



SEMINÁŘ STUDENTŮ ÚFCH JH 2023



Ústav Heyrovského v Praze
23.- 24.5. 2023

Seminář studentů 2023

Sborník příspěvků

**ze studentské konference konané
23. - 24. května 2023
v ÚFCH J. Heyrovského v Praze**

Student Seminar 2023

Collection of abstracts

**of all lectures given at the student conference
held on 23-24 May 2023
in Heyrovský Institute in Prague**

Seminář studentů 2023
Sborník příspěvků ze studentské konference
konané 23.-24. května 2023
v ÚFCH J. Heyrovského v Praze

Kolektiv autorů

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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 (e-Book)

Místo a rok vydání: Praha, 2023

Publikace neprošla jazykovou úpravou

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ISBN 978-80-87351-64-2 (e-Book)

SEMINÁŘ STUDENTŮ 2023

PROGRAM 1. dne konference – úterý 23. května 2023

STUDENT SEMINAR 2023

PROGRAM - Tuesday May 23, 2023

	<i>Předseda- jící/ chairman</i>	<i>Přednášející/ lecturer</i>	<i>Název/ presentation title</i>
9:00-9:10	Zahájení konference „Seminář studentů 2023“ <i>Opening of Annual conference "Seminar of Students 2023"</i>		
9:10-9:25	Jakub Martinka	Václav Ráliš (<i>PřF UK Praha, školitel J. Pinkas</i>)	POLYETHYLENE TERMINATED WITH SILICON AND ITS UTILISATION
9:25-9:40		Karolina Fárníková (<i>VŠCHT Praha, školitelka E. Krupičková Pluhařová</i>)	MOLECULAR SIMULATIONS OF LIPASE: FROM THE LID OPENING TO THE ACTIVE SITE
9:40-9:55		Marek Beneš (<i>VŠCHT Praha, školitelka R. Sokolová</i>)	STUDIUM MECHANISMU OXIDACE PSYCHOAKTIVNÍ LÁTKY 25E-NBOH
9:55-10:10		Mariia Lemishka (<i>školitel J. Dědeček</i>)	MULTISPECTROSCOPIC STUDY OF MOLECULAR OXYGEN DISSOCIATION OVER ZEOLITES
10:10-10:45	PŘESTÁVKA NA KÁVU A ZÁKUSEK (<i>Coffee break in lobby</i>)		
10:45-11:00	Václav Ráliš	Seyed A. M. Bukhari (<i>školitel O. Frank</i>)	SHEDDING LIGHT ON THE INFLUENCE OF STRUCTURAL DEFECTS ON THE BEHAVIOUR OF TWO-DIMENSIONAL MATERIALS
11:00-11:15		Eliška Jiroušková (<i>PřF UK Praha, školitelka R. Sokolová</i>)	ELECTROCHEMISTRY OF NEW PSYCHOACTIVE SUBSTANCES 3 FLUOROPHENMETRAZINE, 4 METHYLPENTEDORNE AND FLUOROMETHOXY- ACETYL FENTANYL
11:15-11:30		Jakub Martinka (<i>školitel J. Pittner</i>)	EXCITED STATE MOLECULAR DYNAMICS ASSISTED BY MACHINE LEARNING
11:30-11:45		Johana Fialová (<i>VŠCHT Praha, školitel J. Fedor, P. Nag</i>)	STUDY OF LOW ENERGY ELECTRON-INDUCED DISSOCIATION OF CF ₃ I USING VELOCITY MAP IMAGING
11:45-13:00	PŘESTÁVKA (OBĚD NENÍ NA KONFERENCI ZAJIŠTĚN) (<i>time for a lunch</i>)		

13:00-13:15	Isabel Králová	David Šťastný (školitel R. Šachl)	TRACKING MEMBRANE PERMEABILIZATION ON SINGLE LIPID VESICLES - METHOD DEVELOPMENT
13:15-13:30		Michaela Hanušová (školitel M. Velický)	FUNDAMENTAL PHYSICS AND CHEMISTRY OF THE INTERFACE BETWEEN MONOLAYER TRANSITION METAL DICHALCOGENIDES AND METALS
13.30-13:45		Jozef Ďurana (školitel M. Fárník)	PHOTODISSOCIATION OF TRIFLUOROACETYL CHLORIDE PROBED BY VELOCITY MAP IMAGING (VMI) TECHNIQUE
13:45-14:00		Zuzana Johanovská (školitel M. Hof)	MICROMANIPULATION AS A NEW INSTRUMENT FOR RESEARCH OF BIOMEMBRANE STRUCTURE AND ITS MECHANICAL PROPERTIES
14:00-14:30	PŘESTÁVKA NA KÁVU A ZÁKUSEK (<i>Coffee break in lobby</i>)		
14:30-14:45	Jozef Ďurana	Maroua Gnioua Omezzine (školitel P. Španěl)	EXPERIMENTAL AND THEORETICAL STUDIES OF GAS PHASE ION MOBILITY AND ENERGETICS: PROTONATED SATURATED AND UNSATURATED ALDEHYDES IN HELIUM
14:45-15:00		Barbora Kocábková (školitel M. Fárník)	MOLECULAR AND CLUSTER MASS SPECTRA OF TRIFLUOROACETYL CHLORIDE
15:00-15:15		Isabel Králová (školitel J. Sýkora)	REGULATION OF THE MEMBRANE CHANNEL ACTION STUDIED BY FLUORESCENCE TECHNIQUES
15:15-15:30		Hlib Lyshchuk (školitel J. Fedor)	DISSOCIATIVE IONIZATION OF MeCpPtMe ₃ : FORMATION OF METHANE AND ETHANE AT SINGLE-COLLISION CONDITIONS WITH ELECTRONS
15:30-15:45		Václav Adamec (PřF UK Praha, školitel: M. Lamač)	TRANSITION-METAL-CATALYSED HYDROGENATION REACTIONS USING THE HYDROSILANE-B(C ₆ F ₅) ₃ SYSTEM AS AN ACTIVATOR
15:45-17:00	PODVEČERNÍ OBČERSTVENÍ (<i>Coffee break in lobby</i>) UKONČENÍ PRVNÍHO DNE KONFERENCE (<i>End of the 1st day of conference</i>)		

PROGRAM 2. dne konference - středa 24.5.2023**PROGRAM - Wednesday May 24, 2023**

	<i>Předseda- jící/ chairman</i>	<i>Přednášející/ lecturer</i>	<i>Název/ presentation title</i>
8:55	Zahájení 2. dne konference „Seminář studentů 2023“ <i>Opening of the 2nd day of Annual conference "Seminar of Students 2023"</i>		
9:00-9:15	Mikuláš Matoušek	Soumya Frederick (školitelka V. Petráková)	VISUALIZING PLASMONIC MISLOCALIZATION USING SINGLE-MOLECULE LOCALIZATION MICROSCOPY
9:15-9:30		Martin Melčák (školitel S. Záliš)	TOWARDS SOLVENT SPECIFIC EFFECTS IN INFRARED SPECTRA OF RHENIUM COMPLEX
9:30-9:45		Abhinav (školitel J. Sýkora)	HYDRATION AND DYNAMICS OF FUNCTION- RELEVANT REGION OF HPUREI
9:45-10:00		Karolina Salvadori (školitel J. Ludvík)	VARIOUS ROLES OF -NO ₂ SUBSTITUENT IN ELECTROCHEMICALLY INVESTIGATED SUPRAMOLECULAR SYSTEMS
10:00-10:30	PŘESTÁVKA NA KÁVU A ZÁKUSEK (<i>Coffee break in lobby</i>)		
10:30-10:45	Barbora Chmelová	Mikuláš Matoušek (školitel L. Veis)	THE CHASE FOR AN INVERTED S-T ORDERING FOR MORE EFFICIENT ORGANIC LEDS
10:45-11:00		Petra Kohútová (školitel M. Hof)	THE FUNCTIONAL PORE FORMATION OF PRO- APOPTIC PROTEINS (BID AND BAX) IN GIANT UNILAMELAR VESICLES AS THE MODEL SYSTEM
11:00-11:15		Priyam Bharadwaz (školitel M. Srnec)	ROLE OF THERMODYNAMICS IN -ATOM ABSTRACTION REACTIVITY OF S- ADENOSYLMETHIONINE ENZYMES
11:15-11:30		Satyam Sahu (školitel M. Velický)	LARGE-AREA MECHANICALLY-EXFOLIATED TWO- DIMENSIONAL MATERIALS ON ARBITRARY SUBSTRATES
11:30-11:45		Federica Scollo (školitel M. Hof)	« SPECIFIC OR NOT SPECIFIC, THAT IS THE QUESTION »: AN OVERVIEW ON GAL-1 - GM1 INTERACTION
11:45-13:00	PŘESTÁVKA (OBĚD NENÍ NA KONFERENCI ZAJIŠTĚN) (<i>time for a lunch</i>)		
13:00-13:15	Mark Niklas Hansen	Barbora Chmelová (školitel R. Šachl)	INTERLEAFLET ORGANIZATION OF MEMBRANE NANODOMAINS: WHAT CAN(NOT) BE RESOLVED BY FRET?
13:15-13:30		Tomáš Imrich (školitelka-konzultantka H. Krýsová)	SYNTHESIS OF DOPED PSEUDOBROOKITE (Fe ₂ TiO ₅) FILMS: PROPERTIES AND APPLICATIONS IN PHOTO(ELECTRO)CATALYSIS

