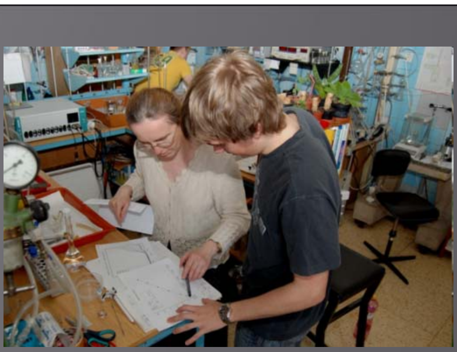

SEMINÁŘ STUDENTŮ ÚFCH JH 2018

Sál Rudolfa Brdičky
ÚFCH JH AV ČR
12. - 13. 6. 2018

Seminář studentů ÚFCH JH 2018

Sborník příspěvků

ze studentské konference konané
12. - 13. června 2018
v sále Rudolfa Brdičky, ÚFCH JH v Praze

Seminar of Students of JHI 2018

Collection of abstracts

of all lectures given at the student conference
held on 12-13 June 2018
in Rudolf Brdička Hall in JHI, Prague

Seminář studentů ÚFCH JH 2018
Sborník příspěvků ze studentské konference
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v sále Rudolfa Brdičky, ÚFCH JH v Praze

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Tisk: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i. Dolejškova 2155/3,
182 23 Praha 8
Vydání: první
Místo a rok vydání: Praha, 2018
Publikace neprošla jazykovou úpravou

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SEMINÁŘ STUDENTŮ ÚFCH JH 2018

PROGRAM 1. dne konference - úterý 12.6.2018

SEMINAR OF STUDENTS JHI 2018

PROGRAM - Tuesday June 12, 2018

	Předseda-jící/ chairman	*Přednášející/ lecturer*	*Název/ title of the prezentation*
8:50	**Zahájení konference „Seminář studentů ÚFCH JH 2018“** *Opening of Annual conference "Seminar of Students JHI 2018"*		
9:00-9:10	*Představení prezentujících z Odd. teoretické chemie* *(Jiří Pittner)* *Presentation of lecturers from the Dep. of Theoretical Chemistry*		
9:10-9:30	**Adam Pastorek**	Jan BRANDEJS *(II. ročník PGS, školitel L. Veis)*	MULTIREFERENCE COUPLED CLUSTERS CORRECTED BY DENSITY MATRIX RENORMALIZATION GROUP
9:30-9:50		Dan BÍM *(III. ročník PGS, školitel M. Srnec)*	BEYOND THE CLASSICAL THERMODYNAMIC CONTRIBUTIONS TO H ATOM ABSTRACTION REACTIVITY
9:50-10:10		Dávid HVIZDOŠ *(II. ročník PGS, školitel R. Čurík)*	DEVELOPMENT OF THEORY FOR THE DISSOCIATIVE RECOMBINATION OF DIATOMIC CATIONS
10:10-10:25		Kamila RIEDLOVÁ *(I. ročník PGS, školitel L. Cwiklik)*	STUDIUM VLIVU ZVOLENÝCH LÉČIV NA MODELU LIPIDOVÉ VRSTVY SLZNÉHO FILMU LIDSKÉHO OKA
10:25-11:00	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** *(Coffee break)*		
11:00-11:10	*Představení prezentujících z Odd. nízkodimenzionálních systémů* *(Martin Kalbáč)* *Presentation of lecturers from the Dep. of Low-dimensional Systems*		
11:10-11:25	**Jan Brandejs**	Lea ASSIES *(diplomantka, školitel M. Kalbáč)*	THERMODYNAMICALLY DRIVEN SELF-ORGANIZATION OF DYNAMIC COVALENT POLYMERS ON GRAPHENE
11:25-11:40		Vladislav BURAVET *(I. ročník PGS, školitel P. Krtil)*	SURFACE SENSITIVITY OF THE FORMALDEHYDE REDUCTION ON TiO_2 CATHODES
11:40-11:55		Jin ZHANG *(I. ročník PGS, školitel M. Shamzy)*	OVERCOMING APPLICATION LIMITATIONS OF GERMANOSILICATE ZEOLITES: POST-SYNTHESISTAILORING THE ACTIVE SITES (change of title)
11:55-12:10		Leoš VALENTA *(diplomant, školitel P. Kovaříček)*	SPATIALLY RESOLVED COVALENT FUNCTIONALIZATION PATTERNS ON GRAPHENE

