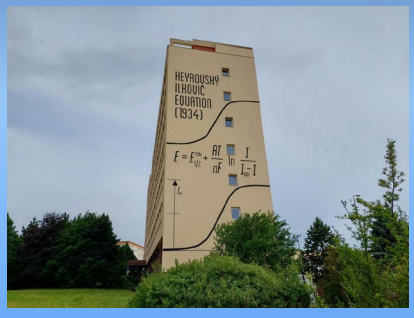
SEMINÁŘ STUDENTŮ ÚFCH JH *2024*



Ústav Heyrovského v Praze

21.5. 2024

Seminář studentů 2024

Sborník příspěvků

ze studentské konference konané
21. května 2024
v ÚFCH J. Heyrovského v Praze

Student Seminar 2024

Collection of abstracts

of all lectures given at the student conference
held on 21May 2024
in Heyrovský Institute in Prague

Seminář studentů 2024
Sborník příspěvků ze studentské konference
konané 21. května 2024
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
Místo a rok vydání: Praha, 2024
Publikace neprošla jazykovou úpravou

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

Bachelor and diploma students (4)
Diplomanti a zájemci z řad bakalářů (4)

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

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

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

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

High school student in project Open Science AS CR

Zajac Václav (*Středoškolský stážista v projektu Otevřená věda AVČR, lektor: M. Jindra)*

PhD Students:
Studenti DSP studia (19)

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

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Jindra Martin *(školitel O. Frank)*

Johanovská Zuzana *(školitel M. Hof)*

Kocábková Barbora *(školitel M. Fárník)*

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Martinka Jakub *(školitel J. Pittner)*

Matoušek Mikuláš *(školitel L. Veis)*

Melčák Martin *(školitel S. Záliš)*

Nguyen Truong An *(školitel Š. Timr)*

Paldusová Kateřina *(školitel M. Cebecauer***)**

Sahu Satyam *(školitel M. Velický)*

Samanta Madhav *(školitel Š. Timr)*

Sedmidubská Barbora *(školitel J. Kočišek)*

Simkovičová Karolina *(školitel Š. Vajda)*

Smeliková Valerie *(školitel M. Kalbáč)*

Referees:

Eva Krupičková Pluhařová
Michal Horáček
Jan Sýkora

SEMINÁŘ STUDENTŮ 2024

PROGRAM– úterý 21. května 2024

STUDENT SEMINAR 2024

PROGRAM - Tuesday May 21, 2024

	Předseda-jící/ ***chairman***	*Přednášející/* ***lecturer***	*Název/* ***prezentation title***
9:00-9:10	**Zahájení konference „Seminář studentů 2024“** *Opening of Annual conference "Seminar of Students 2024"*		
9:10-9:25	**Valerie Smeliková**	Marek Beneš *(VŠCHT Praha, školitelka R. Sokolová)*	STUDY OF THE DEGRADATION MECHANISM OF THE NEW PSYCHOACTIVE SUBSTANCE 25E-NBOH
9:25-9:40		Karolina Fárníková *(VŠCHT Praha, školitelka E. Krupičková Pluhařová)*	COMPUTATIONAL MODELLING OF CO_2 REDUCTION BY COBALTPORPHYRIN CATALYST
9:40-9:55		Petr Vítek*(VŠCHT Praha, školitel S. Valtera)*	OXIDATIVE DEHYDROGENATION OF CYCLOHEXENE ON ATOMICALLY PRECISE $Cu_{5-X}Pd_X$ ($0 \leq X \leq 5$) CLUSTERS
9:55-10:10		Daniel Myšák *(VŠCHT Praha, školitelka E. Krupičková Pluhařová)*	COMPUTATIONAL MODELLING OF GLUTAMATE DEHYDROGENASE IN CROWDED ENVIRONMENT WITH FOCUS ON THE ACTIVE SITE
10:10-10:45	**PŘESTÁVKA NA KÁVU A ZÁKUSEK *(Coffee break in lobby)***		
10:45-11:00	**Barbora Kocábková**	Martin Jindra *(školitel O. Frank)*	LOCALIZED RAMAN SPECTROELECTROCHEMISTRY OF 2D MATERIALS: NOVEL TECHNIQUE FOR STUDYING CHARGE TRANSFER PROCESSES
11:00-11:15		Václav Zajac *(stážista Otevřené vědy AV ČR, lektor M. Jindra)*	PŘÍPRAVA MONOVRSTEV UHLÍKU A JEJICH MODIFIKACE POMOCÍ KONTROLOVANÉ TVORBY DEFEKTŮ
11:15-11:30		Kateřina Paldusová *(školitel M. Cebecauer)*	UNRAVELLING THE ULTRASTRUCTURE OF NEUTROPHIL EXTRACELLULAR TRAPS
11:30-11:45		Oleksandra Labzova *(školitel T. Navrátil)*	A NEW HOLLOW FIBER-BASED LIQUID-PHASE MICROEXTRACTION METHOD FOR THE DETERMINATION OF ANTIHYPERTENSIVE DRUG LERCANDIPINE IN BIOLOGICAL SAMPLES
11:45-12:00		Jakub Martinka *(školitel J. Pittner)*	A SIMPLE APPROACH TO ROTATIONALLY INVARIANT MACHINE LEARNING OF A VECTOR QUANTITY
12:00-13:00	**PŘESTÁVKA (OBĚD NENÍ NA KONFERENCI ZAJIŠTĚN)** *(time for a lunch)*		
13:00-13:15		Valerie Smeliková *(školitel M. Kalbáč)*	INVESTIGATION OF DEFECTS IN 2D MATERIALS USING RAMAN SPECTROSCOPY