13:30-13:45		Khalilullah Umar (školitelka V.Petráková)	HIGH RESOLUTION NEAR INFRARED IMAGING WITH DNA-PAINT
13:45-14:00		Barbora Sedmidubská (školitel J. Kočíšek)	FULLERENOLS AND THEIR INTERACTIONS WITH SECONDARY LOW-ENERGY ELECTRONS
14:00-14:30	PŘESTÁVKA NA KÁVU A ZÁKUSEK (Coffee break in lobby)		
14:30-14:45	David Davidovič	Marta K. Choińska-Młynarczyk (školitel T. Navrátil)	ELECTROCHEMISTRY FOR MEDICAL AND FORENSIC SCIENCE. DETERMINATION OF ILLICIT DRUGS AND BIOLOGICALLY ACTIVE COMPOUNDS USEFUL FOR THE TREATMENT OF PSYCHIATRIC DISEASES
14:45-15:00		Martin Jindra (školitel O. Frank)	REDUCTION AND LARGE-AREA MICROSCOPIC MONITORING OF CONTAMINATION LEVELS OF TRANSFERRED CVD GRAPHENE
15:00-15:15		Mark Niklas Hansen (školitelka V. Petráková)	CONTROLLED ASSEMBLY OF NOBLE METAL NANOPARTICLES AND FLUOROPHORES FOR SUB-DIFFRACTION MANIPULATION OF LIGHT TO STUDY PLASMONIC LIGHT MODULATIONS
15:15-15:30	PŘESTÁVKA (break)		
15:30-15:45	Priyam Bharadwaz	David Davidovič (školitel R. Šachl)	NATURE OF THE INTERACTION BETWEEN ssDNA-LOADED CATIONIC LIPID NANOPARTICLES (cLNPs) AND GIANT UNILAMELLAR VESICLES (GUVs) IN MEMBRANE FUSION
15:45-16:00		Vandana (školitel R. Šachl)	INVESTIGATING THE IN-MEMBRANE FUNCTIONAL/DYSFUNCTIONAL PROTEIN OLIGOMERIZATION IN FGF2 TRANSLOCATION ON VESICLES
16:00-16:15		Hüseyin Evcı (školitel J. Sýkora)	DEVELOPMENT OF NEW SUBSTRATES FOR SUPER-RESOLUTION STUDIES OF SUPPORTED LIPID BILAYERS (SLB) BY GRAPHENE INDUCED ENERGY TRANSFER
16:15-16:25	UZAVŘENÍ KONFERENCE - V SÁLE RUDOLFA BRDIČKY Closing ceremony (in Brdička Hall)		
16:25-17:45	VEČEŘE K UKONČENÍ KONFERENCE (VE VESTIBULU) (Dinner in lobby)		

List of presented students (36)

Seznam prezentujících studentů (36)

Bachelor and diploma students (6)

Diplomanti a zájemci z řad bakalářů (6)

Adamec Václav (PřF UK Praha, diplom. práce, školitel M. Lamač)

Beneš Marek (VŠCHT Praha, bakalář. Práce, školitelka R. Sokolová)

Fárníková Karolina (VŠCHT Praha, bakalář. práce, školitelka: E. Krupičková Pluhařová)

Fialová Johana (VŠCHT Praha, diplom. práce, školitel J. Fedor a P. Nag)

Jiroušková Eliška (PřF UK Praha, diplom. práce, školitelka R. Sokolová)

Ráliš Václav (PřF UK Praha, diplom. práce, školitel J. Pinkas)

PhD Students:

the 1st year doctoral students

Studenti 1. ročníku DSP studia (11)

Bukhari Seyd Adeel Mahmood (školitel O. Frank)

Đurana Jozef (školitel M. Fárník)

Frederick Soumya
(školitelka V. Petránková)

Šťastný David (školitel R. Šachl)

Hanušová Michaela (školitel M. Velický)

Johanovská Zuzana (školitel M. Hof)

Kocábková Barbora (školitel M. Fárník)

Králová Isabel (školitel J. Sýkora)

Lyshchuk Hlib (školitel J. Fedor)

Martinka Jakub (školitel J. Pittner)

Omezzine Gnioua M. (školitel P. Španěl)

PhD Students:

the 2nd - 5th year doctoral students

Studenti 2. až 5. ročníku DSP studia (19)

Abhinav (školitel J. Sýkora)

Bharadwaz Priyam (školitel M. Srnec)

Davidovič David (školitel R. Šachl)

Evcü Hüseyin (školitel J. Sýkora)

Hansen Mark N. (školitelka V. Petránková)

Chmelová Barbora (školitel R. Šachl)

Choińska-Młynarczyk Marta K.
(školitel T. Navrátil)

Imrich Tomáš

(školitelka-konzultantka H. Krýsová)

Jindra Martin (školitel O. Frank)

Kohútová Petra (školitel M. Hof)

Lemishka Mariia (školitel J. Dědeček)

Matoušek Mikuláš (školitel L. Veis)

Melčák Martin (školitel S. Záliš)

Sahu Satyam (školitel M. Velický)

Salvadori Karolina (školitel J. Ludvík)

Scollo Federica (školitel M. Hof)

Sedmidubská Barbora (školitel J. Kočíšek)

Umar Khaliullah

(školitelka V. Petránková)

Vandana (školitel R. Šachl)

Referees:

Tuesday May 23:

Vladimíra Petránková

Jaroslav Kočíšek

Jan Sýkora

Wednesday May 24:

Stefan Swift

Piotr Jurkiewicz

Pamir Nag

Úterý 23. května 2023
Program 1. dne konference (17 příspěvků)

PROGRAM – Tuesday May 23, 2023 (17 presentations)



POLYETHYLENE TERMINATED WITH SILICON AND ITS UTILISATION

Bc. Václav Ráliš

Mgr. Jiří Pinkas, Ph.D.

In our lab we have recently focused on various polyethylenes (PE) terminated with SiR_3 moiety (where $\text{R} = \text{H}, \text{Me}, \text{Ph} \dots$) prepared by hydrosilane/ $\text{B}(\text{C}_6\text{F}_5)_3$ system for the activation of early transition metal halide complexes.¹ These polymers with rather low molecular weight (around 1000 Da) have very low solubility in ordinary organic solvents but it is possible to dissolve them in toluene at higher temperatures.

The subject of our research is the post-modification of these polymers, for example the conversion of the terminal groups to silanols or fluorosilanes and also, we focused on grafting single site catalyst on these materials using hydrosilylation or bonding transition metal directly to the silyl group. Such materials will be further discussed with regard to the catalysis.

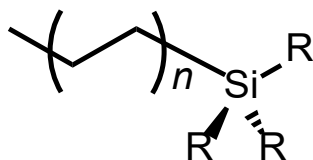


Figure 1 General formula of the polymers, where $\text{R} = \text{H}, \text{Ph}, \text{Me}, \text{F}, \text{Co} \dots$

References:

1. V. Varga, M. Lamač, M. Horáček, R. Gyepes, J. Pinkas, Dalton. Trans. **2016**, 45, 10146-10150

Acknowledgement: This research was supported by the Czech Science Foundation (project 21-01308S)



MOLECULAR SIMULATIONS OF LIPASE: FROM THE LID OPENING TO THE ACTIVE SITE

Karolína Fárníková

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

Lipases are enzymes from the class of hydrolases. Their biological function is to digest fats in small intestine¹. In addition, they can be utilized in industrial processes as catalysts not only in the natural aqueous environment, but also in organic solvents during transesterification or aminolysis². The change of the reaction medium influences activity and selectivity of enzymes. This work focuses on *Candida Antarctica* Lipase B (CALB) in water, acetonitrile and toluene. Specifically, it uses molecular simulations to study opening of the lid (amphiphilic loop in the vicinity of the active site), mechanism of the rate-limiting step and behaviour of the enantiomers³ of the key reaction intermediate. Obtained results will contribute to better understanding of the functioning of this practically used biocatalyst.

References:

1. Kodíček, M., Valentová, O. & Hynek, R. *Biochemie, chemický pohled na biologický svět*. (VŠCHT Praha, 2018).
2. Verger, R. 'Interfacial activation' of lipases: Facts and artifacts. *Trends Biotechnol.* **15**, 32–38 (1997).
3. Kitamoto, Y., Kuruma, Y., Suzuki, K. & Hattori, T. Effect of Solvent Polarity on Enantioselectivity in *Candida Antarctica* Lipase B Catalyzed Kinetic Resolution of Primary and Secondary Alcohols. *J. Org. Chem.* **80**, 521–527 (2015).



STUDIUM MECHANISMU OXIDACE PSYCHOAKTIVNÍ LÁTKY 25E-NBOH

Marek Beneš

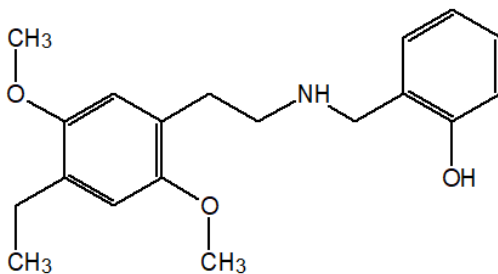
RNDr. Romana Sokolová, Ph.D.

Doc. Martin Kuchař, Ph.D.

Tato práce je zaměřena na studium *in vitro* oxidace látky 2-(((4-ethyl-2,5-dimethoxyfenethyl)amino)methyl)fenolu, známou také pod označením 25E-NBOH, pomocí elektrochemických a spektroeletrochemických metod. Cílem je navržení prvních oxidačních produktů a návrh mechanismu jejich vzniku.