12:10-12:30		Roman NEBEL *(II. ročník PGS, školitel P. Krtil)*	SURFACE SENSITIVITY OF PHOTO-ELECTROCHEMICAL WATER OXIDATION ON TIO$_2$ (ANATASE) SINGLE CRYSTALS
12:30-13:30	**PŘESTÁVKA NA OBĚD** *(Break for lunch)*		
13:30-13:45	***Roman Nebel***	Rebecca PITTKOWSKI *(I. ročník PGS, školitel P. Krtil)*	RUTHENIUM AND IRIDIUM PYROCHLORES WITH DIFFERENT LANTHANIDES AS CATALYSTS FOR OXYGEN EVOLUTION REACTION (OER)
13:45-14:00		Yuyan ZHANG *(I. ročník PGS, školitel J. Čejka)*	SYNTHESIS OF PT-MWW WITH CONTROLLABLE NANOPARTICLE SIZE
14:00-14:10	*Představení prezentujících z Odd. spektroskopie (Martin Ferus)* *Presentation of lecturers from the Dep. of Spectroscopy*		
14:10-14:25	***Roman Nebel***	Jana HRNČÍŘOVÁ (bakalářka, *školitel M. Ferus)*	VZNIK BIOMOLEKUL NA POVRŠÍCH JÍLŮ V PROSTŘEDÍ RANÉ ZEMĚ A MARSU
14:25-14:40		Antonín KNÍŽEK *(diplomant, školitel M. Ferus)*	EXPERIMENTAL STUDY OF CHEMICAL EVOLUTION OF BIOMOLECULES UNDER EARLY EARTH CONDITIONS
14:40-14:55		Adam PASTOREK *(I. ročník PGS, školitel S. Civiš)*	THE STUDY OF THE INFLUENCE OF GAMMA RADIATION ON THE BIOGENIC MOLECULES' FORMATION
14:55-15:45	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** *(Coffee break)*		
15:45-15:50	*Představení prezentujícího z Odd. molekulární elektrochemie a katalýzy (Michal Horáček)* *Presentation of lecturers from the Dep. of Molecular Electrochemistry and Catalysis*		
15:50-16:05	***Dávid HVIZDOŠ***	David DUNLOP (bakalář, *školitel M. Lamač)*	EXPLORING CYTOTOXIC TITANOCENE DIHALIDES
16:05-16:10	*Představení prezentujícího z Odd. chemie iontů v plynné fázi (zajistí vedoucí oddělení nebo jím pověřená osoba)* *Presentation of lecturers from the Dep. Chemistry of Ions in Gaseous Phase*		
16:10-16:30	***Dávid HVIZDOŠ***	Michal LACKO *(II. ročník PGS, školitel P. Španěl)*	A COMBINED SIFT-MS AND PTR-MS STUDY OF PROTON TRANSFER FROM H_3O^+ TO GLYOXAL
16:30-16:40	*Představení mimosoutěžní kategorie středoškolských studentů (stáže v popularizačně vzdělávacím projektu Tři nástroje představí Květa Stejskalová)* *Presentation of lecturers from secondary schools (stays in educational project Three tools)*		
16:40-16:55	***Jana HRNČÍŘOVÁ***	Kristýna POKORNÁ *(středoškolská stáž, školitel M. Horáček)*	PŘÍPRAVA GUANIDINÁTOVÝCH KOMPLEXŮ ZIRKONIA

16:55-17:10***	***Jana HRNČÍŘOVÁ***	Hugo KOCEK *(středoškolská stáž, školitel M. Cebecauer)*	PREPARATION AND CHARACTERIZATION OF CD4 GLYCOPROTEIN MUTANTS FOR FUNCTIONAL AND IMAGING ANALYSIS ON T-CELLS
17:10-17:25***		Adam ŠIMAREK *(středoškolská stáž, školitel J. Pinkas)*	CHLORACE HYDROSILANŮ S POUŽITÍM KATALYZÁTORU $B(C_6F_5)_3$
17:30	**Ukončení prvního dne konference** *(End of the 1st day of conference)*		