13:15-13:30	**Jozef Ďurana**	Michaela Hanušová *(školitel M. Velický)*	METAL-ASSISTED EXFOLIATION OF TMDC 2D MATERIALS IN DIFFERENT ENVIRONMENTS
13.30-13:45		Mikuláš Matoušek *(školitel L. Veis)*	QUANTUM CHEMISTRY WITH CAVITY QED EFFECTS
13:45-14:00		Zuzana Johanovská *(školitel M. Hof)*	MEMBRANE TENSION AND ITS EFFECT ON NANODOMAINS AND OTHER MEMBRANE PROPERTIES
14:00-14:15		Samanta Madhav *(školitel Š. Timr)*	EXPLORING THE CONFORMATIONAL TRANSITIONS OF ADENYLATE KINASE IN A CROWDED MILIEU
14:15-14:45	**PŘESTÁVKA NA KÁVU A ZÁKUSEK *(Coffee break in lobby)***		
14:45-15:00	**Jakub Martinka**	Jozef Ďurana *(školitel M. Fárník)*	INTERACTION OF NAPHTHALENE CLUSTERS WITH LOW-ENERGY ELECTRONS
15:00-15:15		Barbora Kocábková *(školitel M. Fárník)*	ELECTRON ATTACHMENT TO TRICHLOROACETIC ACID CLUSTERS
15:15-15:30		Seyed A. M. Bukhari *(školitel O. Frank)*	INVESTIGATING THE IMPACT OF HELIUM ION IRRADIATION ON TWO-DIMENSIONAL MATERIALS WITH VARIOUS SUBSTRATES
15:30-15:45		Satyam Sahu *(školitel M. Velický)*	DYNAMIC TUNING OF MOS_2 PHOTOLUMINESCENCE VIA THICKNESS MODULATION OF CRSBR IN VAN DER WAALS HETEROSTRUCTURE
15:45-16:00		Daniela G. B.Campoy *(školitel J. Sýkora)*	GRAPHENE INDUCED ENERGY TRANSFER AND ITS APPLICATION IN BIOMEMBRANE RESEARCH
16:00-16:15	**PŘESTÁVKA**		
16:15-16:30	**Zuzana Johanovská**	Hüseyin Evci *(školitel J. Sýkora)*	IONIC STRENGTH AND SOLUTION COMPOSITION DICTATE THE ADSORPTION OF CELL-PENETRATING PEPTIDES ONTO PHOSPHATIDYLCHOLINE MEMBRANES
16:30-16:45		Karolina Simkovičová *(školitel Š. Vajda)*	BRIDGING THE GAP BETWEEN NANO AND SUBNANO CATALYSTS FOR EFFICIENT CO_2 CONVERSION
16:45-17:00		Nguyen Truong An *(školitel Š. Timr)*	ROLE OF OLIGOMERIZATION STATE IN CONFORMATIONAL TRANSITIONS OF HUMAN PLATELET PHOSPHOFRUCTOKINASE
17:00-17:15		Barbora Sedmidubská *(školitel J. Kočišek)*	RRX-001 MOLECULE AND ITS INTERACTIONS WITH SECONDARY LOW-ENERGY ELECTRONS
17:15-17:30		Martin Melčák *(školitel S. Záliš)*	TRYPTOPHAN TO TRYPTOPHAN HOLE HOPPING IN AN AZURIN CONSTRUCT
17:30-17:40	**UZAVŘENÍ KONFERENCE -** *V SÁLE RUDOLFA BRDIČKY* *Closing ceremony (in Brdička Hall)*		
17:40-18:30	**VEČEŘE K UKONČENÍ KONFERENCE** *(VE VESTIBULU)* ***(Dinner in lobby)***		

STUDY OF THE DEGRADATION MECHANISM OF THE NEW PSYCHOACTIVE SUBSTANCE 25E-NBOH

Marek Beneš

Doc. RNDr. Romana Sokolová, Ph.D.
Doc. Martin Kuchař, Ph.D.

This work is focused on the study of in vitro degradation of 25E-NBOH 4-ethyl-2,5-dimethoxy-(N-(2-hydroxybenzyl))phenethylamine (Fig.1.) by electrochemical and spectroelectrochemical methods. The aim is to design the first products and to propose a mechanism for their formation.

Substances of the NBOH group were synthesized for the first time in 2010 with expected applications in medicine. These compounds are very potent agonists of 5HT-serotonin receptors and have quite uncommon combination of hallucinogenic and stimulative effect. The substance 25E-NBOH is currently often abused as an affordable alternative to LSD. The exact mechanism of degradation of 25E-NBOH has not yet been discovered and since proton and electron transfers play an important role in metabolism, electrochemical research on oxidation and discovery of the first products may help to reveal it.

During the lecture, results of cyclic voltammetry and spectroelectrochemistry experiments will be discussed and the proposed mechanisms of generated degradation products will be presented.

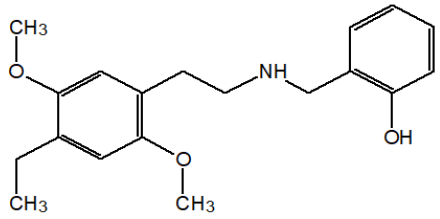

Fig.1.: Chemical structure of 25E-NBOH

Acknowledgement:
This work has been done under the internal support of the J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences (RVO: 61388955).

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COMPUTATIONAL MODELLING OF CO_2 REDUCTION BY COBALTPORPHYRIN CATALYST

Bc. Karolína Fárníková

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

The increasing carbon dioxide (CO_2) levels in the atmosphere correlated with global warming are challenge for humanity. Therefore, there has been an effort to either reduce its production or capture it and use it further [1, 2]. The second option can be realized by catalyzed electrochemical reduction, which leads to various products. To facilitate the electrochemical reduction many catalysts are currently under development.

In our research, we have focused on the details of the catalytic mechanism of the reduction of CO_2 to carbon monoxide, its energetics and how the catalyst can be tuned by alkali metal ions. The catalyst used was a cobalt porphyrin cage. We employed DFT calculations in continuum solvent to model chemical transformation, and classical molecular dynamics where the catalyst is solvated in aqueous solutions of various salts to study the interactions between the catalyst and ions with atomistic resolution. Our results can contribute to optimization and tuning of an environmentally interesting catalyst.

References:

[1] Yu, K. M.; Curcic, I.; Gabriel, J.; Tsang, S. C., Recent advances in CO2 capture and utilization. ChemSusChem 2008, 1 (11), 893–899.
[2] Sun, S.; Sun, H.; Williams, P. T.; Wu, C., Recent advances in integrated CO2 capture and utilization: a review. Sustainable Energy Fuels 2021, 5, 4546–4559.