Látky ze skupiny NBOH byly poprvé syntetizovány v roce 2010 s předpokládaným využitím v medicíně. Tyto sloučeniny jsou chemicky odvozené od fenethylaminu a stejně jako jeho další deriváty (např. MDMA, Amfetamin, atp.) vykazují stimulační a navíc i halucinogenní účinek. V současné době je konkrétně látka 25E-NBOH používána a ilegálně distribuována jako cenově dostupná alternativa k LSD. Přesný mechanismus působení 25E-NBOH nebyl doposud zjištěn a jelikož přenosy protonu a elektronu hrají významnou roli při metabolismu, elektrochemický výzkum oxidace a zjištění prvních produktů může napomoci k jeho odhalení.

Při této práci byla pro výzkum oxidace využita cyklická voltametrie. Při identifikaci produktů byla využita *in situ* IČ a UV-Vis spektroeletrochemie. V další fázi práce budou provedeny oxidační elektrolýzy a následná analýza vzorků na HPLC-DAD a HPLC-MS, dále také biotransformace.

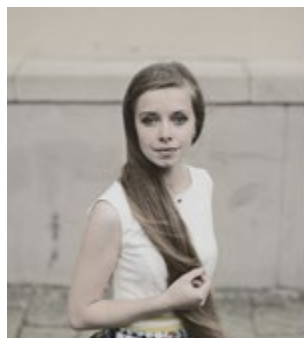


Obr.1.: Chemická struktura látky 25E-NBOH.

References:

Machado, Y.; Coelho Neto, J.; Araújo Lordeiro, R.; Brondi Alves, R.; Piccin, E.; *Forensic Toxicology* 38, 203-215 (2020).

Grafinger, K. E.; Stahl, K.; Wilke, A.; König, S.; Weinmann, W.; *Drug Test. Anal.* 10, 1607–1626 (2018).



MULTISPECTROSCOPIC STUDY OF MOLECULAR OXYGEN DISSOCIATION OVER ZEOLITES

Mgr. Mariia Lemishka

Mgr. Jiří Dědeček, CSc. DSc

Molecular oxygen is eco-friendly, cheap and available oxidant for the hydrocarbons transformation. Moreover, the activation of dioxygen gained significance as a possible key for the usage of methane. The selective oxidation of methane to methanol was suggested to be a promising way of methane utilization with an enormous in both scientific and industrial impact. Nevertheless, the employment of O₂ needs its activation over heterogeneous catalysts, which leads to the formation of the reactive form of oxygen (α -O). Zeolite materials are highly suitable matrices for incorporating transition metal ions (TMI) as catalytically active sites. Zeolites are crystalline microporous aluminosilicate molecular sieves formed by SiO₄ and AlO₄⁻ tetrahedra sharing their corners. Iron-containing zeolites represent important model catalysts for this reaction¹.

In this study, a commercial zeolite FER was selected due to the high concentration of Al pairs responsible for predominant stabilization of iron as Fe(II) in the cationic position. *In-situ* Mössbauer spectroscopy demonstrated O₂ treatment of Fe-FER at 220 °C and subsequent interaction with CH₄. *In-situ* FTIR spectroscopy results confirmed [Fe(IV)=O]²⁺ formed under through-flow conditions was stable till 280 °C. FTIR analysis of gaseous products confirms the presence of the bands characteristic for methoxy species, indicates the methanol formation. Produced methanol was detected in the gas phase by FTIR and mass spectrometry methods².

Concluding, the study has shown that *in-situ* FTIR spectroscopy was the best tool for investigating of α -O formation and stability at elevated temperatures and oxidation properties towards methanol formation. Combination of FTIR, Mössbauer, and XAS studies has shown that two distant Fe(II) centres with planar geometry embedded in FER interact in the redox cycle. The stability of α -O at increased temperatures makes the possibility to facilitate desorption of the oxidation products. That carries out the process more attractive for industrial goals.

References:

¹Tabor, E.; Dedecek, J.; Mlekodaj, K.; Sobalik, Z.; Andrikopoulos, P.C.; Sklenak, S. *Sci. Adv.*, **2020**, 6

²Mlekodaj, K.; Lemishka, M.; Kornas, A.; Wierzbicki, D.K.; Olszowka, J.; Jirglová, H.; Dedecek, J.; Tabor, E. *ACS Catal.*, **2023**, 13, 5, 3345–3355



SHEDDING LIGHT ON THE INFLUENCE OF STRUCTURAL DEFECTS ON THE BEHAVIOUR OF TWO-DIMENSIONAL MATERIALS

Adeel Bukhari

Mgr. Otakar Frank, Ph.D.

Two-dimensional (2D) materials such as graphene and transition-metal dichalcogenides (TMDCs) have been studied extensively across many fields owing to the fascinating physics that occurs in atomically thin layers, resulting in significant leaps in our understanding of their properties. These properties can be influenced by a wide range of factors, one such being structural defects, where the nature and extent of their impact on material behaviour still requires further exploration. Facile methods to quantify the structure-property relation of defects are in demand, with ultra-high vacuum (UHV) systems being required to resolve the structure of defects down to single atoms.

We aim to develop a toolbox for characterising and describing changes induced by defects, which will be created by Helium ion irradiation, with precise control over their positioning. This would involve a set of techniques that are more widely available and can be used in ambient conditions, while at the same time enabling the characterization and quantification of individual defects and their densities. These methods will include Raman spectroscopy and photoluminescence spectroscopy, as well as a range of atomic force microscopy (AFM) based techniques, such as tip-enhanced Raman and photoluminescence spectroscopies and conductive AFM. The mechanical properties of these materials will also be studied through AFM indentation.

Untangling the relationship between distinct kinds of defects and their influence over a materials property allows for informed decision-making when tailoring the properties of devices based on defect-engineered 2D materials.

References:

- [1] A. McCreary, O. Kazakova, D. Jariwala, et al. *2D Mater.*, 8(1):013001, 2021
- [2] O. F. N. Okello, D.-H. Yang, Y.-S. Chu, et al. *APL Mater.*, 9(10):100902, 2021.
- [3] S. Tongay, J. Suh, C. Ataca, et al. *Sci. Rep.*, 3:2657, 2013.
- [4] S. Mignuzzi, A. J. Pollard, N. Bonini, et al. *Phys. Rev. B*, 91(19):195411, 2015
- [5] M. R. Rosenberger, H.-J. Chuang, K. M. McCreary, et al. *ACS Nano*, 12(2):1793–1800, 2018.
- [6] P. Miao, Y.-T. Chen, L. Pan, et al. *J. Chem. Phys.*, 156(3):034702, 2022.
- [7] A. Rodriguez, M. Kalbac, O. Frank. *2D Mater.*, 8(2):025028, 2021
- [8] M. Velický, A. Rodriguez, M. Bouřsa, et al. *J. Phys. Chem. Lett.*, 11(15):6112–6118, 2020.
- [9] G. Hlawacek, A. Götzhauser, eds. *Helium Ion Microscopy. NanoScience and Technology*. Springer International Publishing, Switzerland, 2016.



ELECTROCHEMISTRY OF NEW PSYCHOACTIVE SUBSTANCES 3-FLUOROPHENMETRAZINE, 4-METHYLPENTEDORNE AND FLUOROMETHOXYACETYL FENTANYL

Bc. Eliška Jiroušková

RNDr. Romana Sokolová, Ph.D.

The electrochemistry properties of 3-fluorophenmetrazine (hereinafter referred to as “3-FPM”), 4-methylpentedrone (hereinafter referred to as “4-MPD”) and *meta*-fluoro Methoxyacetyl fentanyl (hereinafter referred to as “FMAcF”) were studied. These compounds are abused as an alternative to classical drugs (ecstasy, cocaine) due to their legal status. New psychoactive substances have been appeared in the drug market recently and they are available online under different cover names, such as “bath salts” or “legal highs”.

The aim of the study is to identify possible metabolic pathways in human organism. Part of the reaction scheme can be an electron transfer coupled with chemical reactions. Therefore, this work is focused on the electrochemical behaviour of substances by means of cyclic voltammetry and UV-Vis and IR spectroelectrochemistry. Next stage of the work will be identification of metabolites using incubation with liver microsomes.

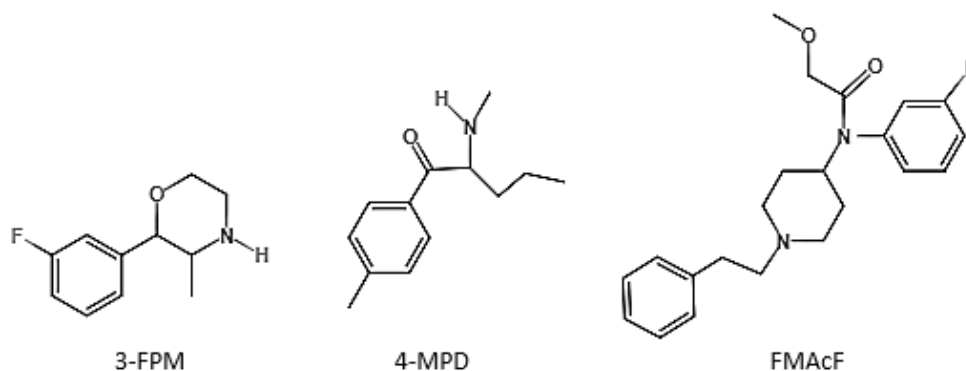


Figure 1: Chemical structure of 3-FPM, 4-MPD and FMAcF.