*** Poznámka ke změně: Byla provedena výměna přednášejících (5.6.2018)

PROGRAM 2. dne konference - středa 13.6.2018

PROGRAM - Wednesday June 13, 2018

	Předseda-jící/ chairman	*Přednášející/ lecturer*	*Název/ title of the prezentation*
8:50	**Zahájení 2. dne konference „Seminář studentů ÚFCH JH 2018“** *Opening of the 2nd day of Annual conference "Seminar of Students JHI 2018"*		
8:55-9:00	*Představení prezentujících z Odd. struktury a dynamiky v katalýze (Jiří Dědeček)* *Presentation of lecturers from the Dep. of Structure and Dynamics in Catalysis*		
9:00-9:20	***Eduard JEŠKO***	Mariia LEMISHKA *(II. ročník PGS, školitel J. Dědeček)*	ALFA OXYGEN FOR SELECTIVE OXIDATION OF HYDROCARBONS OVER BINUCLEAR TRANSITION METAL ION STRUCTURES IN ZEOLITES. FTIR SPECTROSCOPY STUDY
9:20-9:40		Eva VANĚČKOVÁ *(III. ročník PGS, školitel J. Rathouský)*	PHOTOCATALYTIC ABATEMENT OF NOX: NITROUS ACID AS EMERGING POLLUTANT
9:40-9:50	*Představení prezentujících z Odd. dynamiky molekul a klastrů (Michal Fárník)* *Presentation of lecturers from the Dep. of Dynamics of Molecules and Clusters*		
9:50-10:05	***Tomáš CHUM***	Dominika KOLLÁROVÁ *(diplomantka, školitel M. Fárník)*	ŠTÚDIUM MOLEKÚL A KLASTROV HEXAFLUOROPROPYLÉN OXIDU (HFPO)
10:05-10:20		Dan REIMITZ *(I. ročník PGS, školitel J. Kočišek)*	ORGANOMETALLIC COMPOUNDS IN THE CONTEXT OF DNA STRAND BREAK INDUCTION DURING IRRADIATION
10:20-10:40		Kateřina GRYGORIEVA *(III. ročník PGS, školitel M. Fárník)*	LONG-TIMESCALE DYNAMICS IN HYDROGEN-BONDED CLUSTERS: STUDY OF VIBRATIONALLY EXCITED $(HBr)_n$ CLUSTERS

10:40-11:15	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** *(Coffee break)*		
11:15-11:25	*Představení prezentujících z Odd. biofyzikální chemie (Mariana Amaro)* *Presentation of lecturers from the Dep. of Biophysical Chemistry*		
11:25-11:40	***Kateřina GRYGORIEVA***	Ivo VINKLÁREK *(I. ročník PGS, školitel R. Šachl)*	FRET REVEALS INTER-LEAFLET COUPLED NANODOMAINS IN LIPID BILAYERS OF GIANT UNILAMELLAR VESICLES
11:40-12:00		Martin PIŽL *(II. ročník PGS, školitel S. Záliš)*	VIBRATIONAL SPECTRA OF TRANSITION METAL COMPLEXES: AN ANHARMONIC APPROACH
12:00-12:15		Kristián SKÁLA *(I. ročník PGS, školitel R. Šachl)*	PREPARATION OF PROAPOPTOTIC PROTEIN BAX
12:15-12:35		Tomáš CHUM *(PGS student, školitel M. Cebecauer)*	THE IMPACT OF PROTEIN TRANSMEMBRANE SEGMENT ON PROTEIN LOCALISATION IN LIVING CELLS
12:35-13:45	**PŘESTÁVKA NA OBĚD** *(Break for lunch)*		
13:45-14:05	***Martin PIŽL***	Eduard JEŠKO *(II. ročník PGS, školitelka M. Amaro)*	INVESTIGATING THE INTERACTION BETWEEN THE PRION PROTEIN AND MODEL MEMBRANES BY FLUORESCENCE CORRELATION SPECTROSCOPY
14:05-14:10	*Představení prezentujících z Odd. elektrochemických materiálů (Otakar Frank)* *Presentation of lecturers from the Dep.of Electrochemical Materials*		
14:10-14:25	***Martin PIŽL***	Martin JINDRA *(bakalář, školitel O. Frank)*	IN-SITU SPECTROSCOPY METHODS TOWARDS BETTER UNDERSTANDING OF STRESS AND CHARGE TRANSFER MECHANISMS IN 2D-3D SYSTEMS
14:25-14:40		*Jaroslava ŘÁHOVÁ (I. ročník PGS, školitel O. Frank)*	LOCAL PHOTOCURRENT CHARACTERIZATION OF GRAPHENE-SILICON SCHOTTKY JUNCTION
14:40-15:15	**PŘESTÁVKA NA KÁVU A ZÁKUSEK** *(Coffee break)*		
15:15-15:25	*Představení prezentujících z Odd. elektrochemie v nanoměřítku (Magda Hromadová)* *Presentation of lecturers from the Dep. of Electrochemistry in Nanoscale*		
15:25-15:45	***Mariia LEMISHKA***	Anna MAKRLÍKOVÁ *(III. ročník PGS, školitel T. Navrátil)*	ELECTROCHEMICAL METHODS FOR DETERMINATION OF HOMOVANILLIC, VANILLYLMANDELIC, AND 5-HYDROXYINDOLE-3-ACETIC ACIDS IN HUMAN URINE
15:45-16:00		Michal NOVÁK *(I. ročník PGS, školitelka M.Hromadová)*	CHARACTERIZATION OF PRISTINE AND Si - MODIFIED Zr SURFACE BY ATOMIC FORCE MICROSCOPY AND ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY
16:00-16:20		Štěpánka SKALOVÁ *(III. ročník PGS, školitel T. Navrátil)*	DOXORUBICIN HYDROCHLORIDE AND ITS DETERMINATION IN A MICRO VOLUME CELL USING DIFFERENTIAL PULSE CATHODIC STRIPPING VOLTAMMETRY