OXIDATIVE DEHYDROGENATION OF CYCLOHEXENE ON ATOMICALLY PRECISE $Cu_{5-x}Pd_x$ ($0 \leq x \leq 5$) CLUSTERS

Petr Vítek

Ing. Stanislav Valtera

In this study, atomically precise $Cu_{5-x}Pd_x$ ($0 \leq x \leq 5$) clusters on zirconia (ZrO_2) support were tested during oxidative dehydrogenation (ODH) of cyclohexene. The subnanometer size of the clusters gives them different properties compared to bulk materials. They are not only composition-dependent [1] but also size-dependent [2], which offers a vast possibility of modifying their behavior. The support has a significant effect on the final nanocatalyst properties through the cluster-support interaction by influencing charge transfer between the cluster and the support [3].

To investigate the composition role in the cluster activity and selectivity, the cluster size was kept constant at exactly five atoms. During testing, we focused on changes in the obtained activity and selectivity between clusters with different composition. As predicted, the swapping of one atom in a cluster had a significant effect on their properties, altering their activity while maintaining high selectivity toward benzene.

References:

[1] Valtera S.; Jašík J.; Vaidulych M.; Olszówka J.; Zlámalová M.; Tarábková H.; Kavan L. and Vajda Š.; The Journal of Chemical Physics **2022**, 156

[2] Jašík J.; Valtera S.; Vaidulych M.; Bunian M.; Lei Y.; Halder A.; Tarábková H.; Jindra M.; Kavan L.; Frank O.; Bartling S. and Vajda Š., Faraday Discuss **2023**, 242, 70–93

[3] Xinzhe L.; Sharon M.; Yiyun F.; Jun L.; Perez-Ramirez J.; Jiong L.; Nature Reviews Chemistry **2023**, 7, 754–767

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

Daniel Myšák

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

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

Using all-atom classical molecular dynamics [1] we simulated Glutamate dehydrogenase (GDH), an important enzyme in the metabolic branching point of all living organisms [2]. Our model systems contained bovine GDH trimer under various conditions (pH, crowder – glucose, dextran) [3]. We characterized motion of the protein domains surrounding the active site, variety of possible active site conformations as well as different substrate conformations. Next, we obtained spatially resolved picture of the crowder molecules around the protein. We discuss the effect of the environment on the above-mentioned quantities and compare with experimental data. These observations can help to explain how enzymes behave in cell's crowded environment.

References:

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LOCALIZED RAMAN SPECTROELECTROCHEMISTRY OF 2D MATERIALS: NOVEL TECHNIQUE FOR STUDYING CHARGE TRANSFER PROCESSES

Ing. Martin Jindra

Mgr. Otakar Frank, Ph.D.

Previous studies on the Raman spectroelectrochemistry of graphene have primarily utilized samples with poorly defined characteristics, which has limited the clarity and applicability of the results.

This research introduces a microdroplet setup that addresses these limitations by enabling precise localization of measurements on the basal plane of graphene crystals. This localized approach not only resolves issues related to sample definition but also enhances the quality of spectroscopic data.

Utilizing this novel setup, we have observed defect-related processes during charge transfer events in graphene, which are crucial for understanding its electrochemical properties. Furthermore, for the first time, our method provides access to the anti-Stokes region in Raman spectroelectrochemistry, offering new insights into the understanding of vibrational processes.

This experimental breakthrough opens up new fields for further in-depth studies of graphene and, potentially, other two-dimensional materials.

References:

Jindra M.,Velický M.,Bouša M., Abbas G., Kalbáč M. and Frank O., *The Journal of Physical Chemistry Letters* **2022** *13* (2), 642-648, DOI: 10.1021/acs.jpclett.1c03466

Abbas G., Sonia F. J., Jindra M., Červenka J., Kalbáč M., Frank O. and Velický M., *The Journal of Physical Chemistry Letters* **2023** *14* (18), 4281-4288 DOI: 10.1021/acs.jpclett.3c00814

PŘÍPRAVA MONOVRSTEV UHLÍKU A JEJICH MODIFIKACE POMOCÍ KONTROLOVANÉ TVORBY DEFEKTŮ

Václav Zajac

Ing. Martin Jindra

Strukturní defekty hrají klíčovou roli v modifikaci fyzikálních vlastností materiálů. Tato práce se zabývá přípravou monovrstev grafenu a možnostmi jejich modifikace pomocí kontrolované tvorby defektů. Vzorky exfoliovaného grafenu byly charakterizovány Ramanovou spektroskopií a mikroskopií atomárních sil a následně modifikovány pomocí kyslíkového plazmatu a ozonu. Během jednotlivých experimentů byly měněny podmínky expozice monovrstev grafenu kyslíkovému plazmatu a ozonu a byl pozorován vliv těchto podmínek na koncentraci defektů v grafenu C_D^2 na jeho povrchové vlastnosti (topografie, adheze aj.). Na závěr je srovnána praktická využitelnost obou metod, včetně jejich výhod a nevýhod.

References:

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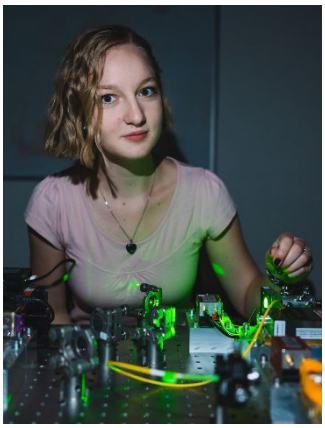
Práce v rámci středoškolské stáže v projektu Otevřená věda AV ČR.



UNRAVELLING THE ULTRASTRUCTURE OF NEUTROPHIL EXTRACELLULAR TRAPS

Mgr. Kateřina Paldusová

Marek Cebecauer, PhD.

Neutrophils are the most abundant white blood cells in human body. They represent the first line of immune defence against pathogens and other malfunctions. While combating microbes, neutrophils employ several mechanisms: phagocytosis, degranulation, and NETosis. Although NETosis was first described in 2004 [1], there is still a lot of unknown about this process. The basic principle of NETosis is in the release of neutrophil extracellular traps (NETs) consisting of DNA and antimicrobial proteins, e.g., neutrophil elastase (NE) and myeloperoxidase (MPO). Two main types of NETosis have been proposed. Lytic type is characterised by the rupture of plasma membrane and expulsion of nuclear and granular contents in the form of pre-assembled NETs. During vital NETosis, neutrophils release the DNA and granular content via vesicular pathway while maintaining their plasma membrane integrity. In this case, NETs assemble extracellularly [2]. Our hypothesis is that the molecular ultrastructure of NETs differs with respect to the mechanism of their origin, inducing stimulus, and local physico-chemical conditions such as temperature and/or oxido-reductive disbalance associated with inflammation. We are planning to employ a panel of chemical and bacterial stimuli, immuno-biochemical assays and high-end super-resolution microscopy techniques to confirm (or negate) our hypothesis.