Acknowledgement

The work has been supported by the Czech Academy of Sciences (RVO: 61388955).

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EXCITED STATE MOLECULAR DYNAMICS ASSISTED BY MACHINE LEARNING

Mgr. Jakub Martinka

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

Molecular dynamics of excited states is an important field of study of many biochemically important molecules and phenomena. A full quantum mechanical description is computationally unfeasible, fortunately, Tully's fewest switches surface hopping method, which is based on the calculation of a set of molecular dynamics trajectories, satisfies the statistical character of quantum description and can be used to study these phenomena.

However, even these calculations are using costly multireference methods and are thus computationally demanding, which limits their applicability. In recent years, machine learning has become a successful technique that has significantly improved the speed and accuracy of results of traditional computational methods. However, in the case of molecular dynamics of excited states, the use of this technique is still a great challenge, which has not yet received sufficient attention. Combining these techniques with non-adiabatic molecular dynamics methods can enable the study of biochemically important molecules and phenomena.

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STUDY OF LOW ENERGY ELECTRON-INDUCED DISSOCIATION OF CF₃I USING VELOCITY MAP IMAGING

Bc. Johana Fialová

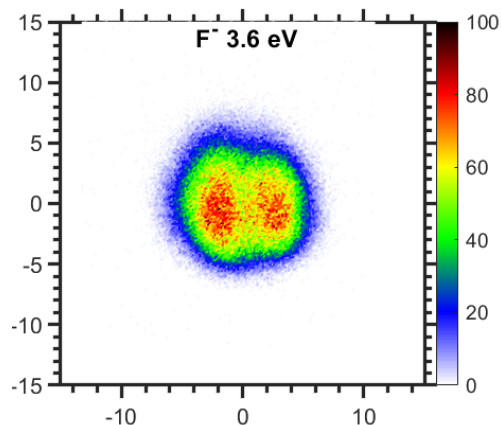
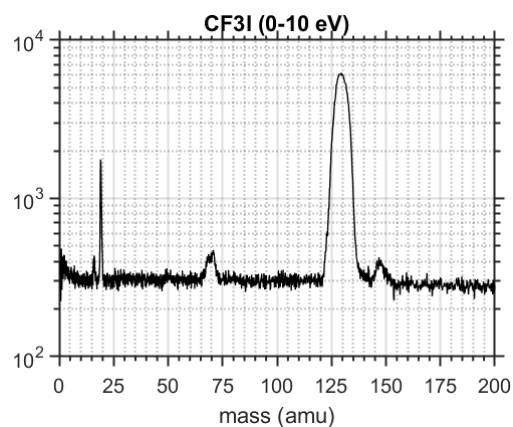
Juraj Fedor PhD.

Pamir Nag PhD.

Dissociative electron attachment (DEA) is an effective method of reducing reactive halogen derivatives by collisions with electrons, upon which the inert halogen ions are formed. Velocity map imaging (VMI) is a technique that reveals the dynamics of this process. The electron beam is crossed with a molecular beam of the studied molecule, leading to negative ions' creation. The VMI spectrometer measures their time of flight (TOF) and kinetic energies by utilizing a time- and position sensitive delay line detector.

My study is focused on the molecule trifluoroiodomethane (CF₃I) as it could be a potential substitute for environmentally detrimental tetrafluoromethane (CF₄), which is used in plasma processing (semiconductor industry). The advantage of CF₃I is its short lifetime in the atmosphere (a few days), in comparison, the atmospheric lifetime of CF₄ is 50 000 years (the short lifetime of CF₃I is caused by photolytic cleavage of the CF₃-I bond). This

creates a need to understand the electron-induced chemistry of this compound and its dynamics. For this purpose, we utilize the VMI spectrometer. In my lecture, the results of the analysis of previously measured data by Pamir Nag PhD. will be presented.





TRACKING MEMBRANE PERMEABILIZATION ON SINGLE LIPID VESICLES - METHOD DEVELOPMENT

Mgr. David Šťastný

Doc. RNDr. Radek Šachl PhD.

Protein complexes are challenging systems to study, especially when these complexes form on lipid membranes only for a short period of time. This is also the case of fibroblast growth factor 2 (FGF2), a protein that has many physiological and pathological functions in the human organism. Despite being heavily studied for many years, it remains unclear how the protein is translocated into the extracellular space where it performs its function.

To understand such systems we developed a method called double leakage single GUV assay (DLSGA). It utilizes giant unilamellar vesicles (GUVs) mimicking native cellular membranes. In a single experiment, up to 300 individual GUVs are imaged for the content of a leakage dye that reports on the presence of FGF2 pores. During three measurements and under different conditions, detailed information about pore-opening dynamics is gained for each GUV.

By using this method, we were able to confirm the role of Y81 in hastening insertion of FGF2 oligomers into the membrane. We were also able to observe differences in the formation of FGF2 pores by distinct FGF2 variants with mutated cysteines. Our experiments revealed that FGF2 with mutated C95 (which can only form dimers) is able to form stable pores to a similar degree as the wild type variant of the protein (which can form higher oligomers). This experiment thus confirms that dimers as well as the higher oligomer species insert efficiently into the membrane and underpin the importance of dimers for translocation of the protein.

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FUNDAMENTAL PHYSICS AND CHEMISTRY OF THE INTERFACE BETWEEN MONOLAYER TRANSITION METAL DICALCOGENIDES AND METALS

Mgr. Michaela Hanušová

Ing. Matěj Velický Ph.D.

Monolayer transition-metal dichalcogenides (TMDCs) have recently captured significant attention due to their potential applications in many areas, including electrochemistry, photovoltaics, etc.^{1,2}

Various exfoliation techniques have been explored so far. However, a suitable route for obtaining large areas of monolayers on different substrates remains challenging. Gold-assisted exfoliation has attracted interest due to the high yields of monolayer flakes. The use of other noble metals could theoretically also lead to successful exfoliation. But their use is limited due to their susceptibility to oxidation in air-prepared samples.^{3,4}

Herein, we investigate the ways for obtaining large-area monolayer flakes on different substrates using different metal deposition techniques. We use mechanical exfoliation of TMDCs onto metallic surfaces under ambient and controlled atmosphere conditions. That prevents undesirable oxidation of the substrate surface.

In my presentation, I will discuss the characterization of prepared samples by Raman spectroscopy and atomic force microscopy.

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PHOTODISSOCIATION OF TRIFLUOROACETYL CHLORIDE PROBED BY VELOCITY MAP IMAGING (VMI) TECHNIQUE

Mgr. Jozef Ďurana

doc. Mgr. Michal Fárnik, Ph.D., DSc.

Trifluoroacetyl chloride (CF_3COCl) plays – as any other halogenated carbonaceous chemical compound – important role in the ozone layer depletion. It is certainly not as potent as common chlorofluorocarbons (CFC), yet it still bears a lot of information about the decomposition and the environmental fate of mentioned chemicals in the Earth's atmosphere. Since the stratosphere, where ozone layer resides, is a domain of photochemistry, it is only natural to study interaction of CF_3COCl with UV light in details. Additionally, study of this photo dissociative processes should be carried out in atmospherically relevant environment, namely on ice particulates.

In the experiment, photodissociation of CF_3COCl molecules is investigated by the Velocity Map Imaging technique (VMI). The resonance-enhanced multiphoton ionization (REMPI) process, using dye laser producing ultraviolet light at wavelength of 235 nm is used to detect Cl fragments after the dissociation. From the fragment velocity vector, detailed molecular level information about the photodissociation process is deduced.

Three main scenarios are investigated: a) CF_3COCl coexpansion in helium, b) CF_3COCl coexpansion in argon and c) pick up of CF_3COCl on argon clusters.

Information gathered from this experiment will be used to further explore the behavior of halogenated compounds in the polar stratospheric clouds.



MICROMANIPULATION AS A NEW INSTRUMENT FOR RESEARCH OF BIOMEMBRANE STRUCTURE AND ITS MECHANICAL PROPERTIES

Mgr. Zuzana Johanovská

prof. Dr.rer.nat. Martin Hof, DSc.

In cells, various membrane events are influenced and sometimes even controlled by changing of the tension on the membrane or their curvature (for example movement of the cells, influence on membrane proteins etc.). Micromanipulation technique brings new, so far not fully explored possibilities to this biomembrane research, as it enables direct modifications of membrane mechanical properties of giant unilameral vesicles (GUVs), simulating cell membrane.

The combination of micromanipulation with other methods such as fluorescence microscopy will allow us to open the door to other exciting experiments we plan to perform in later stages of this project. Especially we are interested in the combination of micromanipulations with our frequently used method MC-FRET, which allows us to detect and characterize membrane nanodomains. Also studying of the peptide-membrane interactions and influence of the peptides on mechanical properties of the cells is planned in near future.

My lecture will however focus mainly on the basics of micromanipulation as the new method, which we are currently introducing here at Heyrovsky Institute in Fluorescence group. Also some future outlook will be provided, as well as first obtained results.