16:20-16:40	***Mariia LEMISHKA***	Vojtěch HRDLIČKA *(III. ročník PGS, školitel T. Navrátil)*	HOLLOW FIBRE MICROEXTRACTION AND VOLTAMMETRIC DETECTION OF HOMOVANILLIC AND VANILLYLMANDELIC ACID
16:40-17:15	**PŘESTÁVKA** *(Break)*		
17:15	**SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ KONFERENCE -** *V SÁLE RUDOLFA BRDIČKY* *Closing ceremony - results announcement (in Brdička Hall)*		
17:30	**SLAVNOSTNÍ VEČEŘE K UKONČENÍ KONFERENCE** *(VE VESTIBULU)* *(Dinner in lobby)*		

Seznam prezentujících studentů (35)

Kategorie I (18)

Diplomanti. magistři a zájemci z řad bakalářů (7)

Assies Lea *(diplomantka, školitel M. Kalbáč)*

Dunlop David *(bakalář, PřF UK, školitel M. Lamač)*

Hrnčířová Jana *(bakalářka, PřF UK, školitel M. Ferus)*

Jindra Martin *(bakalář, VŠCHT, školitel O. Frank)*

Knížek Antonín *(diplomant, PřF UK, školitel M. Ferus)*

Kollárová Dominika *(diplomantka, VŠCHT, školitel M. Fárník)*

Valenta Leoš *(diplomant VŠCHT, školitel P. Kovaříček)*

Studenti 1. ročníku DSP (11)

Buravet Vladislav *(školitel P. Krtil)*

Novák Michal *(školitekal M. Hromadová)*

Pastorek Adam *(školitel S. Civiš)*

Pittkowski Rebecca *(školitel P. Krtil)*

Reimitz Dan *(školitel J. Kočišek)*

Riedlová Kamila *(školitel L. Cwiklik)*

Řáhová Jaroslava *(školitel O. Frank)*

Skála Kristián *(školitel R. Šachl)*

Vinklárek Ivo *(školitel R. Šachl)*

Zhang Jin *(školitelka M.Shamzy)*

Zhang Yuyan *(školitel J. Čejka)*

Mimosoutěžní kategorie (3)

Středoškolští stážisté:

Kocek Hugo *(Gymnázium Nad Štolou, Praha 7, školitel M. Cebecauer)*

Pokorná Kristýna *(Gymnázium Roudnice nad Labem, školitel M. Horáček)*

Šimarek Adam *(MSŠCH Praha 1, školitel J. Pinkas)*

Kategorie II (14)

Studenti 2. ročníku DSP (7)

Brandejs Jan *(školitel L. Veis)*

Ješko Eduard *(školitelka M. Amaro)*

Hvizdoš Dávid *(školitel R. Čurík)*

Lacko Michal *(školitel P. Španěl)*

Lemishka Mariia *(školitel J. Dědeček)*

Nebel Roman *(školitel P. Krtil)*

Pižl Martin *(školitel S. Záliš)*

Studenti 3. ročníku DSP (6)

Bím Daniel *(školitel M. Srnec)*

Grygoryeva Kateřina *(školitel M. Fárník)*

Hrdlička Vojtěch *(školitel T. Navrátil)*

Makrlíková Anna *(školitel T. Navrátil)*

Skalová Štěpánka *(školitel T. Navrátil)*

Vaněčková Eva *(školitel J. Rathouský)*

Studenti 4. a vyšších ročníků DSP (1)

Chum Tomáš *(školitel M. Cebecauer)*

Hodnotící komise:

Michal Fárník
Jaroslav Kočišek
Petr Kovaříček

THERMODYNAMICALLY DRIVEN SELF-ORGANIZATION OF DYNAMIC COVALENT POLYMERS ON GRAPHENE

Lea Assies

Ing. Petr Kovaříček, Ph.D.,
RNDr. Ing. Martin Kalbáč, Ph. D.

