS_2 monolayers with defects introduced by helium-ion irradiation. Samples were prepared by metal-assisted exfoliation on gold and by conventional Scotch tape exfoliation on SiO_2. Clean suspended monolayers were obtained using a hole-patterned substrate combined with the metal-assisted approach, enabling direct comparison of suspended and gold-supported regions.

Electrical characterization by Kelvin probe force microscopy and conductive AFM showed a decrease in work function with increasing ion dose, indicating n-type doping. At the same time, conductivity of MoS_2 on gold decreased with defect density, suggesting Schottky barrier formation at the interface.

Optical measurements using Raman, photoluminescence, and tip-enhanced spectroscopy revealed defect-related Raman modes, shifts of the E_2g and A_2g peaks, and a clear substrate dependence. The B/A excitonic emission ratio increased with ion dose, and power-dependent behavior was observed for the defect emission peak.

High-resolution transmission electron microscopy of suspended samples revealed several defect types, which were correlated with the optical and electrical response. These results underscore the importance of understanding defect effects in 2D materials for future defect-engineered applications.

References:

[1] Majumder, Sudipta, et al. "Unveiling the correlation between defects and high mobility in MoS2 monolayers." ACS Applied Materials & Interfaces 17.7 (2025): 10942-10953
[2] Gontijo, Rafael N., et al. "Resonant Raman scattering study of strain and defects in chemical vapor deposition grown MoS2 monolayers." Small 21.28 (2025): 2310685.

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

Daniel Myšák

Mgr. Ing. Eva Krupičková Pluhařová, 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 molecular dynamics simulations, we studied effects of pH, different substrates and crowded environment on glutamate dehydrogenase (GDH) structure and dynamics [1]. Our current research focuses on the ligand access, since under certain conditions product release represents the rate-limiting step [2]. Using **enhanced sampling methods** (steered MD and umbrella sampling), we modeled and quantified substrate release pathways. Several exit routes were identified and grouped into three dominant ones (see Figure 1). Optimized pulling simulations under different solvent conditions revealed how **molecular crowding** influences the **Gibbs free energy profiles** and **substrate release mechanisms** of GDH.

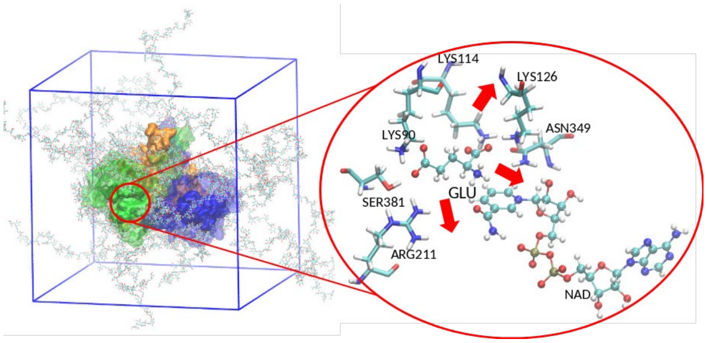


Figure 1: Our model system with zoom into the active site and highlighted three leaving paths.

[1] Rosario G. et al. Can macromolecular crowding help regulate glutamate dehydrogenase activity? ACS Omega. 2025 Oct 30;10. doi:10.1021/acsomega.5c07618

[2] Bera AK. et al. Allosteric regulation of glutamate dehydrogenase deamination activity. Scientific Reports. 2020;10:16785. https://doi.org/10.1038/s41598-020-73743-4

ELECTROCHEMISTRY OF TAMOXIFEN

Bc. Vojtěch Bičák

RNDr. Alan Liška, Ph.D.

This work deals with the electrochemistry of tamoxifen mainly in a non-aqueous environment. Although tamoxifen has already been studied electrochemically and several papers have been published on its electrochemistry, none of them provide specific evidence of its electrochemical products and the mechanisms of their formation. Our goal was to conduct a thorough electrochemical study of tamoxifen primarily in a non-aqueous environment, revealing the products of its electrochemical oxidation and reduction and the mechanism of their formation. For the electrochemical characterization of tamoxifen, we used DC polarography, cyclic voltammetry, and voltammetry on a rotating disk electrode. The products of electrochemical oxidation and reduction were prepared by preparative electrolysis of tamoxifen. The products were analyzed using NMR, EPR and UV-VIS spectroelectrochemistry. The results obtained were compared with those reported in the literature.

References:

FijaŁek, Z.; Chodkowski, J.; Warowna, M. Polarographic studies of drugs of triphenylethene derivatives: Part I. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, **1987**, *226* (1-2), 129–136.

Garrido, J.; Quezada, E.; Fajín, J.; Cordeiro, M.; Garrido, E.; Borges, F. Electrochemical Oxidation of Tamoxifen Revisited. International Journal of Electrochemical Science **2013**, *8* (4), 5710–5723.

Wu, K.; Wyck, S. J. V.; Geiger, W. E. Nonaqueous electrochemical oxidation of tamoxifen. J. Electroanal. Chem. 2016, 783, 140–145.