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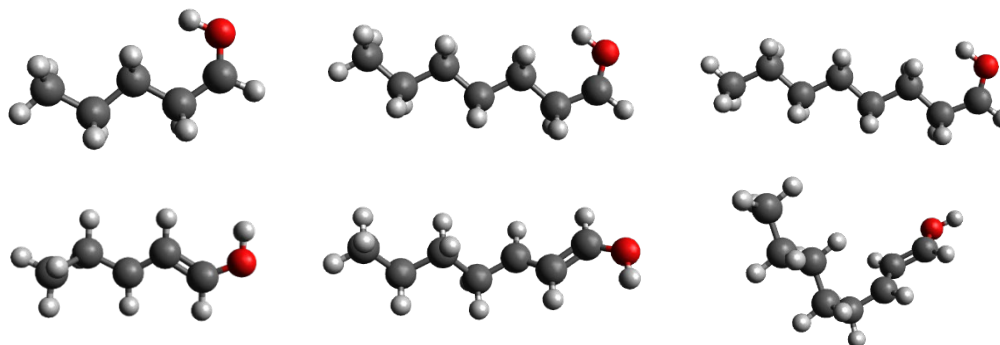


EXPERIMENTAL AND THEORETICAL STUDIES OF GAS PHASE ION MOBILITY AND ENERGETICS: PROTONATED SATURATED AND UNSATURATED ALDEHYDES IN HELIUM

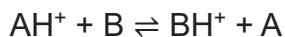
Maroua Omezzine Gnioua, MSc.

Prof. RNDr. Patrik Španěl, Dr. rer. nat.

To gain a further understanding of the ion-molecule reactions important for trace gas mass spectrometric analysis, theoretical calculations and experimental measurements were carried out for selected classes of volatile organic compounds (VOC). Quantum chemistry calculations based on the density functional theory, DFT, were performed using the ORCA software to study the structures and energetics of ions. The total enthalpies of the neutral aldehyde molecules and ions resulting from their protonation in reactions with H_3O^+ were calculated at the B3LYP 6-311++G(d,p) level of theory including the D4 dispersion correction for the standard temperature and pressure. The calculations were performed for several optimized structures of each of the ions.



The dipole moments and polarizabilities were also calculated for all neutral molecules. The Selected Ion Flow Drift Tube Mass Spectrometry (SIFDT-MS) was used to measure the mobilities and energies of protonated aldehyde ions under different reduced electric field intensities (E/N). The aim is to accurately determine the rate coefficients for forward and backward proton transfer reactions between different aldehydes



from which other thermochemical parameters can be reliably obtained such as equilibrium rate constants and the changes in Gibbs free energy.

Acknowledgements

This work has been supported by the Czech Science Foundation (project no. 21-25486S, Selected ion flow drift tube mass spectrometry with negative ions and nitrogen carrier gas).



MOLECULAR AND CLUSTER MASS SPECTRA OF TRIFLUOROACETYL CHLORIDE

Ing. Barbora Kocábková

Doc. Mgr. Michal Fárník, Ph.D. DSc.

Every volatile halogenated hydrocarbon is a potential threat to the ozone layer. Thus, it is advantageous to have enough information about its interactions in low density conditions. Supersonic molecular beams provide us with a controlled environment able to simulate conditions in the stratosphere (composition, density, radiation). Results presented here take part in a study of trifluoroacetyl chloride (CF_3COCl) behavior in cluster systems with this part focusing on molecule and molecular cluster spectra yielded by 70 eV electrons ionization and mild ionization with low energy electron attachment.

The measurements were carried on the CLUB apparatus [1]. Molecular beam was produced by a continuous supersonic expansion of a 1.5% (pressure-wise) mixture of CF_3COCl and helium through a 50 μm wide conical nozzle at 1.5 bar. Clusters were formed in co-expansion of CF_3COCl (3.5%) with argon under higher source pressure (3.8 bar). Mass spectra of CF_3COCl were measured using a time-of-flight reflectron mass spectrometer with electron beam ionization.

The fragmentation patterns of the positively and negatively charged clusters differ significantly, which points to a different ion chemistry in these species. At the same time, the combined data from the positive and negative ion mass spectra allow us to infer information about the neutral cluster structure. From a practical point of view, the behavior of these molecules in clusters can mimic their chemistry in atmospheric aerosols necessary for understanding of various processes in atmospheric chemistry.

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REGULATION OF THE MEMBRANE CHANNEL ACTION STUDIED BY FLUORESCENCE TECHNIQUES

Mgr. Isabel Králová

*prof. Dr. rer. nat. Martin Hof, DSc.
Mgr. Jan Sýkora, Ph.D.*

In our work, we focus on a membrane voltage-gated hydrogen channel H_v1 which is a selective proton channel that facilitates large fluxes of protons across biological membranes. H_v1 is controlled by transmembrane voltage and pH gradient. The H_v1 channel is crucial for the extrusion of protons to maintain a balanced cytosolic pH. Several studies have revealed a strong relationship between pH balance, cancer development, and the overexpression of the H_v1 channel, which has been proposed as a marker of malignancy in cancer.

In addition to the transmembrane domain, H_v1 also contains an outer element that can potentially function as a proton antenna. The dynamic interactions of this extra-membrane domain with lipid membrane may function as a regulatory factor of proton transfer. To test this hypothesis, H_v1 will be investigated using a fluorescence technique based on Förster resonance energy transfer (FRET) between tryptophans present in the outer domain of H_v1 and a head group of fluorescently labeled lipids embedded in the membrane.

As the study of membrane proteins in their natural environment of membranes is still challenging, we plan to employ an assay based on the nanodiscs, which are natural membrane fragments solubilized by a copolymer, diisobutylene maleic acid (DIBMA). In order to develop and tune the FRET assay, the data of DIBMA nanodiscs and artificial membranes containing model transmembrane peptide needs to be profoundly characterized and understood.

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DISSOCIATIVE IONIZATION OF MeCpPtMe₃: FORMATION OF METHANE AND ETHANE AT SINGLE-COLLISION CONDITIONS WITH ELECTRONS

Hlib Lyshchuk

Mgr. Juraj Fedor, Ph. D.

This study aims to understand chemical reactions that are fundamental to the dissociative ionization of trimethyl(methylcyclopentadienyl)platinum(IV) (MeCpPtMe₃), of common FEBID precursor of Platinum. Previous studies which probed electron-driven chemistry of this precursor using surface-science technique [1, 2] revealed a surprising phenomenon, namely that is not the methyl radical which is primarily released upon electron irradiation, but rather the methane molecule. The gas-phase study of Engman et al. [3] provided a large number of interesting data, however, it did not address this question.

In the present work, gas-phase MeCpPtMe₃ was irradiated with electrons of controlled energy, and the positive product ions were analyzed in a reflectron time-of-flight mass spectrometer (RTOF). By fitting complex isotope patterns, we identified the contributions of specific fragment ions to peaks in the mass spectrum. Additionally, the appearance energy for the parent molecule and selected groups of peaks corresponding to the loss of one and two methyl groups were determined. To support the experimental data, quantum calculations were performed. The comparison of the experimental and calculated appearance energies suggests that methane and ethane are formed already in the binary collisions of the precursor with electrons at electron energies close to the ionization threshold.

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TRANSITION-METAL-CATALYSED HYDROGENATION REACTIONS USING THE HYDROSILANE- $B(C_6F_5)_3$ SYSTEM AS AN ACTIVATOR

Bc. Václav Adamec

RNDr. Martin Lamač, Ph.D.

MSc. Urbán Béla Ph.D.

Catalytic utilizing the strong Lewis acid $B(C_6F_5)_3$ and silanes are studied in many organic transformations. Recently, our team has reported the use of borane-silane together with sandwich complexes of VI.B group and it was used for olefin polymerization and hydrodehalogenation reactions. We it subsequently decided to probe the capability of this system for hydrogenations, in this case, selective semi-hydrogenation of acetylenes.

The aim of this research is to find ideal catalyst and conditions for hydrogenation of diphenyl acetylene, test other substrates, and investigate the reaction mechanism and factors influencing the selectivity. So far, we have discovered that semi-hydrogenation of diphenyl acetylene using some group 4 metallocenes leads selectively to *Z*-stilbene. Other products were in some cases also identified, such as the fully saturated product (diphenylethan) and hydrosilylated product.

In my talk, I will provide an overview of the tested organometallic pre-catalysts and reaction conditions as well as some reaction kinetics investigations.

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Středa 24. května 2023
Program 2. dne konference (19 příspěvků)

PROGRAM – Wednesday May 24, 2023 (19 presentations)



VISUALIZING PLASMONIC MISLOCALIZATION USING SINGLE- MOLECULE LOCALIZATION MICROSCOPY

Soumya Frederick, MSc.

Petráková Vladimíra doc. Ing. Ph.D.

Plasmonic coupling with fluorophores introduces a mislocalization in the emission position where the far-field microscopy detects an apparent fluorescence emission position that deviates significantly from the actual molecule position. The magnitude and nature of this deviation include information about the position and orientation of the plasmonically coupled fluorophore. By understanding the mechanism of the fluorescence shift, we can create tools for the spatial manipulation of light at the nanoscale.

To study the effect, we combine superresolution microscopy, DNA nanotechnology (DNA origami) and plasmonic nanoparticles. To quantify the fluorescence shift, we use the DNA origami that allows the positioning of fluorophores and plasmonic nanoparticles with nanometer precision. We use the DNA-PAINT technique for visualization of the structure with resolution below the diffraction limit. We evaluate the magnitude of the fluorescence shift and enhancement in presence of nanoparticles with various sizes. We further aim to target the enhancement mechanism by controlling the spectral overlap between the plasmon resonance, fluorophore absorption, and emission and study the implications of the enhancement mechanism on position shifts. Understanding how the enhancement mechanism drives the shift will enable to control the shift by engineering the plasmonic structures for desired effects.



TOWARDS SOLVENT SPECIFIC EFFECTS IN INFRARED SPECTRA OF RHENIUM COMPLEX

Ing. Martin Melčák

RNDr. Mgr. Jan Heyda, Ph.D.