References:

1. Brinkmann, V., Reichard, U., Goosmann, C., Fauler, B., Uhlemann, Y., Weiss, D.S., Weinrauch, Y., Zychlinsky, A., 2004. Neutrophil Extracellular Traps Kill Bacteria. Science 303, 1532–1535. https://doi.org/10.1126/science.1092385
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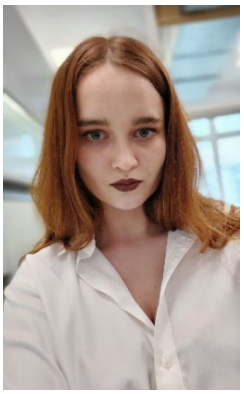

A NEW HOLLOW FIBER-BASED LIQUID-PHASE MICROEXTRACTION METHOD FOR THE DETERMINATION OF ANTIHYPERTENSIVE DRUG LERCANDIPINE IN BIOLOGICAL SAMPLES

Labzova Oleksandra, MSc.

Assoc. Prof. Ing. Renáta Šelešovská, Ph.D.

Prof. Ing. Tomáš Navrátil, Ph.D.

Lercanidipine (LCN) is a new calcium entry-blocking agent used in the treatment of hypertension. Some patients have a poor absorption of LCN, which is manifested by an increased concentration of LCN in their urine. A sufficiently sensitive, rapid, and simple method for the determination of LCN allows objective treatment monitoring and dosage optimization. Several chromatographic and spectrophotometric methods have been developed for the determination of LCN in clinical samples, mostly using expensive, complicated, and bulky equipment, e.g. HLPC/MS/MS. This study aimed to develop a sufficiently sensitive and inexpensive method for the determination of LCN in clinical samples using hollow fiber-based liquid phase microextraction (HF-LPME) in combination with square wave voltammetry (SWV) on a screen-printed boron-doped diamond electrode (SP-BDDE). HF-LPME is an environmentally friendly sample preparation method using disposable porous polypropylene tubes as a liquid membrane support with a surprisingly good synergy with electrochemical detection - SWV at SP-BDDE is highly sensitive, while HF-LPME provides the necessary sample cleanup. Moreover, due to the relatively low polarity of LCN (log $P_{(octanol/water)}$ = 6.4), high preconcentration factors can be achieved. The optimum conditions were SWV with amplitude 0.075 V, potential step 0.004 V, and frequency 10 Hz; and HF-LPME with donor solution pH 7, acceptor solution pH 3, dodecane as supported liquid membrane, extraction time 30 min and stirring speed 500 rpm. Under the optimized conditions, the limits of quantification and detection were 1.1 and 3.3 nmol L^{-1}, respectively. The applicability of the developed method was verified on human urine, blood serum, and blood plasma spiked with 20 and 100 nmol L^{-1} LCN.

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Acknowledgments

This research has been supported by The University of Pardubice (Project No. SGSFChT_2024_003).

A SIMPLE APPROACH TO ROTATIONALLY INVARIANT MACHINE LEARNING OF A VECTOR QUANTITY

Mgr. Jakub Martinka

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

Machine learning of potential energy surfaces is well-established approach, especially for electronic ground state. Simulations including excited states present additional challenge, due to the requirement of calculating nonadiabatic coupling, which has a vectorial form. Vector or tensor properties depend on the orientation of the molecule, and ML predictions need to be invariant (covariant) with respect to rotation. If the properties cannot be obtained by differentiation, as is the case for energy gradients, special techniques have to be used, or the covariance could, in principle, be achieved automatically by adding many different orientations of the molecule to the training set, which can be very costly.

Various solutions have been proposed, such as constructing an auxiliary scalar quantity for NAD couplings or embedding rotational equivariance into neural network design. In contrast, we present a simpler alternative: a three-step approach utilizing the molecular tensor of inertia. First, the molecule is rotated to its principal axes, ensuring vector properties are computed consistently for ML training. Next, ML model predicts the vector property relative to this orientation using a training set with properties in the principal axes coordinate system. Finally, the ML estimate is transformed back to the original orientation, ensuring proper covariance. We tested this technique using MLatom and Newton-X on the 1,2-dichloroethane molecule's dipole moment along MD trajectories.

References:

Y. Zhang, J. Jiang, B. Jiang (2023), Machine learning, Dipole moments, Multipole moments, Polarizability, Tensorial properties, In. P. O. Dral (Ed.), *Quantum Chemistry in the Age of Machine Learning*, (pp. 453-465).

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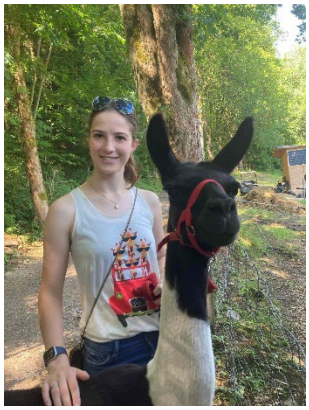

INVESTIGATION OF DEFECTS IN 2D MATERIALS USING RAMAN SPECTROSCOPY

Ing. Valerie Smeliková

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

Two-dimensional (2D) materials are a class of materials with exceptional properties due to their unique structure. They typically consist of one individual layer with a thickness on the atomic level. In recent years, they have gained considerable attention thanks to their exclusive properties and the associated almost unlimited application potential, for example in nanotechnology, electronics, sensor technology and energy storage. The structure of 2D materials are often presented as an ideal crystal with no imperfections, however presence of defects is inevitable and defects can play a significant role for the performance of any device [1,2]. In certain cases, the presence of a specific type of defect is desirable as it can be used to achieve certain specific capabilities of a 2D material [1].