Jain, R.; Radhapyari, K.; Vikas Voltammetric quantification of tamoxifen. Drug Test Anal. **2011**, *3* (10), 743-747

Falahieh, Z. D; Jalali, M; Alimoradi, M. Cyclic voltammetry behavior of tamoxifen in different electrolytes, electrochemical characterization, and its measurement by differential pulse anodic voltammetry. Turkish Journal of Chemistry, **2017**, *41* (6), 826-844.

ATOMICALLY PRECISE CuPd PENTAMER CLUSTERS FOR CATALYTIC DEHYDROGENATION OF CYCLOHEXENE

Petr Vítek

RNDr. Štefan Vajda, CSc., Dr.habil

Subnanometer clusters are a unique class of material whose properties can drastically differ from bulk. Due to their size, quantum effects become predominant, and minor changes in composition [1] or size [2] can lead to a significant change in properties. Additionally, cluster-support interaction can further affect the behavior of clusters, not only in terms of mobility, but by altering the electronic structure. This provides us with an additional parameter to fine-tune the catalytic properties [3].

In the present study, atomically precise $Cu_{5-n}Pd_n$ ($0 \leq n \leq 5$) clusters deposited on ultra-thin zirconia (ZrO_2) support prepared by atomic layer deposition (ALD), were tested during oxidative dehydrogenation (ODH) of cyclohexene. The monometallic Cu_5 was inactive, while Pd-containing clusters showed catalytic activity, with non-monotonic dependence on Pd content. The selectivity was 100% toward benzene formation with no evidence of formation of undesired CO_2. Surprisingly, under ODH conditions, reaction produced not only H_2O, but also H_2. It was observed that oxygen is crucial for the reaction to proceed, but by adjusting its concentration in the gas feed, the reaction pathway can be controlled and shifted toward H_2 production. This can be used for hydrogen storage where cyclohexene/benzene system can be used as an energy-efficient liquid organic hydrogen carrier (LOHC).

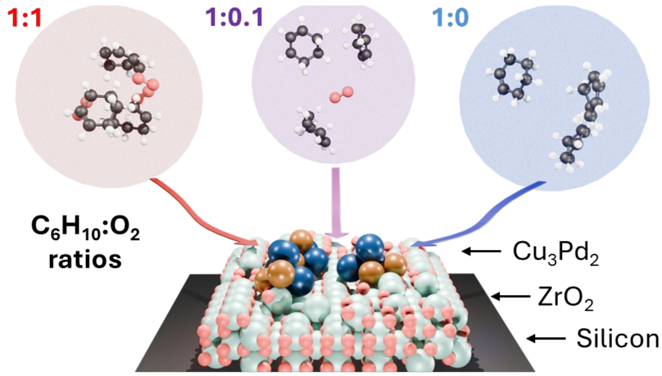


Figure 1: Schematic representation of size-selected Cu_2Pd_3 clusters exposed to various oxygen concentrations during oxidative dehydrogenation of cyclohexene

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 $Cu_{4-n}Pd_n$ ($0 \leq n \leq 4$) tetramer clusters: the effect of cluster composition and support on performance”. *Faraday Discuss.* 242 **2023**

„ZELENĚJŠÍ“ ROZPOUŠTĚDLA PRO PULZNÍ VOLTAMETRICKOU ANALÝZU PESTICIDU FOLPETU NA UHLÍKOVÝCH PRACOVNÍCH ELEKTRODÁCH

Michal Ševčík+++
Gymnázium Karviná

*Ing. Lenka Janíková, Ph.D.****

Elektrochemické metody se pro vysokou citlivost a nízké pořizovací náklady používají ke stanovení širokého spektra látek. Rozšířenou elektrochemickou metodou je voltametrie vycházející z původní Heyrovského polarografie. Voltametrie ve většině případů pro analýzu využívá elektrolyty založené na vodných prostředích tlumivých roztoků či zředěných roztoků anorganických kyselin a solí.

Folpet je derivát kyseliny ftalové, který patří mezi širokospektrální fungicidy s kontaktním mechanismem účinku. Jedná se o látku, která ve vodě podléhá rychlé hydrolýze. Při prvotním studiu elektrochemického chování folpetu prostřednictvím diferenční pulzní voltametrie bylo zjištěno, že je nutné využití nevodných prostředí. Jako analyticky nejvhodnější se ukázal chloristan lithný rozpuštěný v dimethylformamidu, přičemž se jedná o toxikologicky významné látky.

Ve 21. století naléhá na lidskou činnost v oblasti chemického průmyslu i výzkumu potřeba udržitelnosti, ochrany životního prostředí a živých organismů. Pro analytickou chemii lze tuto potřebu subsumovat pod zelenou analytickou chemii, jejímž cílem je vývoj udržitelnějších analytických metod prostřednictvím miniaturizace a omezení předúpravy vzorků, snížení objemu vznikajících odpadů a vystříhání se použití toxikologicky významných látek.