Dynamic polymers, “dynamers”, employ reversible linkages either directly in the polymer backbone or as crosslink between the individual chains.[1] Lately, conjugated polymer semiconductors, containing extended π-systems, are of big interest, because they can be doped into electrically conducting state,[2] they are flexible and processable in solution and thus show great potential for optoelectronic and electrochemical devices.[3] From the numerous covalently dynamic bonds identified so far, imines are one of the very few species providing a double bond, which is needed if an extended conjugation is required upon polymer formation.[4]

The goal of the project is to synthesize dynamic conjugated polymers, which selectively assemble on graphene into periodic structures. For this purpose, bifunctional aromatic aldehyde monomers with long aliphatic side-chains have been synthesized, condensed with diamines and the reaction conditions optimized. The synthesized polymers have been characterized in solution as well as on the surface and the dynamic character of the polymer was demonstrated. Deposition of the polymers was carried out by spincoating and then compared to layers prepared by on-surface reaction. Self-assembly on the molecular scale was studied by scanning probe microscopies. Using photolithography, patterned graphene has been prepared and used as a confined 2D space in which the polymerization can take place. Setting the spatial boundaries should promote directionality of the polymerization and thus lead to highly ordered polymers on the surface with periodic assembly over a long distance, similarly to the small molecule physisorption on graphite governed by the free energy of adsorption, i.e. both the adsorption enthalpy and entropy loss on adsorption.[5]

References:

[1] **a)** N. Roy, B. Bruchmann, J.-M. Lehn, *Chem. Soc. Rev.* **2015**, *44*, 3786-3807; **b)** M. Kathan, P. Kovaříček, C. Jurissek, A. Senf, A. Dallmann, A. F. Thünemann, S. Hecht, *Angew. Chem., Int. Ed.* **2016**, *55*, 13882-13886.

[2] C. R. Hauer, G. S. King, E. L. McCool, W. B. Euler, J. D. Ferrara, W. J. Youngs, *J. Am. Chem. Soc.* **1987**, *109*, 5760-5765.

[3] A. Fallahi, M. Alahbakhshi, E. Mohajerani, F. Afshar Taromi, A. R. Mohebbi, M. Shahinpoor, *The Journal of Physical Chemistry C* **2015**, *119*, 13144-13152.

[4] **a)** S. J. Rowan, S. J. Cantrill, G. R. L. Cousins, J. K. M. Sanders, J. F. Stoddart, *Angew. Chem., Int. Ed.* **2002**, *41*, 898-952; **b)** M. E. Belowich, J. F. Stoddart, *Chem. Soc. Rev.* **2012**, *41*, 2003-2024.

[5] Ciesielski, A.; El Garah, M.; Haar, S.; Kovaříček, P.; Lehn, J.-M.; Samorì, P. *Nat. Chem.* **2014**, *6* (11), 1017–1023.

BEYOND THE CLASSICAL THERMODYNAMIC CONTRIBUTIONS TO H-ATOM ABSTRACTION REACTIVITY

Ing. Daniel Bím

RNDr. Martin Srnec, PhD.

The mononuclear and binuclear non-heme iron (NHFe and $NHFe_2$) enzymes play an essential role in a broad range of biochemical transformations, including, *inter alia*, the functionalization of unreactive C–H bonds of organic substrates. Due to their versatility in Nature, much effort has been devoted to preparation of novel (bioinspired) $NHFe_{(2)}$ catalysts. An important common theme for all of these species is that their chemistry is closely related to their redox properties, which are in turn determined by many factors: variability in oxidation, spin, and protonation states, molecular charges, types of ligands, coordination geometries (ligand fields), and solvent (protein) environments.