Raman spectroscopy emerges as a powerful tool for probing and characterizing defects in 2D materials. By analyzing the vibrational modes of the material, Raman spectroscopy provides valuable insights into the presence and nature of defects, offering a non-destructive and sensitive means of defect detection [3]. One possible procedure for creating defects is to expose the 2D material to ion beam or plasma in ultra-high vacuum (UHV) environment, which ensures minimal interference from impurities and provides an ideal platform for precise control of experimental conditions. As defects in graphene can be efficiently studied by Raman spectroscopy we used graphene as a probe for investigating defects in MoS_2/graphene heterostructure. In this vein we exposed both materials to the same doses of ions and study in detail how specific number of defects affects Raman spectra of both materials.

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METAL-ASSISTED EXFOLIATION OF TMDC 2D MATERIALS IN DIFFERENT ENVIRONMENTS

Mgr. Michaela Hanušová

Ing. Matěj Velický Ph.D.

Transition-metal dichalcogenides (TMDC) 2D materials have captured significant attention due to their electronic, mechanical and optoelectronic properties unattainable in their bulk form.[1,2]

While various methods for obtaining monolayers have been explored, achieving large-scale production of high-quality TMDC monolayers remains challenging. Mechanical exfoliation seems to be the way to produce high-quality monolayers. In addition, gold-assisted mechanical exfoliation has been shown to be a scalable and efficient method for producing large-area monolayers. Although other metals could potentially lead to successful exfoliation, their tendency to oxidize in air-prepared samples limits their applicability.[3,4]

Herein, we investigate the metal-assisted exfoliation of TMDCs under different conditions, including ambient, controlled atmosphere and ultrahigh vacuum (UHV). We explore the influence of the exfoliation method on the quality of the monolayers, interfacial strain, charge doping and heterogeneity at the interface.

In my presentation, I will discuss the characterization of the interface using a combination of Raman spectroscopy, atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM).

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QUANTUM CHEMISTRY WITH CAVITY QED EFFECTS

Mgr. Mikuláš Matoušek

RNDr. Libor Veis, Ph.D.

Although the DMRG method originated in solid state physics, it has also been successful in quantum chemistry, where it provides an excellent description of strongly correlated electrons. For linear molecules, DMRG offers superior performance to other multireference methods, while for other problems it can still give results on par with QMC or selected-CI.

We took the MOLMPS program[1] developed in our group, which can run massively parallel DMRG calculations, and generalized it, so it can use general Hamiltonians with multiple particle types. Such Hamiltonians occur in many areas of quantum chemistry, one example being non-Born-Oppenheimer quantum chemistry, where DMRG was first used by M. Reihers group[2]. Here the wavefunction includes one or more hydrogen nuclei, which therefore are treated at the quantum level. The second quantized Hamiltonian then contains not only creation and annihilation operators for the electrons, but also for the nuclei.

Further options where we need to introduce new particle into the Hamiltonian include exotic molecules containing other subatomic particles, such as positrons[3]. The advantage of our code is that it is written to be general, not focusing on a single Hamiltonian, and as such allows for implementation of new Hamiltonians easily, without need to introduce changes into the code. In this presentation, we will show how our implementation works and demonstrate its performance on a new challenging problem.

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MEMBRANE TENSION AND ITS EFFECT ON NANODOMAINS AND OTHER MEMBRANE PROPERTIES

Mgr. Zuzana Johanovská

Prof. Martin Hof

Micromanipulation technique brings quite new, so far not fully explored possibilities to biomembrane research, as it enables direct modifications of membrane mechanical properties of giant unilamellar vesicles (GUVs), simulating cellular membranes.

Thus we can study protein membrane interactions, structure of the membrane and other various phenomena occurring within the periphery of the cells.
These experiments can be carried out for example by aspiration of GUVs into thin microcapillaries (diameter in range of ca 6 to 10 μm) and thus affecting their membrane tension.

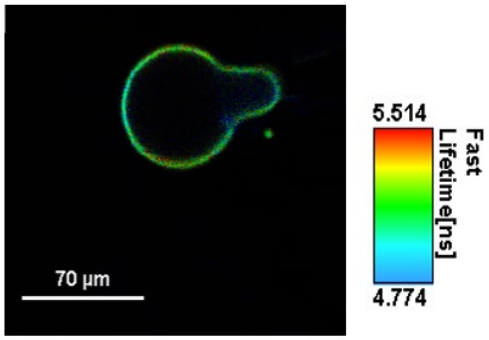

Fig. 1 FLIM image of aspirated GUV

The combination of micromanipulation with other methods such as fluorescence microscopy allows us to open the door to exciting experiments. Especially we are interested in the combination of the micromanipulation technology with our frequently used method MC-FRET (connection of Monte Carlo simulations and time resolved experimental measurements of FRET), which allows us to detect and characterize membrane lipid clustering and formation of lipid nanodomains under various mechanical conditions.

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EXPLORING THE CONFORMATIONAL TRANSITIONS OF ADENYLATE KINASE IN A CROWDED MILIEU

MSc. Madhav Samanta

Mgr. Štěpán Timr, Ph.D.

Inside living cells, enzymes are exposed to a highly crowded and complex environment. These conditions, which are far from those in conventional in-vitro assays, can alter enzyme activity in non-trivial ways. To understand these effects, detailed insights from molecular simulations are highly desirable.

In this work, we employ all-atom molecular dynamics (MD) simulations to investigate the impact of molecular crowding on adenylate kinase (AK3L1) as a model enzyme. We describe how crowding affects conformational changes and substrate binding, which are linked to enzyme activity.

The results help to rationalize previous experimental observations reporting altered kinetic parameters of adenylate kinase in the presence of crowding. Our study is a step towards a better understanding of enzyme behavior within the complex milieu of living cells.

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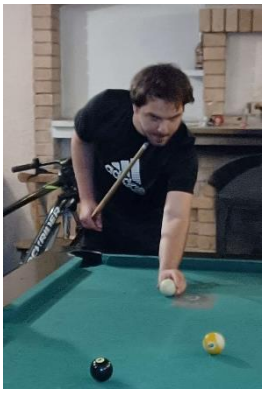

INTERACTION OF NAPHTHALENE CLUSTERS WITH LOW-ENERGY ELECTRONS

Mgr. Jozef Ďurana

doc. Mgr. Fárník Michal Ph.D., DSc.