V rámci této práce, byla provedena přehledová studie zaměřená na voltametrii v prostředí nevodných základních elektrolytů, do které bylo zahrnuto 46 původních prací. Na základě výsledků přehledové studie byly zvoleny kandidátní iontové složky a „zelenější“ rozpouštědla základního elektrolytu pro voltametrická měření na pracovní elektrodě ze skelného uhlíku a pracovní elektrodě z borem dopovaného diamantu v katodické potenciálové oblasti.

Elektrochemické chování folpetu v navržených základních elektrolytech bylo srovnáno s využitím square wave voltametrie a cyklické voltametrie. Vzhledem k charakteristice poskytovaných signálů a vypočteným statistickým parametrům byly zvoleny čtyři konkrétní „zelenější“ základní elektrolyty pro další výzkum na pracovní elektrodě ze skelného uhlíku.

Posunem ve výzkumu je bližší diagnostika řídicího elektrodového děje, který byl popsán difúzním koeficientem, koeficientem přenosu náboje, heterogenní konstantou přenosu elektronů a počtem přenášených elektronů. V původním základním elektrolytu složeném z chloristanu lithného a dimethylformamidu bylo díky square wave voltametrii dosaženo vyšší selektivity stanovení folpetu.

Design zelené analytické metody narazil na nízkou přesnost a selektivitu stanovení, navržená zelená analytická metoda neposkytovala spolehlivé výsledky stanovení folpetu. Z výsledků výzkumu vyplývá, že snaha o zvýšení udržitelnosti analytických metod může v případě voltametrie v nevodných základních elektrolytech narazit na nespolehlivost metody. Nejudržitelnějším rozpouštědlem ve voltametrické analýze je voda, jiná rozpouštědla by měla představovat krajní možnost vyhrazenou pro analyty, které jsou ve vodě nestabilní.

Další výzkum v oblasti „zelenějších“ rozpouštědel nevodných základních elektrolytů pro voltametrickou analýzu se může ubírat směrem ke směsným vícesložkovým rozpouštědlům nebo atypickým elektrolytům, jako jsou silné anorganické kyseliny v protických i aprotických organických rozpouštědlech, které otevírají definitorickou otázku, co je to nevodné prostředí, když všechny formy anorganických kyselin včetně koncentrovaných obsahují nezanedbatelný podíl vody.

Reference

[1] Vobořil J., Žemlová L., Janíková L., Ševčík M., Matvieiev O. et al., in: Navrátil T., Fojta M., Schwarzová K. (Eds.), *Proc. 44th Mod. Electrochem. Methods*, Best servis (2025) 176
[2] Mansour F. R., Bedair A., *Sustain. Chem. Pharm*. 47 (2025) 102157
[3] Pena-Pereira F., Wojnowski W., Tobiszewski M., *Anal. Chem*. 92 (2020) 10076
[4] Płotka-Wasylka J., Namieśnik J., *Green Analytical Chemistry: Past, Present and Perspectives*, Springer (2019)

Poděkování

Grantový projekt Univerzity Pardubice „Výzkum perspektivních metod a postupů v oblastech environmentálního a chemického inženýrství a udržitelného managementu chemických podniků“ (reg. č. SGS_2025_002)

Grantový projekt Univerzity Pardubice „Studium inovativních metod a procesů environmentálního a chemického inženýrství a udržitelného managementu chemických podniků“ (reg. č. SGS_2026_002).

+++ *Práce realizována v rámci středoškolské stáže na Univerzitě Pardubice*
*** *Ústav environmentálního a chemického inženýrství, Univerzita Pardubice*

DIDAKTICKÁ PRAXE V CHEMII A JEJÍ APLIKACE VE ŠKOLNÍ VÝUCE

Tadeáš Vícha

Ing. Květoslava Stejskalová, CSc.

Tato práce vycházející ze stáže na Ústavu fyzikální chemie J. Heyrovského v projektu Otevřená věda AV ČR se zaměřuje na praxi v didaktice chemie. V rámci této stáže byla také realizována laboratorní výuka na pětidenní letní chemické škole „Uhlík v Boru 2025“, zaměřená na propojení teoretických poznatků s experimentální činností.

Získané zkušenosti byly následně aplikovány při výuce na základních školách, kde byly realizovány tematické bloky zaměřené například na Tyndallův jev, typy chemických reakcí nebo pH, vždy s důrazem na aktivní zapojení žáků.

Na základě těchto zkušeností je diskutováno využití experimentální výuky a její přínos pro porozumění chemickým jevům a rozvoj zájmu žáků o přírodní vědy.

BORON-DOPED DIAMOND ELECTRODES IN HIGHLY CONCENTRATED CHAOTROPIC ELECTROLYTES: A (SPECTRO)-ELECTROCHEMICAL STUDY

Ing. Petr Čech

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

Boron-doped diamond (BDD) is a promising electrode material owing to its exceptional physical, chemical, and electrochemical stability, enabling applications in electrochemistry and electrosynthesis. BDD is further characterized by a wide electrochemical potential window and low background current, making it well-suited for studies in demanding electrolyte environments [1], [2].