Based on our experimentally calibrated methodology for the calculation of reduction potentials of NHFe complexes, we studied the effect of redox properties of selected non-heme $Fe^{IV}O$ species on their H-atom-abstraction reactivity. This allowed us to discover the simple thermodynamic descriptor η, denoted as the “asynchronicity factor”, arising from a differential contributions of redox and acidobasic properties of H-atom acceptor and donor. Being correlated to the reorganization energy λ from Marcus theory of electron transfer, the parameter η represents a new and general concept in reactions involving the hydrogen atom transfer. As such, it provides a straightforward guideline for a tailored design of efficient and selective H-atom-transfer catalysts. Variations in effective redox and acidobasic contributions through the modification of an axial ligand in the coordination sphere of a catalytic site (demonstrated for the large set of non-heme $Fe^{IV}O$ complexes) served as an example of such a strategy.

MULTIREFERENCE COUPLED CLUSTERS CORRECTED BY DENSITY MATRIX RENORMALIZATION GROUP

Mgr. Jan Brandejs

RNDr. Libor Veis, Ph.D.

The single-reference coupled clusters (CC) is nowadays a method of choice for accurate description of weakly correlated molecules.
Nevertheless, the situation is dramatically different for strongly correlated (multireference) systems, where no single Slater determinant dominates the wave function and the usual single reference approaches break down. Since many chemically interesting compounds and particularly reaction intermediates have multireference character, development of methods capable of treating such systems is an important task.

As an example of a method suitable for treating strongly correlated systems, we cite the density matrix renormalization group (DMRG). It is known for its great efficiency for relatively large active spaces and for its ability to precisely capture the static correlation. It is, however, computationally prohibitive to brute-force DMRG to capture dynamic correlation by including all virtual orbitals into the active space. It seems thus interesting to exploit pathways to benefit from the combination of the DMRG with another method.

We consider combining DMRG with CC, in particular multireference Mukherjee's CC — the former robustly describing the static correlation and the latter to obtain the remaining dynamic correlation — with the aim of accurate, balanced, and efficient treatment of both. In our implementation, first a calculation using the DMRG method is done in the active space. A subsequent multireference CC calculation for the rest of the Hilbert space is then able to compute the remaining dynamic correlation absent in DMRG itself.
Most recently we have applied this method to benchmark systems with complex electronic structure, namely cyclobutadiene and tetramethylethylene.

SURFACE SENSITIVITY OF THE FORMALDEHYDE REDUCTION ON TiO_2 CATHODES

Vladislav Buravet, MSc

Doc. Ing. Petr Krtil, CSc.

Carbon dioxide (CO_2) is one of the most important greenhouse gases and represents the largest human contribution to the climate change. Although there are chemical technologies capable of converting the CO_2 to valuable chemicals like fuel (e.g. Fischer-Tropsch process), they remain dependent on fossil fuels both for energy and for the source of hydrogen.

The electrochemistry can in principle provide a technology linking the renewable electricity sources with CO_2 valuation. The CO_2 reduction is a multielectron process which is difficult to control in terms of activity and selectivity. The state of art catalysts are based on Cu and Ag, the potential of non-metal catalyst is poorly understood so far.

TiO_2 has received great attention as a catalyst due to high efficiency, low cost and lack of toxicity. It was shown that TiO_2 (anatase) with different surface orientation possess different catalytic activity in water splitting process[1]. Two types of TiO_2-anatase catalysts, dominated by {001} and {101} surface orientation, were investigated in present work. Catalytic activity on formaldehyde reduction was analyzed as formaldehyde is known to be an intermediate on the pathway of CO_2 reduction[2] so the use of formaldehyde avoids hindrances caused by low solubility of carbon dioxide in aqueous solutions. Products of formaldehyde reduction were detected online using differential electrochemical mass spectroscopy (DEMS) technique.

The reduction of formaldehyde on TiO_2 in 0.1M $KHCO_3$ solution (pH=9.3) is accompanied by vigorous hydrogen evolution reaction (HER). Based on the DEMS data the HER dominates, and the charge efficiency of the formaldehyde reduction on TiO_2 amounts to 26% and 14% on the {001} and {101} surfaces, respectively. Methane and methanol are detected as the main volatile products on both types of surfaces. TiO_2 with {001} surface orientation is determined as catalytically more active. However, TiO_2 with {101} facets shows higher selectivity in the reduction of formaldehyde towards methane and methanol, as higher amounts of these products are created at lower current passing for the formaldehyde reduction.

References

1. Minhová-Macounová, K.; et. al., *The J. Phys. Chem. C*. 2017, *121(11)*, 6024-6032
2. Eggins, B. R.; et. al., *J. Chem. Soc* 1988, *(16)*, 1123-1124.