Ing. Stanislav Záliš, CSc.

Ultrafast intersystem crossing (ISC) in transition metal complexes represents a challenging process for both experimental and theoretical investigation. Two computational approaches have been employed to study the relaxation processes during the ISC of complex $[\text{Re}(\text{bpy})(\text{CO})_3\text{Cl}]$ (bpy = 2,2'-bipyridine) in explicit dimethylsulfoxide solvent. Several relaxation processes has been identified along with their time scales and physical nature. Using state-of-the-art non-adiabatic molecular dynamics we have described the relaxation of “molecular spin-orbit wave packet”, and successive vibrational relaxation in non-adiabatic regime. We have connected the non-adiabatic simulations to the experiment through the fluorescence decay. Along with the non-adiabatic approach, adiabatic trajectories in one electronic state were employed, enabling to reach time scales longer than ps and to study the relaxation of the solvent molecules. In accord with the experiment, we have observed the fast shift of frequencies and revealed the correlation with proximal solvent relaxation.

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HYDRATION AND DYNAMICS OF FUNCTION-RELEVANT REGION OF HPUREI

Abhinav, MSc

Mgr. Jan Sýkora, Ph.D.

About two-thirds of people on the planet suffer from *Helicobacter pylori* infection. This gram-negative bacterium causes severe gastritis, ulcers, gastric adenocarcinoma, and even cancer by flourishing in the digestive tract. *H. pylori* enables the proton-gated urea channel HpUrel to survive in the stomach's highly acidic environment. Specifically, urea molecules can enter the cytosol upon drop in periplasmic pH, thanks to HpUrel action in the periplasmic inner membrane. After the urea is digested by urease enzymes, carbon dioxide and ammonia are produced, which are subsequently transported back to the periplasm to adjust the pH to neutral. The activity of HpUrel at low pH is largely modulated by six key amino acid residues in periplasmic loop 2 (PL2). Our research aims to relate proton transfer to the hydration and dynamics in the proximity of these crucial amino acid residues to determine the mechanism of PL2 in opening and closing of HpUrel. Here, we attempt to label the HpUrel protein site-specifically with a dye that is environment-sensitive and monitor the hydration and mobility by means of time-dependent fluorescence shift at these functionally important areas. Our research will help to understand the role of these locations in the complex proton gating process.

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VARIOUS ROLES OF -NO₂ SUBSTITUENT IN ELECTRO- CHEMICALLY INVESTIGATED SUPRAMOLECULAR SYSTEMS

Ing. Karolína Salvadori

prof. RNDr. Jiří Ludvík, CSc.

Supramolecular chemistry is an interdisciplinary area providing a suitable way of connection between different fundamental objectives.^[1] As an interdisciplinary field, it combines the knowledge and experience of synthesis, analytical chemistry including spectroscopic methods, and other disciplines. Because electrochemistry brings benefits such as high selectivity in connection with facile operation, eco-friendly conditions, or economical aspects relating to lower demands for chemical agents and space, the application of this methodology in supramolecular chemistry is desirable. Unfortunately, this is still rather rare. This could be explained due to a lack of knowledge of the electrochemical redox mechanism, which significantly differs for different molecules because of the interplay of all functional groups present in their structure. However, the clue to understanding the redox behaviour of polyfunctional molecules is hidden in detailed analysis of electrochemical results on molecular level.

In our research -NO₂ substituted sulfonamides, ureas, and sulfonimides were thoroughly studied. We decided to take advantage of the presence of the nitro group which is known for its electrochemical and optical properties. The electrochemical behaviour of aromatic nitro compounds in polar aprotic solvents is thoroughly documented^[2] and usually corresponds to two separate processes - after the first reversible one-electron formation of radical anion the second three-electron four-proton irreversible process follows yielding to the corresponding hydroxylamine derivative. However, in the cases of sulfonamides and urea-substituted structures, the nitro group was reduced in the sense of auto-protonation.^[3] Therefore, we decided to apply nitro group as a probe, reflecting acid-base or complexation properties of original molecules in the presence of different anions. On the other hand, in the case of sulfonimides the nitro group served as a strong electron-withdrawal substituent facilitating electrochemically involved cleavage of the system. This ability allowed us to prepare the structures, which were synthetically unavailable, and could be later utilized as anion receptors.

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THE CHASE FOR AN INVERTED S-T ORDERING FOR MORE EFFICIENT ORGANIC LEDS

Mgr. Mikuláš Matoušek

RNDr. Libor Veis , Ph.D.

Organic LEDs became a common element of many everyday devices. Despite their widespread use, there are still many limitations. One of the most fundamental issues is that due to the random electron hole recombination at the luminophore, 75% of the conduction electrons excite the luminophore to a triplet state which cannot be used for light emission. This sets a theoretical limit of OLED efficiency to only 25%.

We present our search for molecules which have the first excited singlet state lower in energy than the triplet, which would allow us to use the reverse intersystem crossing process to recover some of the triplet excitations, improving the total efficiency of OLED devices beyond this theoretical limit.

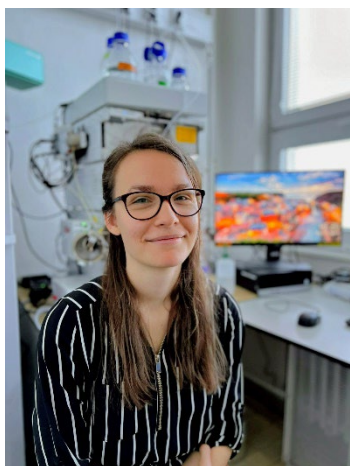
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THE FUNCTIONAL PORE FORMATION OF PRO-APOPTIC PROTEINS (BID AND BAX) IN GIANT UNILAMELAR VESICLES AS THE MODEL SYSTEM

Mgr. Petra Kohútová

prof. Martin Hof, Dr. rer. nat., DSc.

Apoptosis, also called programmed cell death, is essential in multicellular organism. This highly regulated mechanism functions as the quality control, during which the dysfunctional/ unwanted cells are removed in response to pro-apoptotic factors. There are two ways how the cell undergoes the apoptosis, extrinsic and intrinsic (mitochondrial) pathway. The key step in intrinsic pathway of apoptosis is the permeabilization of the mitochondrial outer membrane (MOM) and release of some of the mitochondrial proteins (for instance: cytochrome *c*, part of the electron transport chain). Many proteins participate in the process of apoptosis, for example members of the Bcl-2 protein family, covering two subgroups, anti- and pro-apoptotic proteins. Whether the cell undergoes apoptosis depends also on the balance between these two subgroups of proteins.

We use giant unilamellar vesicles (GUVs) as a simplified model membrane system to examine how pro-apoptotic proteins (Bid and Bax) form a functional pore into the membrane. The lipid composition of liposomes is phosphatidylcholine (PC), phosphatidylethanolamine (PE) and cardiolipin (CL). CL is a negatively charged, which plays a crucial role in binding pro-apoptotic proteins to the membrane, where Bax tends to form pores.

With the help of an advanced dual(+1) fluorescence correlation spectroscopy (dual(+1) FCS), technique invented in our laboratory, we correlate Bax/Bid in-membrane oligomerization in membrane permeabilization (pore formation).

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ROLE OF THERMODYNAMICS IN -ATOM ABSTRACTION REACTIVITY OF S- ADENOSYLMETHIONINE ENZYMES

Priyam Bharadwaz

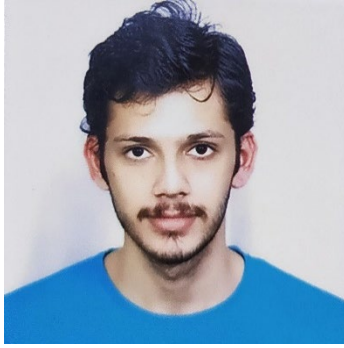
Mauricio Maldonado-Domínguez, Ph.D.

Mgr. Martin Srnec, Ph.D.

Hydrogen atom abstraction (HAA) is ubiquitous in nature, which relies on concomitant transfer of one proton and one electron from a substrate to an oxidant. An important superfamily of enzyme that extensively engaged in HAA is the Fe₄S₄-bound S-adenosylmethionine (SAM) via a [4Fe-4S] cluster and SAM to initiate a diverse set of radical reactions. The initial stage of this catalytic mechanism can be described by the homolytic reductive cleavage of the C-S⁺ bond of SAM enabled by intramolecular homolytic electron transfer from the [Fe₄S₄]¹⁺ cluster to SAM resulted in the formation of methionine and strongly oxidizing 5'-deoxyadenosyl (dAdo•) radical. After that the associated dAdo• radical undergoes HAA in the presence of substrate to generate a substrate radical. Despite a large number of dAdo• mediated HAA reactions, till date, the computationally accessible thermodynamic contributions to dAdo• catalytic efficiency is still unexplored. Herein, we investigate the chemical behavior of the range of substrates involve in HAA with SAM in the presence of auxiliary oxidant CH₃•, in aqueous media. We also analyze their complete (diagonal and off-diagonal) thermodynamic properties and their relationship to reactivity. Using this, we investigate their chemical properties with dAdo• radical in two different media – in aqueous vs enzyme-like environment, the latter of which is represented by two the prototypical radical SAM enzymes pyruvate formate-lyase activating enzyme (PFL-AE) and lysine 2,3-aminomutase (LAM) – with the aim to elucidate how the protein environment affect its catalytic function.