In this work, a comprehensive electrochemical and in situ Raman spectroelectrochemical (SEC) study of BDD electrodes in highly concentrated aqueous electrolytes is presented. Sodium perchlorate ($NaClO_4$) and sodium thiocyanate (NaSCN) were selected as the two most chaotropic salts of the Hofmeister series, representing tetrahedral and linear anion geometries respectively. The high ionic strength introduces strongly corrosive conditions toward conventional electrode materials, while simultaneously suppressing oxygen and hydrogen evolution at the electrode surface. Chaotropic ions disrupt the hydrogen bond network and thereby also extend the electrochemical stability window of the solvent. Both salts were studied at high concentration and compared against dilute $NaClO_4$ to isolate the effect of concentration [3].

Preliminary results indicate that $NaClO_4$ at high concentration yields a potential stability window exceeding 3 V, consistent with effective suppression of water decomposition. In contrast, NaSCN exhibits an asymmetric window: while the cathodic limit is extended, early oxidation of the SCN^- anion restricts the anodic window, demonstrating that anion redox stability competes with and overrides the water-stabilization effect. Dilute $NaClO_4$ shows a moderately narrower window on both sides, confirming the role of concentration. In situ Raman SEC measurements were performed to characterize the electrode-electrolyte interface across the potential range, with spectral and electrochemical analysis ongoing.

References:
[1] Macpherson, J.V., *Phys. Chem. Chem. Phys.* **2015**, 17, 2935-2949
[2] Živcová, Z.V., *Electrochimica Acta*, **2013**, 87, 518-525
[3] Gomez Vazquez, D. *J. Am. Chem. Soc.* **2025**, 147, 35953-35961

SLOW DANCING IN A CROWDED ROOM: EFFECT OF MACROMOLECULAR CROWDING ON DYNAMICS OF ADK

MSc. Samanta Madhav

Mgr. Štěpán Timr, Ph.D.

Biological cells have complex interiors filled with proteins, membranes, sugars, and other biomolecules. Traditional in vitro assays, which study enzymes in isolation, overlook how these crowded environments modulate enzyme function. Here, we examine adenylate kinase (ADK), an enzyme whose activity depends on large domain motions and conformational changes. Previous experiments reported an increase in ADK activity in the presence of macromolecular crowders and attributed this enhancement to excluded volume effects. To obtain a comprehensive all-atom description of crowder interactions with ADK and to determine whether effects beyond excluded volume impact ADK function, we performed extensive molecular dynamics simulations of ADK in the presence of synthetic crowders. From the resulting trajectories, we constructed Markov state models to characterize the conformational landscape and transition kinetics of the protein under crowded conditions. Our findings show that crowders interact intimately with the enzyme and that these interactions affect its conformational equilibrium. Moreover, crowder interactions can alter enzyme activity by modulating reactant positions in the active site and influencing the conformational fluctuations of key active site residues. By characterizing the impact of synthetic crowders on ADK conformation and dynamics, this work advances our understanding of enzyme function in crowded environments that mimic the cellular interior.

References:

(1) Rastogi, H.; Chowdhury, P. K. Understanding Enzyme Behavior in a Crowded Scenario through Modulation in Activity, Conformation and Dynamics. Biochim Biophys Acta Proteins Proteom 2021, 1869 (11). https://doi.org/10.1016/j.bbapap.2021.140699.

(2) Lu, J.; Scheerer, D.; Haran, G.; Li, W.; Wang, W. Role of Repeated Conformational Transitions in Substrate Binding of Adenylate Kinase. Journal of Physical Chemistry B 2022, 126 (41), 8188–8201. https://doi.org/10.1021/acs.jpcb.2c05497.

(3) Zheng, Y.; Cui, Q. Multiple Pathways and Time Scales for Conformational Transitions in apo-Adenylate Kinase. Journal of Chemical Theory and Computation 2018 14 (3), 1716-1726. https://doi.org/10.1021/acs.jctc.7b01064.

UNRAVELING THE OXIDATION MECHANISM OF THE TOPICAL DRUG TAPINAROF WITH A MULTIDISCIPLINARY APPROACH

Mgr. Lucie Dostálková

doc. RNDr. Romana Sokolová, Ph.D.

Tapinarof (Fig. 1) is a topical non-steroidal therapeutic compound used in VTAMA® cream. It is employed for the treatment of various conditions such as plaque psoriasis (a chronic, multisystem inflammatory skin disease) and atopic dermatitis [1,2]. Studying its redox characteristics in model neutral aqueous media can provide valuable insights into its metabolic pathways in the skin as a topical drug. In this work [3], we focused on studying its oxidation mechanism using electrochemical, spectroelectrochemical (SEC), and LC-MS methods.