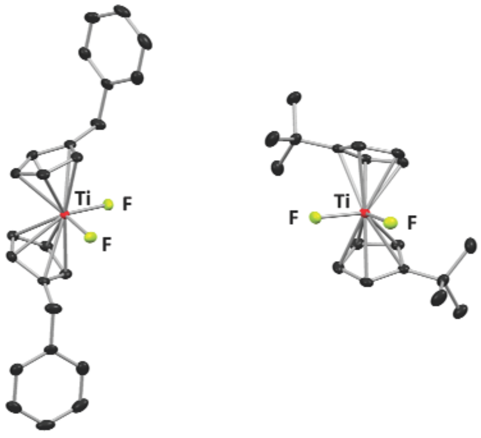
EXPLORING CYTOTOXIC TITANOCENE DIHALIDES

David Dunlop

RNDr. Martin Lamač Ph.D.

Various metallocenes have been shown to possess interesting cytotoxic activity, making them potential anti-tumor agents. The cytotoxic properties of the so called „sandwich complexes" are strongly dependent on both the metals and the fine tuning of their ligands.

The goal of this talk is to share the challenges posed by the synthesis of selected titanocene dihalides and the approaches we have applied to their solution, the results of NMR and X-ray diffraction analysis of the isolated complexes and some of the preliminary results of their cytotoxic parameters.



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Acknowledgements

This work has been supported by the Czech Science Foundation (project no. 17-05838S).

LONG-TIMESCALE DYNAMICS IN HYDROGEN-BONDED CLUSTERS:

STUDY OF VIBRATIONALLY EXCITED $(HBr)_n$ CLUSTERS

Ing. Kateřina Grygoryeva

Doc. Mgr. Michal Fárník, Ph.D., DSc.

Hydrogen bonding is recognized as one of the vital interactions defining structural and dynamical behavior of many systems in physics, chemistry and biology.[1] Its properties can be conveniently studied on hydrogen halide (HX) clusters, which exhibit hydrogen bonding of variable strength decreasing in the row HF–HCl–HBr–HI from almost covalent to nearly van der Waals interactions.[2] Hydrogen halides are relatively simple diatomic molecules, which facilitates the theoretical treatment of their clusters at high ab initio level. Thus $(HX)_2$ dimers served as benchmark systems for ab initio quantum mechanical calculations contributing to the development of the hydrogen bond theory.[3,4]

One of intriguing questions to be answered concerns the flow of energy in these clusters. Specifically, how does vibrational excitation affect the cluster, and what are its relaxation pathways? In this work, we investigate the effect of vibrational excitation on hydrogen bromide clusters $(HBr)_n$ and on their photodissociation dynamics. In particular, we excite one quantum of HBr stretch vibration at wavelengths corresponding to HBr molecules located in various clusters. For comparison, we also excite bare molecules. Free molecules and molecules in clusters are then photodisociated by a UV-laser pulse; their H-fragments are ionized and their velocities are recorded using a Velocity map imaging (VMI) method. VMI images recorded at different delays between IR and UV laser pulses suggest a presence of fast relaxation dynamics in vibrationally excited clusters; however, it cannot be quantified in our experiment with ns resolution. Nevertheless, these images also show a much longer dynamics happening on a slower time-scale: hundreds of nanoseconds.

Acknowledgments:
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HOLLOW FIBRE MICROEXTRACTION AND VOLTAMMETRIC DETECTION OF HOMOVANILLIC AND VANILLYLMANDELIC ACID

Mgr. Vojtěch Hrdlička

Doc. Dr. Ing. Tomáš Navrátil

Homovanillic acid (HVA) and vanillylmandelic (VMA) acid are end-stage metabolites of dopamine and epinephrine in human body. These compounds are biomarkers of various neurological, metabolic and oncological disorders, *e.g.* neuroblastoma, the most common extracranial cancer in infants. The determination of HVA and VMA in human fluids is important for clinical applications as well as for large scale pre-emptive screenings.

Hollow fibre microextraction is a relatively new method for biological sample preparation. The hollow fibres are typically made from thin porous polypropylene (pore diameter 0.2 µm). The fibre serves either as a separator between phases (*e.g.* water/1-octanol) in two phase extraction, or more commonly, as a carrier of a water immiscible liquid membrane. Utilization of liquid membrane in a three-phase system features low consumption of organic phase and possible extraction of ionisable species into aqueous phase. Acidic species are extracted from acidic solution through organic liquid membrane to the basic solution inside the fibre. The aqueous extract is also convenient for subsequent voltammetric detection.