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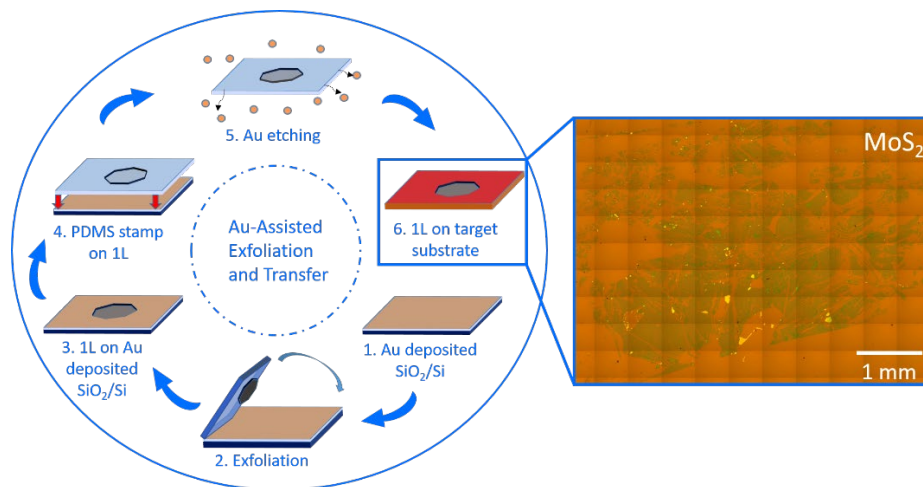


LARGE-AREA MECHANICALLY-EXFOLIATED TWO-DIMENSIONAL MATERIALS ON ARBITRARY SUBSTRATES

Satyam Sahu M.Sc.

Mgr. Matěj Velický, Ph.D.

Layered materials play a crucial role in modern device-based applications due to their unique properties, which can be unlocked through the exfoliation of layered crystals to monolayers. While several exfoliation methods have been developed, Au-assisted exfoliation has recently shown potential for producing large-area monolayers. However, this method promotes charge transfer that limits (opto)electronic applications of exfoliated materials. Here, we present a method of preparing large-sized monolayer flakes using Au-assisted exfoliation followed by chemical etching of Au. We characterize the samples using photoelectron and optical spectroscopic techniques and fabricate field-effect transistors and photodetectors to demonstrate the suitability of our method for large-area optoelectronic devices. Our findings highlight the technique's ability to preserve the material's intrinsic physical and chemical properties, opening up new possibilities for a wider range of applications.



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« SPECIFIC OR NOT SPECIFIC, THAT IS THE QUESTION »: AN OVERVIEW ON GAL-1 - GM1 INTERACTION

Msc. Federica Scollo

Prof. Dr. rer. nat. Martin Hof, DSc.

Galectins are a ubiquitous family of galactose-binding proteins, they possess one or more β -sandwich carbohydrate recognition domain/s (CRD/s) by which they interact with molecules having a galactoside moiety. Among all of them, galectin-1 is of great interest, being implicated in T-cells communication. Gal-1 is believed to express its function by binding specifically the monosialotetrahexosylganglioside (GM1). The above-mentioned binding has been hypothesized and indirectly shown in previous works, either employing too sophisticated or non-physiologically relevant systems. [1] [2]

In this work, we investigate the interaction of galectin-1 with different types of physiologically relevant model membranes containing GM1. We employed a combination of experimental techniques, both fluorescence-based and label-free techniques, i.e. Förster Resonance Energy Transfer (FRET), confocal Fluorescence Microscopy, Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D) and Isothermal Titration Calorimetry.

To the best of our knowledge, our data show for the first time that galectin-1 is interacting with model lipid membranes and, more importantly, the data suggest a specific interaction with GM1.

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INTERLEAFLET ORGANIZATION OF MEMBRANE NANODOMAINS: WHAT CAN(NOT) BE RESOLVED BY FRET?

Ing. Barbora Chmelová

doc. RNDr. Radek Šachl, Ph.D.

The Plasma membrane consists of two highly asymmetric layers and is compartmentalized into small heterogeneities (nanodomains) whose mutual position within the bilayer is determined by strong interleaflet interactions. Regarding nanodomain organization four scenarios have been considered: perfect registration across the membrane, independent distribution, anti-registration (nanodomains in the opposing leaflets are repelled), or presence in only one membrane leaflet. Due to nanodomain characteristics, it is highly challenging to distinguish these scenarios from each other. We have therefore developed a powerful method called MC-FRET (Förster resonance energy transfer analyzed by Monte-Carlo simulations) that can determine the size, concentration, and organization of lipid rafts. The aim is to find the limits of MC-FRET by discovering membrane parameters responsible for yielding sufficient/optimal resolution. We generated and analyzed in-silico time-resolved fluorescence decays for a large set of virtual as well as real donor/acceptor pairs with variously distributed nanodomains to identify conditions that gave satisfactory or unsatisfactory resolution. Overall, FRET is a robust method that under specific conditions reveals otherwise difficult-to-reach characteristics of membrane lipid nanodomains.

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SYNTHESIS OF DOPED PSEUDOBROOKITE (Fe_2TiO_5) FILMS: PROPERTIES AND APPLICATIONS IN PHOTO(ELECTRO)CATALYSIS

Ing. Tomáš Imrich

prof. Dr. Ing. Josef Krýsa
Ing. Hana Krýsová, Ph.D.

Pseudobrookite (Fe_2TiO_5) is of interest in various photo(electro)chemical applications. It is a medium wide bandgap (2.1 eV, indirect) n-type semiconductor [1]. Imrich et al. [2] prepared for the first-time phase pure undoped Fe_2TiO_5 films and characterized their optical and photo(electro)chemical properties.

The aim of the work was the synthesis of pseudobrookite films and their detailed physical and photo(electro)chemical characterization. Precursor films were deposited by spray pyrolysis (SP) at 550 °C on fluorine doped tin oxide (FTO) on borosilicate glass using iron (III) acetylacetonate and titanium diisopropoxide bis(acetylacetonate) in methanol, with a [Fe]:[Ti] ratio slightly below 2:1. As the dopant, tin (Sn) was used by adding it directly into the precursor solution. SP was followed by annealing in air at 700 °C. A long duration of annealing was required for completing the process of the formation of the desired Fe_2TiO_5 phase (60 hours).

The level of doping was set to 1 mol % based on previous experiments with hematite ($\alpha\text{-Fe}_2\text{O}_3$) photoanodes. Doping had a beneficial effect and resulted in an increase in photocurrents (approximately 2.5 times higher than undoped Fe_2TiO_5 under AM 1.5 irradiation (100 mW/cm²)). Optimized photoanodes were used in long-term polarization in acidic media (e.g., 0.1 M H_2SO_4).

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HIGH RESOLUTION NEAR INFRARED IMAGING WITH *DNA-PAINT*

Khalilullah Umar, MSc.

Doc. Ing. Vladimíra Petráková, Ph.D.

One of the limiting factors in single molecule localization microscopy (SMLM) including DNA – Point Accumulation in Nanoscale Topography (DNA-PAINT), lies in the limited range of fluorophore which hinders the technique from reaching their full potential. DNA – PAINT is limited to the use of organic fluorophores that do not cover well the near-infrared and the infrared region, have small stoke shift leading to spectra crosstalk [1], thus, inhibiting its application.

We proffer a solution to this problem using non-conventional photoluminescent probes such as (NV-) fluorescent nanodiamonds and gold nanoclusters. Both photoluminescent probes are capable of emission in the biologically inactive infra-red, have large stoke shift, and high penetrating capability of infrared light [2], thus enabling imaging deep into tissues, as well as, for other nanophotonic applications.

Here photoluminescent probes will be used in imaging of DNA nanostructures, several intrinsic and extrinsic factors required for optimizing the imaging condition will be studied. The efficiency of the photoluminescent probe and resolution of resulting image will be compared to that of common organic dyes having near infrared emission.

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FULLERENOLS AND THEIR INTERACTIONS WITH SECONDARY LOW-ENERGY ELECTRONS

Ing. Barbora Sedmidubská

Mgr. Jaroslav Kočíšek, Ph.D.

Ing. Marie Davidková, CSc.

Buckminsterfullerene C₆₀ is the smallest fullerene - a nano-sized spherical carbon molecule with 20 hexagonal and 12 pentagonal rings that can scavenge low-energy electrons (LEE) in a wide range of energies. Fullerenes can form stable π - π complexes [Castro, 2017] and for years have been studied as possible carriers of drugs due to the ease of their modification (endo/exo-hedral) [Kazemzadeh, 2019]. It resulted in many targeted therapy models so as complexes for photodynamic therapy [Sharma, 2011]. But, can fullerenes be interesting for chemo-radiotherapy as well?

The question can be partially answered by studying their interactions with secondary LEE, which are forming as secondary species in the irradiated tissue. [Sanche, 2009] The same happens in a present experiment of pulse radiolysis. It uses very short pulses of highly accelerated electrons for irradiation of solution and formation of secondary species in the solution. These species, including LEE are detected by the means of transient absorption spectroscopy. Relative concentrations of secondary species are monitored as a function of time. Processes occurring faster than in 100 ns can be studied on the ELYSE (lysis by electrons) platform at Institute de Chimie Physique, Orsay, France [Belloni, 2005], which was used in the present study.

The subject of study are fullerlenols (C₆₀(OH)_n) with OH groups on their surface, as they are water-soluble derivatives of C₆₀ more suitable for possible use in medicine. In my lecture, the first results of picosecond pulse radiolysis on fullerlenols in water solution are presented, their activity with LEE and their potential in radiosensitizing role in chemo-radiotherapy.