The findings from cyclic voltammetry measurements in a phosphate buffer suggest that in the oxidation process, the same number of protons and electrons is involved, and the reaction is followed by an ECE mechanism. The participation of water and subsequent formation of a keto group was confirmed by infrared SEC. After oxidative electrolysis at constant potential, the mixture of oxidation products was analysed by liquid chromatography coupled with mass spectrometry, which confirmed the structures of the proposed products. Based on all the employed methods, supported by theoretical calculations, we proposed the oxidation mechanism of tapinarof in aqueous media.

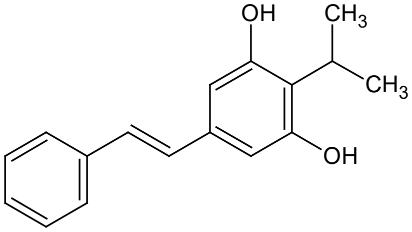


Fig. 1. Chemical structure of tapinarof

References:

[1] Maglangit, F.; Yu, Y.; Deng, H. *Nat Prod Rep.* **2021**, 38, 782-821.

[2] Keam, S.J. *Drugs.* **2022** 82, 1221–1228.

[3] Dostálková, L.; Papoušková, B.; Zatloukalová, M.; Kabeláč, M.; Vacek, J.; Sokolová, R. *Chem Commun*. **2026**, submitted.

H-ATOM ABSTRACTION SELECTIVITY IN PROZAC DERIVATIVES: INSIGHTS FROM THE OFF-DIAGONAL THERMODYNAMICS CONTROLLED THROUGH THE MODULAR DESIGN OF OXIDANTS

MUSKAN SHARMA MSC.

RNDr. Martin Srnec, Ph.D., DSc.

Hydrogen Atom Transfer (HAT) is a key mechanistic step in many enzymatic and chemical C–H activation processes, directly impacting oxidative metabolism and drug stability. Prozac (Fluoxetine), a widely used antidepressant, undergoes metabolic transformations where selective activation of C–H bonds play a crucial role. In Prozac, two major sites for hydrogen abstraction are available: the tertiary C–Ha and the primary C–Hb positions. Understanding the reaction selectivity and its control is essential for predicting metabolic outcomes.

In this study, we employ the concept of off-diagonal thermodynamics to dissect the contributions of asynchronicity and frustration to the reaction barrier of the reaction between Prozac and quinuclidine radical, in addition to a well-known linear free energy relationship. Our results consistently show that Hb abstraction exhibits a more favorable off-diagonal contribution to the barrier, which results in a lower activation barrier, while Ha abstraction is associated with greater off-diagonal contribution leading to a higher barrier. These findings are in accord with the mechanistic trends established by Srnec et al., which demonstrates that modulating off-diagonal terms governs HAT reactivity.

Further, derivation of the quinuclidine by attaching a redox-active module modulates both off-diagonal thermodynamic parameters as well as the reaction energy, through all of which one may control barrier heights.

With that we provide a comprehensive understanding of how structural modifications and its chemo-selectivity influence HAT reactivity in Prozac derivatives, with potential implications for drug metabolism prediction and design of selective functionalization pathways.

References:

[1] M. Maldonado-Domínguez, M. Srnec, *Inorg. Chem.* ***2022****, 61, 18811–18822.*

INVESTIGATING INTERLAYER DECOUPLING IN EXFOLIATED TMDCS ON METAL SUBSTRATES

Mgr. Michaela Hanušová

Ing. Matěj Velický Ph.D.

Monolayers of transition metal dichalcogenides (TMDCs) such as MoS_2 have captured significant attention due to their unique electronic and optical properties unattainable in their bulk form [1,2].

Among various preparation methods, the gold-assisted exfoliation has emerged as an effective technique for selectively obtaining large-area monolayers. However, its underlying mechanism is still a subject of debate [3]. While other metals can also facilitate exfoliation, their practical use is limited by oxidation of their surface [4].

Herein, we present a systematic study of MoS_2 exfoliated onto different metal substrates under controlled atmospheric conditions. Through a combination of photoelectron spectroscopy techniques and Raman spectroscopy, we probe the interfacial interactions and their impact on the MoS_2 monolayer properties and decoupling in multilayers

Our findings demonstrate that the choice of metal substrate plays a critical role in modifying interfacial behaviour, leading to distinct electronic structures and Raman signatures. Furthermore, the observed evolution from substrate-coupled to quasi-freestanding behaviour with increasing thickness provides new insight into the mechanisms governing metal-assisted exfoliation and interlayer decoupling. These findings contribute to a deeper understanding of substrate–material interactions in two-dimensional systems.

References:

1. Mak, K. F. et al. *Phys Rev Lett 105*, **2010**, 136805
2. Splendiani, A. et al. *Nano Lett 10*, **2010**, 1271-1275
3. Ziewer, J. et al. *Adv Mater*, **2024**, 2419184
4. Hanušová, M. et al. *Nano Lett 25*, **2025**, 12995-13002

SPECTROSCOPIC READOUT OF WATER PERMITTIVITY WITHIN PROTEINS LUMEN

Davide Burattini, MSc.