Naphthalene (Np) is a simple astrochemically relevant polycyclic aromatic hydrocarbon. In our present study, we focus on its clusters [1].

We generate the clusters in a supersonic expansion of naphthalene with various buffer gasses (He, Ne, Ar, Kr) under different expansion conditions and probe them via time-of-flight mass spectroscopy.

After a low-energy electron attachment, Np_n^- anions ($n \geq 3$) are observed in the mass spectra. The monomer anion Np^- is not present at all (due to its negative electron affinity), and the dimer is only observable in co-expansion with Ar and Kr at higher expansion pressures, where the mixed neutral clusters Np_nRg_m (Rg = Ar, Kr) are formed. This occurrence suggests the formation of the naphthalene dimer anion through the electron attachment to a mixed cluster and subsequent evaporation of the rare gas atoms.

We conclude that naphthalene dimer anion cannot be produced by the electron attachment directly to the isolated naphthalene dimer, instead, it requires a stabilization by evaporation of the rare gas atom(s) from the mixed clusters. Thus, the naphthalene dimer anions observed in previous experiments were formed under conditions, where frequent collisions occurred and most likely the dimer anions were stabilized by the collisions [2].

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ELECTRON ATTACHMENT TO TRICHLOROACETIC ACID CLUSTERS

Ing. Barbora Kocábková

Assoc. Prof. Michal Fárník

Even though the use hydrochlorofluorocarbons (HCFCs) is being abandoned, residues of those compounds will be present in the environment for several more generations due to their chemical resilience. One of the degradation products is trichloroacetic acid (TCA, CCl_3COOH) formed in the atmosphere during oxidative degradation of HCFCs. We explore interactions of TCA molecules and clusters with low energy electrons, particularly the electron attachment (EA) and dissociative electron attachment (DEA).

The experiment was done using the CLUB apparatus. Particle beam was produced by a continuous supersonic co-expansion of sample vapors with a buffer gas (Ar or He) through a 90 μm wide conical nozzle. Helium was used to generate a beam of individual molecules, while clusters were formed in argon. After low energy electron attachment, the beam was probed with reflectron time-of-flight mass spectrometer.

The dominant dissociation process after the electron attachment (DEA) is the C—Cl bond cleavage resulting in Cl^- anion. This pathway by far dominates all other dissociation reactions in the isolated TCA molecule, namely HCl + CO_2 dissociation yielding CCl_2^-, HCl evaporation leading to CCl_2COO^-, and H abstraction resulting in CCl_3COO^-. On the contrary, the cluster series is dominated by the H abstraction channel yielding $TCA_n{\cdot}CCl_3COO^-$ series with *n* up to about 5. Thus the clustering changes the DEA process significantly switching the major dissociation pathway towards the one of the weakest populated in the isolated molecule. This interesting effect of the environment on the intramolecular chemistry will be discussed.

INVESTIGATING THE IMPACT OF HELIUM ION IRRADIATION ON TWO-DIMENSIONAL MATERIALS WITH VARIOUS SUBSTRATES

Adeel Bukhari

Supervisor - Otakar Frank

Structural defects in two-dimensional materials (2DM) present an as of yet unanswered question in terms of their influence on the properties of materials. Since the concentration of defects present in a 2DM has been shown to impact their behaviour, creating defect-engineered 2DMs provides another avenue towards devices tailor-made for specific applications.[1]

Here we introduce defects in precise positions, with controlled fluences, in monolayers of molybdenum disulfide (MoS_2) and platinum diselenide ($PtSe_2$) using helium ion microscopy.[2] We characterise the dependence of the optical, electrical, and mechanical properties of the 2DM on the concentrations of defects created with a range of methods that include optical spectroscopies and atomic force microscopy-based methods such as kelvin probe force microscopy.[3]

Gaining further insight into the role that structural defects play in determining the behaviour of a 2DM brings us one step closer to rational design when it comes to tailoring the properties of defect-engineered 2DMs.

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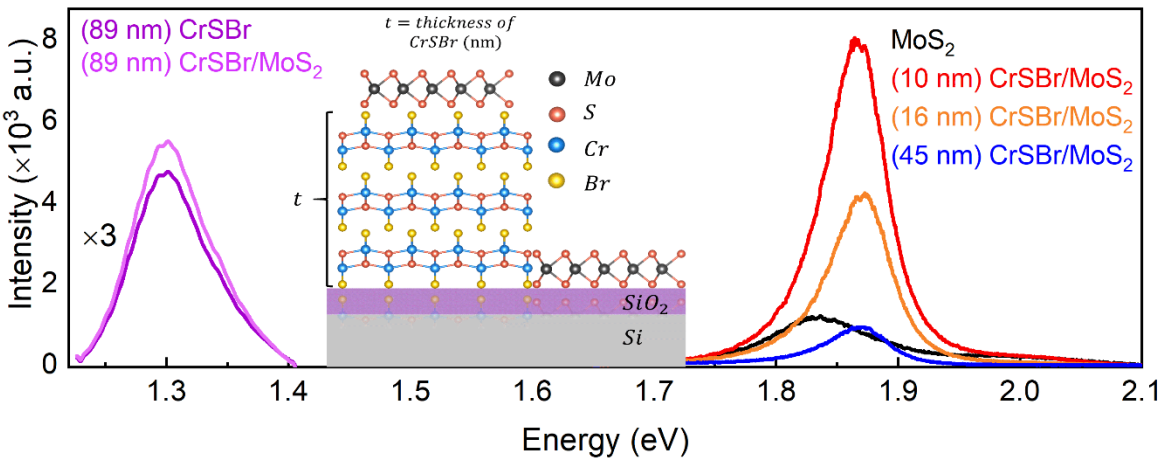
DYNAMIC TUNING OF MoS_2 PHOTOLUMINESCENCE VIA THICKNESS MODULATION OF CrSBr IN VAN DER WAALS HETEROSTRUCTURE

Satyam Sahu M.Sc.