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ELECTROCHEMISTRY FOR MEDICAL AND FORENSIC SCIENCE. DETERMINATION OF ILLICIT DRUGS AND BIOLOGICALLY ACTIVE COMPOUNDS USEFUL FOR THE TREATMENT OF PSYCHIATRIC DISEASES

Mgr. Marta Choińska-Młynarczyk

prof. Ing. Tomáš Navrátil, Ph.D.

Medicine and forensic science is one of the most challenging. It requires very sensitive, selective, and fast methods of determination. On the other hand, the equipment should be easy to manufacture and handle, as well as it should give repeatable and accurate information. 3D-printed electrodes fulfill all of these requirements which indicates the huge development of techniques based on them. From year to year, they are more popular in medical and forensic research.

Because of the fast development of 3D-printed electrochemistry, I decided to use it in my doctoral thesis for the determination of biologically active compounds. I decided to use in my research compounds that can be used as treatment and illicit drugs, especially psilocybin (and its derivative psilocin) and lysergic acid diethylamide. Each of them has high potency and may be used hallucinogenic compound or as a pain relief drug, antidepressant and anti-anxiety drug or to decrease addiction.

In my lecture, I will present the last results from my research concentrated on LSD, psilocin, and psilocybin determined at laboratory-manufactured carbon fiber-PLA electrodes.

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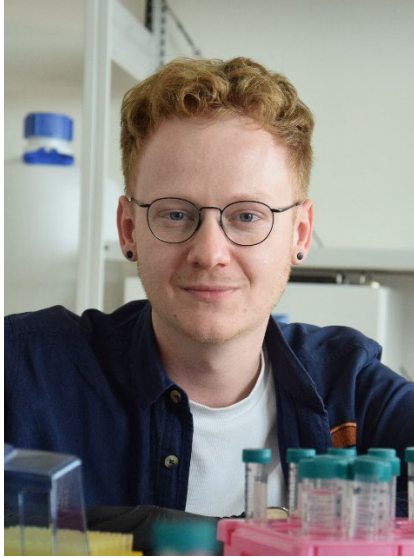


REDUCTION AND LARGE-AREA MICROSCOPIC MONITORING OF CONTAMINATION LEVELS OF TRANSFERRED CVD GRAPHENE

Ing. Martin Jindra

Mgr. Otakar Frank, Ph.D.

The key step in the industrial preparation of graphene-based devices is the transfer of the graphene grown by chemical vapor deposition (CVD) from the metal catalyst onto technologically relevant substrates. The standard transfer technique involves using a supporting polymer layer [typically poly(methyl methacrylate), PMMA], which, after its removal, leaves residual contamination that negatively affects the graphene's physical properties. Thus, we explored the ability of basic organic solvents (acetone, isopropanol, methanol and their combinations) to clean the transferred graphene layers and investigated techniques for monitoring their contamination at the macroscale. All of the more intense cleaning procedures resulted in a lower level of surface contamination compared to the commonly used acetone-based approach. Atomic force microscopy (AFM) and micro-Raman spectroscopy (mRS) revealed lower roughness and charge doping with the increased level of cleaning, respectively. At the macroscopic level, ellipsometric contrast micrography (ECM) and Brewster angle microscopy (BAM) showed the level of contamination directly. In terms of contamination monitoring, the advantage of ECM and BAM, compared to the AFM or mRS techniques, is their screening velocity, which can easily exceed $5 \text{ mm}^2 \text{ min}^{-1}$ with micrometre resolution, which allow us to easily scan the whole sample area. Therefore, these techniques could be an important part of future industrial graphene-based technologies.



CONTROLLED ASSEMBLY OF NOBLE METAL NANOPARTICLES AND FLUOROPHORES FOR SUB- DIFFRACTION MANIPULATION OF LIGHT TO STUDY PLASMONIC LIGHT MODULATIONS

Mark Niklas Hansen, MSc.

Doc. Ing. Vladimíra Petráková, Ph.D.

Various photonic phenomena rely on precise positioning of photon sources in close arrangements with nanometer precision. Here, we construct a versatile platform for the controlled assembly of plasmonic nanoparticles and fluorophores to study the modulations and enhancement of light emitted by the plasmon-coupled fluorophore. We employ DNA nanotechnology for this effort, taking advantage of the programmable nature of DNA spatial configuration. By using the DNA origami technique, nanoparticles of different shape, size, and material can be precisely spatially arranged.

In contrast to traditional organic fluorophores, we also show the potential of our structures to utilize nitrogen-vacancy (NV) center-containing nanodiamonds. Since NV centers possess broad absorption and emission, a large Stokes shift, and are resistant to photobleaching, they are ideal candidates for exploring the phenomena observed in plasmon-coupled fluorophores.

We confirm successful assembly of a variety of nanostructures by Atomic Force Microscopy and Transmission Electron Microscopy, as well as preliminary optical characterization attempts. In the future, we are planning to investigate the plasmonic enhancement of coupled NV centers and potential shifts in their projected position based on the assembly design.

NATURE OF THE INTERACTION BETWEEN ssDNA-LOADED CATIONIC LIPID NANOPARTICLES (cLNPs) AND GIANT UNILAMELLAR VESICLES (GUVs) IN MEMBRANE FUSION

MSc. David Davidović

Doc. RNDr. Radek Šachl, Ph.D.

Lipid nanoparticles (LNPs) have shown great potential as nucleic acids delivery vehicles, but with limited efficacy. In order to successfully deliver cargo to the cytosol, LNPs need to overcome the challenge of membrane fusion-mediated escape from endosomal compartments. However, the mechanism that drives this process is not yet fully grasped. In this work, the interaction of cationic lipid-containing LNPs with the negatively charged lipids on the surface of the endosomal-mimicking giant unilamellar vesicles (GUVs) was studied employing a wide variety of Fluorescence methods, both Microscopy and Spectroscopy. We investigated the extent and kinetics of membrane fusion between the two structures as a function of LNPs with various helper lipid contents. We characterized the internal structure of novel formulations of LNPs and we showed the importance of the LNPs' lipid composition on their fusogenic properties. By studying this model system, we gain insights into how LNPs are trapped and processed at the anionic endosomal membrane prior to nucleic acids release. This could foster the identification of new strategies to improve the efficacy of LNP-based gene delivery systems.



INVESTIGATING THE IN-MEMBRANE FUNCTIONAL/DYSFUNCTIONAL PROTEIN OLIGOMERIZATION IN FGF2 TRANSLOCATION ON VESICLES

Vandana, MSc

doc. RNDr. Radek Šachl, Ph.D.

Fibroblast Growth Factor 2 (FGF2) is a protein that has many extracellular roles, such as wound healing, cell differentiation or metastasis. It is highly produced and released by malignant cells during tumorigenesis. FGF2 is secreted from cells via an unconventional secretory pathway. In the presence of phosphatidylinositol-4,5-bisphosphate PI(4,5)P₂ lipids, FGF2 oligomerises in the membrane, followed by in-membrane oligomerisation and pore formation. These are the critical steps in FGF2 translocation through the membrane. To study the protein pore formation process, we used synthetic free-standing lipid bilayers known as giant unilamellar vesicles (GUVs) to explore protein oligomerisation. We used a lipid bilayer with a complex composition mimicking that of plasma membranes.

The Dual(+1) FCS approach can investigate protein oligomerisation in the (in-)membrane. To distinguish functional oligomers from non-functional aggregates, we present a single statistical molecule and individual vesicle assay for determining the brightness of individually diffusing in-membrane oligomers and correlating their oligomerisation state with membrane pore formation. Importantly, time-dependent membrane pore development was studied using a group of single vesicles. This research shows that assessing oligomeric states alone does not provide a comprehensive knowledge of the structure-function connection of membrane-inserted oligomers. This approach allows for the correlation of in-membrane protein surface concentration change with the oligomeric state change. And also helps us to correlate membrane permeability with the pore state.

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DEVELOPMENT OF NEW SUBSTRATES FOR SUPER- RESOLUTION STUDIES OF SUPPORTED LIPID BILAYERS (SLB) BY GRAPHENE INDUCED ENERGY TRANSFER

Mgr. Hüseyin Evci

Mgr. Jan Sýkora, Ph.D.

Fluorescence microscopy is a widely used technique in biological research. Intrinsically it suffers from low spatial resolution on the order of hundreds of nanometers in lateral plane and several microns in the axial direction. A recent rapid development of novel techniques achieved nano-metric resolution in lateral dimension.¹ In contrast, there still exists a high demand for robust techniques shrinking the axial resolution to the desired nanometer scale. One of the most promising approaches is Graphene Induced Energy Transfer (GIET) developed by Prof. Enderlein group.² In brief, fluorescence is quenched in a distance-dependent manner by the atomically-thin graphene sheet. As the range of the energy transfer occurs up to ~ 30 nm, for instance lipid bilayers with the thickness of 5 nm can be resolved with the GIET technique in detail. Here, I attempt to fabricate the graphene based supports for the formation of lipid bilayers, which would enable to study glycosylation, vesicle formation, or receptor desensitization by GIET. Specifically, the graphene supports are cushioned with Pyrene-PEG polymer, where pyrene interacts with the graphene and PEG helps to minimize the effect of the graphene on the bilayer behavior. The experiments were focused on the formation of the supported lipid bilayers (SLB) containing negatively charged lipids on these newly prepared substrates and the lateral mobility in SLBs were characterized.

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SEMINÁŘ STUDENTŮ ÚFCH JH 2023

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