RNDr. Jan Sýkora, Ph.D,

Water molecules forming the hydration shell of proteins show different physicochemical properties than bulk water [1]. This interfacial water behavior plays a key role in biological processes such as protein translocation and insertion in membranes [2]. For instance, water permittivity alters the pKa of amino acids, providing an unknown contribution to the aforementioned tasks. Measuring water permittivity within protein lumen is not straightforward due to the close conformation of these macromolecules, thus becoming difficult to correlate this parameter with protein functions. To overcome this problem, the aim of the project is to establish a permittivity calibration scale and use it to measure the water permittivity within the bacterial translocon secYEG. We will attach BADAN, a solvatochromic fluorescent dye, to a model peptide and test it in a broad range of solvents with known permittivity, then use steady-state and time-resolved fluorescence spectroscopy to measure the dye response to this parameter and establish a calibration scale. We will express secYEG, reconstruct it into a model lipid system and measure the permittivity within the translocon using a BADAN labelled construct able to open, enter secYEG and form a stalled translocation intermediate [3]. Repeating the experiment for different mutant of secYEG and with different lipid compositions, we will investigate if alterations in structure and function of the complex affect the permittivity. Finally, we will asses the proper localization of the construct within secYEG using FRET and FCCS, to investigate if different positions inside the translocon show different permittivity. The expected results are to establish a universal spectroscopic tool to measure permittivity and resolve this parameter within secYEG to correlate it with protein functions.

References:

[1] Laage, D et al. 2017. Chem. Rev.
[2] Capponi et al 2015. PNAS.
[3] Kedrov et al. 2011. The EMBO Journal.

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 form and disassemble in response to external conditions. Such assemblies have been identified across various pathways, including glycolysis, oxidative phosphorylation, and purine synthesis. However, the molecular mechanisms driving their formation and functional relevance remain poorly characterized.

Enzyme clustering is often hypothesized to enhance pathway efficiency by increasing local enzyme and substrate concentrations. However, in crowded cellular environments, clustering also introduces additional effects arising from macromolecular crowding and transient enzyme-substrate interactions, which may either enhance or suppress pathway efficiency. To understand these effects in detail, we develop a coarse-grained computational model capturing the main phenomena involved**.** We focus on active-site occupancy as a key observable, motivated by the fact that many enzymes operate in reaction-limited regimes. By varying enzyme-enzyme interactions, enzyme-substrate non-specific interactions, and crowder-substrate interactions (purely repulsive versus attractive), we show that different clusters can have strongly opposing effects on active site occupancy. We further find that active site occupancy depends on the properties of nonspecific enzyme-substrate interactions, such as their range and anisotropy, and that crowders can enhance or decrease the active site occupancy depending on the type of interaction present in the assembly.

Our simulations suggest that enzyme clustering does not always lead to an increase in active site occupancy; the effect is highly sensitive to various interactions present within the system. These findings will inform the development of more realistic models of metabolic pathways by incorporating the effects of dynamic enzyme assemblies.

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.

SIMULATION AND EXPERIMENTAL STUDIES OF TRANSPORT OF CELL-PENETRATING PEPTIDES ACROSS BIOLOGICAL MEMBRANES

MSc. Krishna Pradhan

Doc. Radek Šachl RNDr, Ph.D

Doc. Mario Vazdar, Ph.D.

.

The efficient intracellular delivery of therapeutic agents remains a major challenge in biophysics due to the selective permeability of biological membranes. Cell-penetrating peptides (CPPs) offer a promising solution via passive translocation, yet the underlying molecular mechanisms and the influence of membrane asymmetry are not yet fully understood.

This research investigates the "arginine magic" phenomenon, focusing on how guanidinium like-charge ion pairing facilitates peptide-membrane interactions. We employ a synergistic approach using all-atom molecular dynamics simulations and experimental fluorescence spectroscopy.

The study focuses on the formation of transient pores and the "train-like" translocation mechanism induced by peptide aggregation and membrane destabilization. Current experimental efforts involve the preparation of asymmetric vesicles to better mimic biological environments.

In my lecture, I will discuss the project's theoretical framework and the preliminary stages of characterizing peptide adsorption and binding. These preliminary steps are essential for quantifying the free energy barriers and molecular determinants of CPP transport.

References:

- Vazdar, M., et al. *Acc. Chem. Res.* **2018**, 51, 1455-1464.
- Allolio, C., et al. *Proc. Natl. Acad. Sci.* **2018**, 115, 11923-11928.
- Bartoš, L.; Vácha, R. *Biophys. J.* **2024**, 123, 693-702.
- Doktorova, M., et al. *Nat. Protoc.* **2018**, 13, 2086–2101.