Dr. Matěj Velický, Supervisor

Dr. Otakar Frank, Co-supervisor

This study investigates the tunability of photoluminescence (PL) properties of molybdenum disulphide (MoS_2) in a heterostructure composed of MoS_2 and chromium sulphide-bromide (CrSBr). By systematically varying the thickness of CrSBr in proximity of MoS_2 and employing various spectroscopic techniques, we explore the dynamic modulation of the MoS_2 PL intensity and spectral composition. Our findings reveal intriguing changes in MoS_2 PL behaviour correlated with different thicknesses of CrSBr, shedding light on potential tailoring of the optoelectronic functionalities within van der Waals heterostructures. This work contributes to the understanding of the interplay between 2D materials and offers insights for future applications in optoelectronic devices.



GRAPHENE INDUCED ENERGY TRANSFER AND ITS APPLICATION IN BIOMEMBRANE RESEARCH

MSc Daniela Guadalupe Blanco Campoy

Jan Sýkora, PhD

In recent years, super-resolution microscopy techniques have seen a tremendous revolution with respect to spatial details. In order to study lipid bilayers which is a highly dynamic self-assembly, with a typical thickness of approximately 5 nm, a high axial spatial resolution is required. Graphene Induced Energy Transfer (GIET) belongs to one of the methods that can resolve axial distances of fluorescent emitters with nanometer resolution. This technique relies on graphene induced fluorophore quenching, which results in reducing its lifetime in a distance dependent manner. The resolving power of GIET is tremendous enabling to distinguish the membrane organization in bottom and top leaflets.

In our research we aim to design and fabricate the substrates suitable for GIET studies on Supported Lipid Bilayer (SLB). For this purpose, we employ the graphene sheet attached to the glass support being covered with Pyrene-Polyethylene Glycol (PEG) cushions. For the optimal SLB formation we have tested several PEG polymers with different lengths, different terminal functional groups and various ways of preparation to prevent the interactions of the lipid molecules with the glass support. The proper SLB deposition has been verified by combination of fluorescence techniques: fluorescent recovery after photobleaching (FRAP) and Fluorescence Correlation Spectroscopy (FCS) to monitor the lateral mobility of labeled lipid, and fluorescence lifetime imaging (FLIM) to address the thickness of the formed lipid system attached to the substrate.

The herein designed systems can be potentially used for manifold biophysical applications, such as the study of motility and coupling of asymmetric bilayers, lipid flip-flop between leaflets in a single bilayer, or of the interaction of fluorescently labeled peptides and proteins with lipid bilayers.

Acknowledgements. Grant Nr. 22-25953S provided by the Czech Science Foundation

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IONIC STRENGTH AND SOLUTION COMPOSITION DICTATE THE ADSORPTION OF CELL-PENETRATING PEPTIDES ONTO PHOSPHATIDYLCHOLINE MEMBRANES

Mgr. Hüseyin Evci

Mgr. Jan Sýkora, Ph.D.

Interaction between arginine-rich positively charged peptides with neutral zwitterionic phosphocholine (PC) bilayers is a key step in the translocation of those potent cell-penetrating peptides into the cell interior. In the past, it is shown both theoretically and experimentally that polyarginines (R9) adsorb to the neutral PC-supported lipid bilayers in contrast to polylysines (K9). Recent contributions showed some contradictions in characterizing this interaction[1,2]. Therefore, we systematically studied the interaction between R9 or K9 peptides and the POPC bilayer by means of fluorescence cross-correlation spectroscopy (FCCS) experiments and aided by molecular dynamics (MD) simulations. Using FCCS experiments with R9 and K9 fluorescently labeled with Oregon Green 488 and POPC liposomes stained with Atto633-DOPE, we first demonstrated that the binding of R9 to POPC is tighter by almost 2 orders of magnitude compared to that of K9. Finally, upon the addition of an excess of either Na+ or Ca2+ ions with R9, the total fluorescence correlation signal is lost, which implies the unbinding of R9 from the PC bilayer, in agreement with the predictions from MD simulations. Support from Grant 22-25953S from the Czech Science Foundation is greatly acknowledged.

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BRIDGING THE GAP BETWEEN NANO AND SUBNANO CATALYSTS FOR EFFICIENT CO_2 CONVERSION

Mgr. Karolína Simkovičová

RNDr. Štefan Vajda, CSc. Dr.habil.

The production of value-added products (e.g., methane, methanol, etc.) from carbon dioxide and hydrogen offers a promising avenue for sustainable energy production and CO_2 utilization. However, under mild conditions, CO_2 hydrogenation presents a significant challenge due to the high stability of the CO_2 molecule. In recent years, significant research efforts have been devoted to exploring novel catalytic systems for this conversion process. In this presentation, we will focus on bridging the gap between nanosized and subnanometer-sized catalysts to enhance the efficiency and selectivity of CO_2 conversion.

Firstly, we will discuss the activity of micro-mesoporous iron oxide supported CuO nanoparticles. This catalyst exhibits high surface area and enhanced dispersion of active sites, promoting efficient CO_2 activation and subsequent hydrogenation reactions. The combination of Cu and Fe is taking advantage of copper's ability to activate hydrogen and promoting hydrogen spillover, and iron oxide's role in Fischer-Tropsch synthesis by the in-situ generated Fe_5C_2 for yielding longer hydrocarbon chains [1].

Secondly, we will delve into the emerging field of subnanometer-sized supported clusters. By tailoring the size and composition of clusters, the electronic and geometric properties of the clusters can be fine-tuned, thereby enabling the proper adjustment of their catalytic activity and selectivity. This can be further enhanced by the synergy of different metals within bimetallic clusters [2]. In a previous study, it was shown that Cu_4 clusters are active in methanol synthesis [3] and a recently published study on bimetallic tetramer clusters predicted that the substitution of one Cu atom with an atom of Pd can efficiently tailor the catalytic properties of the cluster-based catalysts [4]. Hence, we utilize a combination of Cu and Pd in tetramer clusters to study their catalytic activity in CO_2 conversion.