PORTABLE VOLTAMMETRIC PLATFORM FOR THE SENSITIVE DETECTION OF SALINOMYCIN USING SILVER AMALGAM SCREEN-PRINTED ELECTRODES

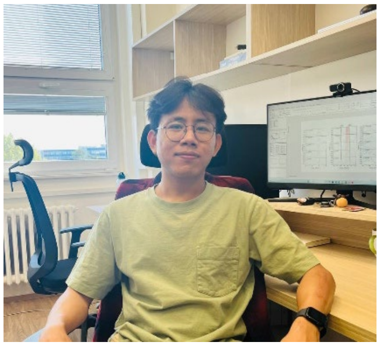
MSc. Sofiia Ivakh

Bohdan Josypčuk, Ph.D.

Electrochemical analysis of compounds undergoing reduction at highly negative potentials is frequently hindered by the limited cathodic potential window of conventional electrode materials, primarily due to the onset of hydrogen evolution. To address this constraint, the present work focuses on the development and evaluation of silver amalgam screen-printed electrodes (AgA-SPEs) as an advanced sensing platform for the determination of salinomycin, a veterinary antibiotic with increasing environmental and biomedical relevance.

AgA-SPEs were fabricated through controlled chronocoulometric deposition of mercury onto commercially available silver screen-printed substrates. Among the tested compositions, a silver-to-mercury ratio of 1:1 exhibited the most favorable performance, combining an enhanced hydrogen overpotential with good signal stability and reproducibility. This optimized electrode was subsequently employed for the development of a differential pulse voltammetric method targeting salinomycin. The proposed sensing approach provides a sensitive, cost-effective, and disposable tool suitable for on-site monitoring. It holds promise for applications in pharmaceutical analysis, environmental monitoring, and emerging biomedical research, particularly in light of the growing interest in salinomycin as a potential anticancer compound.

This work was supported by the Czech Science Foundation (Project 25-16569S), the Grant Agency of Charles University (GAUK project 176424) and the Specific University Research (SVV) program.



SEQUENTIAL GOLD-ASSISTED EXFOLIATION FOR ULTRACLEAN TMDC HETEROSTRUCTURES WITH STRONG INTERLAYER COUPLING

MSc. Chan Thar Soe

Dr. Matěj Velický, Supervisor
Dr. Otakar Frank, Co-supervisor

Gold-assisted exfoliation enables the production of large-area, high-quality two-dimensional transition metal dichalcogenide (TMDC) monolayers(1). TMDC heterostructures are particularly interesting because they host interlayer excitons whose properties depend strongly on interlayer coupling and the interface quality. Conventional polymer-based transfer methods, such as PDMS, often introduce residues, bubbles, and wrinkles that degrade the interface and affect interlayer coupling in the heterostructures(2). In this work, we prepare MoS_2 and WSe_2 heterostructures by sequential exfoliation directly onto a gold substrate, producing contamination-free interfaces and atomically flat heterostructures. Atomic force microscopy (AFM) is first used to examine the interface, confirming wrinkle- and bubble-free surfaces with high uniformity. Fast Fourier transform (FFT) analysis of the AFM topographic images reveals moiré patterns, indicating low-angle stacking between the TMDC layers. In the high-frequency Raman region, we observe the activation and intensity enhancement of the geometry-forbidden E_{1g} mode and the symmetry-forbidden A_{2u} mode after the formation of the heterostructure. In addition, the emergence of the interlayer breathing mode in the low-frequency Raman spectra provides strong evidence of interlayer coupling between the stacked layers. Overall, this work demonstrates a contamination-free approach for fabricating high-quality TMDC heterostructures and provides a useful platform for probing intrinsic interlayer interactions.

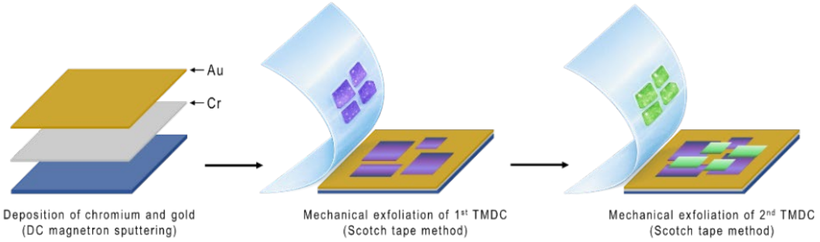


Figure 1: Schematic of sequential gold-assisted exfoliation of TMDC heterostructures.

References:

1. Velický M, Donnelly GE, Hendren WR, McFarland S, Scullion D, DeBenedetti WJI, et al. Mechanism of Gold-Assisted Exfoliation of Centimeter-Sized Transition-Metal Dichalcogenide Monolayers. ACS Nano. 2018;12(10):10463-72.
2. Khestanova E, Ivanova T, Gillen R, D'Elia A, Gallego Lacey ON, Wysocki L, et al. Robustness of Momentum-Indirect Interlayer Excitons in MoS2/WSe2 Heterostructure against Charge Carrier Doping. ACS Photonics. 2023;10(4):1159-68.