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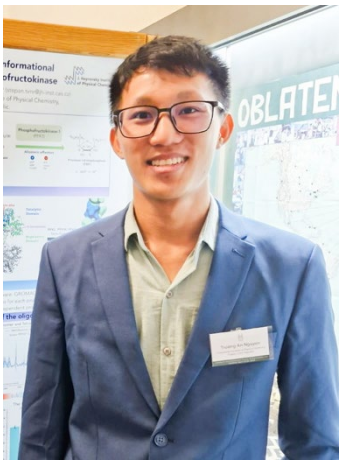

ROLE OF OLIGOMERIZATION STATE IN CONFORMATIONAL TRANSITIONS OF HUMAN PLATELET PHOSPHOFRUCTOKINASE

Truong An Nguyen

Mgr. Štěpán Timr Ph.D.

Glycolysis is a crucial metabolic pathway which is subjected to regulation via a range of mechanisms and the disturbances of which have been linked with diseases. The enzyme Phosphofructokinase-1 (PFK1), catalyzes the rate-limiting conversion of fructose-6-phosphate to fructose-1,6-bisphosphate, is a key flux controller of the glycolytic pathway. However, a full mechanistic understanding of this regulation, which has been suggested to involve changes in the oligomerization state of the enzyme, is still lacking. Here we perform fully atomistic molecular dynamics simulations of the human platelet PFK1 isoform (PFKP) in several different oligomerization and ligand-binding states. Our extensive simulations show that the conformational flexibility of functionally relevant parts of the PFKP structure is significantly altered by changes in the oligomerization state. Moreover, by delivering a state-dependent correlation network analysis, the work forms a basis for a deeper understanding of the allosteric regulation of PFKP. The aim is to provide detailed microscopic insights into the mechanisms underlying PFK1 function and its isoform-specific regulation.

RRX-001 MOLECULE AND ITS INTERACTIONS WITH SECONDARY LOW-ENERGY ELECTRONS

Barbora Sedmidubská, Ing.

Mgr. Jaroslav Kočišek, PhD
Ing. Marie Davídková CSc.

The molecule of RRx-001 ($C_5H_6BrN_3O_5$, 2-Bromo-1-(3,3-dinitroazetidin-1-yl)ethan-1-one) is studied for use in chemoradiotherapy (phase 3 in clinical studies- final phase before licence), due to its minimal toxicity and property to make tumor cells radiosensitive [Oronsky, 2021]. Such molecule is called radiosensitizer and causes the effect of chemoradiotherapy to be as high as possible, so-called synergistic. But what are the reaction mechanisms contributing to the already proven synergism in the case of this molecule?

Our goal is to study these processes and obtain information that could help with the design of novel radiosensitizers. RRx-001 contains one bromine and two nitro groups with high electron affinities, playing chemically interesting roles when competing for incoming low-energy electrons (LEE). In the case of electron-affine molecules, the synergism can have a source in the interaction of such a molecule with very reactive secondary LEE forming in large quantities during water radiolysis after irradiation of living tissue [Sanche, 2009].

Therefore, in the present study, we focus mainly on the reactivity of RRx-001 with secondary LEE. For this, we also use the technique of pulse radiolysis. It utilizes short pulses of highly accelerated electrons to irradiate the solution, followed by the formation of secondary species. These species, including LEE, are detected using transient absorption spectroscopy. Relative concentrations of secondary species are measured as a function of time. Processes occurring in orders of picoseconds up to nanoseconds can be studied on the ELYSE (lysis by electrons) platform at the Institute de Chimie Physique, Orsay, France [Belloni, 2005], which was used in the present study.

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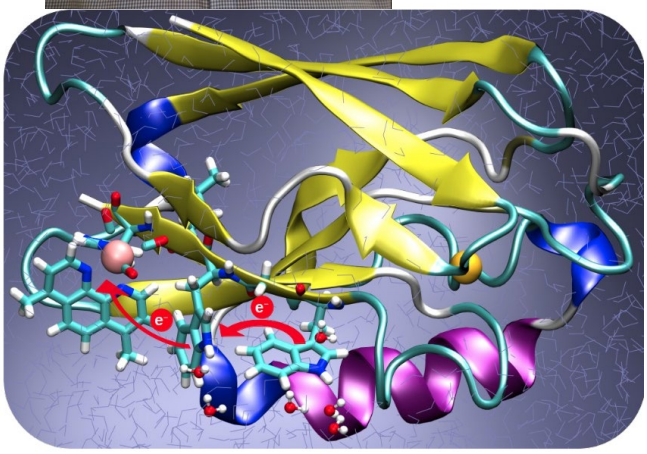
TRYPTOPHAN TO TRYPTOPHAN HOLE HOPPING IN AN AZURIN CONSTRUCT

Ing. Martin Melčák

doc. RNDr. Mgr. Jan Heyda, Ph.D.
Ing. Záliš Stanislav CSc.



Azurine enzymes present ideal systems to investigate the factors controlling multistep electron transfer (hole hopping). Gaining deeper understanding of these mechanisms presents an opportunity to reveal principles leading to the design of materials capable of efficient photochemical charge separation for light energy conversion and/or photocatalysis.

In this work, electron transfer (ET) between neutral and cationic tryptophan residues in the azurin construct [Re^{I}(H126)-$(CO)_3$(dmp)](W124)(W122)Cu^{I} (dmp = 4,7-Me_2-1,10-phenan-throline) was investigated by Born−Oppenheimer quantum mechanics/molecular mechanics/molecular dynamics (QM/MM/MD) simulations [1].

More specifically, we focused on $W124^{\bullet+}$ ← W122 ET, which is the middle step of the photochemical hole-hopping process between Rhenium dye at the protein surface and a copper in the protein interior: $*Re^{II}(CO)_3(dmp^{\bullet-})$ ← W124 ← W122 ← Cu^{I}. For this sequential hopping process nearly 10,000-fold acceleration over single-step tunneling was reported [2].

In accordance with experiments, UKS-DFT QM/MM/MD simulations identified forward and reverse steps of $W124^{\bullet+}$ ↔ W122 ET equilibrium, as well as back ET from $W124^{\bullet+}$ that restores the initial $*Re^{II}(CO)_3(dmp^{\bullet-})$ state [3].

Simulations were further used to characterize stability and hydration of individual electronic states and to identify a sensitive correlation between ET probability (hopping yield) and relative orientations of $Re(CO)_3$(dmp) and W124.

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SEMINÁŘ STUDENTŮ ÚFCH JH 2024

Sál Rudolfa Brdičky a vestibul
Ústavu Heyrovského v Praze

21.5.2024