MECHANISTIC INSIGHTS INTO ALLOSTERIC REGULATION OF HUMAN PHOSPHOFRUCTOKINASE-1

MSc. Truong-An Nguyen

Mgr. Timr Štěpán Ph.D.

As a highly allosterically regulated enzyme that catalyzes the rate-limiting step of glycolysis, phosphofructokinase-1 (PFK1) serves as a key regulatory point in the pathway. However, a full mechanistic understanding of its regulation is still lacking. This work investigates the molecular basis for the differential allosteric regulation of PFK1, where the enzyme is inhibited by high-energy signal ATP yet activated by low-energy signals AMP and ADP. While recent structural studies identified an activating site for AMP and ADP, the mechanism excluding ATP from this activating site remains unknown. Using replica exchange umbrella sampling (REUS) simulations, we determine how ligand phosphate groups govern the specificity of binding to the activating site. Our results indicate that ATP's longer phosphate moiety samples more alternative conformations, becoming stabilized in non-activating poses that displace it from the binding site, thereby suggesting the selective binding mechanism of the activating site.

References:

Lynch, E.M., Hansen, H., Salay, L. et al.. Nat Commun 15, 7323 (2024).

VOLTAMMETRIC DETERMINATION OF TRAZODONE IN URINE USING BORON-DOPED DIAMOND ELECTRODE AFTER HOLLOW-FIBER MICROEXTRACTION

Msc. Oleksandra Labzova
Supervisors:
Assoc. Prof. Ing. Renáta Šelešovská, Ph.D.
Prof. Ing. Tomáš Navrátil, Ph.D.

This study presents a highly sensitive voltammetric method for the determination of Trazodone (TZ) using disposable screen-printed boron-doped diamond electrodes (SP-BDDEs), including the elucidation of the electrooxidation mechanism using HPLC/MS, supported by DFT calculations. To overcome the complications associated with the analysis of complex biological matrices, such as human urine, the electrochemical detection was integrated with hollow-fiber liquid-phase microextraction (HF-LPME) with isoamyl benzoate-supported liquid membrane. Systematic parameter optimization yielded a low limit of detection (*LOD*) of 12 nmol L^{-1}, and a limit of quantification (*LOQ*) of 36 nmol L^{-1}, with a linear range of 0.02 to 1.0 µmol L^{-1}. Validated through the analysis of authentic urine samples at therapeutic concentration levels (20 and 100 nmol L^{-1}), this approach offers a cost-effective, portable, and "green" analytical alternative to traditional chromatographic techniques. Its simplicity and high sensitivity make it particularly suitable for routine clinical monitoring, pharmacokinetic studies, and decentralized near point-of-care applications.

References:
Wang, J.; Wang, J.; Zhang, C.; Li, G. Front. Pharmacol. **2025**, 16, 1531496.
Shi, X.; Wu, Y.; Hang, T.; Xu, X.; Ding, L.; Tian, Y.; Wen, A. J. Chromatogr. B **2008**, 871, 90–94.
Stahl, S. M. CNS Spectr. **2009**, 14, 536–546.
Brogden, R. N.; Heel, R. C.; Speight, T. M.; Avery, G. S. Drugs **1981**, 21, 401–429.
Bossini, L.; Casolaro, I.; Koukouna, D.; Cecchini, F.; Fagiolini, A. Expert Opin. Pharmacother. **2012**, 13, 1707–1717.
Labzova, O.; Hrdlička, V.; Šelešovská, R.; Navrátil, T. Talanta **2025**, 293, 128038.
Payán, M. R.; López, M. Á. B.; Fernández-Torres, R.; Mochón, M. C.; Ariza, J. L. G. Talanta **2010**, 82, 854–858.
Saraji, M.; Farajmand, B.; Ensafi, A. A.; Allafchian, A. R.; Zare, Z. M. Talanta **2010**, 82, 1588–1593.
Kauffmann, J.-M.; Vire, J.-C.; Patriarche, G. J.; Nunez-Vergara, L. J.; Squella, J. A. Electrochim. Acta 1987, 32, 1159–1162.

WHEN PHONONS TALK TO EACH OTHER

Satyam Sahu, Ph.D.

Phonon–phonon interactions govern energy redistribution and dissipation in solids, yet they are often described within weak, perturbative frameworks that overlook their behavior under strong excitation. In this talk, I explore how vibrational modes in two-dimensional materials evolve when driven into nonlinear regimes, where the lattice response departs from simple harmonic behavior and different phonon populations begin to interact, compete, and exchange energy. Using power-dependent Raman spectroscopy, we access steady-state nonequilibrium conditions in systems such as CrSBr, CrSBrCl and MoS_2/CrSBr heterostructures, revealing signatures of mode-selective enhancement and suppression that reflect underlying nonlinear coupling pathways. These effects highlight how anisotropy, electronic resonances, and interlayer interactions can reshape phonon dynamics far from equilibrium, providing new opportunities to control energy flow and lattice excitations in low-dimensional quantum materials.

Student Seminar 2026
Conference centre in Hejnice Monastery
May 13-14, 2026