The lecture presents possibilities of HVA and VMA hollow fibre microextraction followed by voltammetric detection. Various aspects of extraction and determination of HVA/VMA in very small volumes or inside the fiber itself will be discussed, including suitable liquid membranes, electrode materials and experimental setup.

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VZNIK BIOMOLEKUL NA POVRŠÍCH JÍLŮ V PROSTŘEDÍ RANÉ ZEMĚ A MARSU

Jana Hrnčířová

RNDr. Martin Ferus, Ph.D

Původ a vznik života je velmi komplikovanou otázkou, kterou se lidstvo snaží vyřešit už celá staletí. Jednou z představ je teorie vědecké abiogenze, jejíž autor je Alexandr Ivanovič Oparin[1]. Teorie abiogeneze vysvětluje vznik života chemickou cestou od formování základních stavebních kamenů biogenních látek, jako jsou například aminokyseliny nebo nukleové báze, až po spontánní vznik prvního živého chemického systému. Oparinova práce byla pouze teoretická a prvního experimentálního ověření se dočkala až v roce 1953 ve slavném Millerově pokusu[2]. Povedlo se nasyntetizovat aminokyseliny a další biomolekuly za prebiotických podmínek – účinky elektrických výbojů na směs chemikálií. Výsledky byly ovšem v konfliktu s představou RNA světa a Centrálním dogmatem molekulární biologie. Vzniku aminokyselin translací musí předcházet vznik nukleových bází transkripcí. Z tohoto pohledu tak detekce aminokyselin znamenala potvrzení syntézy sekundárních produktů metabolismu živých soustav a nikoliv ověření vzniku prvotních chemických látek – bází nukleových kyselin. Naše experimenty se zabývají vznikem nukleových bází termolýzou formamidu s různými druhy jílů v přítomnosti železného meteoritu na rané Zemi či Marsu, kde panovalo před 4 miliardami let prostředí podobné tehdejší Zemi. Jde tedy o objasnění vlivu volného železa v meteoritu a vlivu železa vázaného v jílech vznikajících vodní alterací kráterů po impaktech meteoritů či jiných na železo bohatých hornin a minerálů[3]. Díky kvantově mechanickým výpočtům doktorky Šponerové[4] jsme navrhli reakční schéma, které objasňuje vznik nukleových bází hned několika reakčními cestami prostřednictvím různých meziproduktů, jako jsou aminacetonitril, formamidin nebo dimer formamidu. Ty se nám povedlo spektroskopicky identifikovat ve spektrech termolyzovaných vzorků. Raná Země byla v mnoha ohledech podobná dnešnímu Marsu. Povrch na Marsu je velmi bohatý na obsah železa, zatímco železo na povrchu rané Země, které se sem dostalo i díky impaktům meziplanetární hmoty, která obsahuje více železa než horniny nacházející se na Zemi, se postupem času zakoncentrovalo do jádra planety vlivem deskové tektoniky. Právě vyšší obsah železa v povrchové hornině mohl být důležitým faktorem při vzniku mnoha biomolekul, což se také prokázalo našimi experimenty.

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DEVELOPMENT OF THEORY FOR THE DISSOCIATIVE RECOMBINATION OF DIATOMIC CATIONS

Mgr. Dávid Hvizdoš

Mgr. Roman Čurík, Ph.D.

Dissociative recombination (DR) is a complicated yet highly important process in molecular plasma dynamics. It is the process of neutralization of molecular ions by incoming electrons and their subsequent dissociative breakup. Much of the complexity of this problem stems from the presence of a long-range Coulomb interaction. This makes implementing exact numerical models problematic or downright impossible. DR cross sections are thus typically calculated using approximative methods.

In the previous year we reported on our work [1] that tested the well known frame transformation method [2] adapted to the case of DR using a nuclear basis of Siegert pseudostates [3] and compared it with an exact numerical model for the simple case of H_2^+ DR. The first approach used several additional approximations and came up with decently correct results. There were, however, several discrepancies between the exact and approximative models. We can now show how these discrepancies are caused by two factors: neglecting the energy dependence of quantum defects and using a slightly incomplete nuclear basis. We will also present how the results drastically improve once we overcome these hurdles.

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THE IMPACT OF PROTEIN TRANSMEMBRANE SEGMENT ON PROTEIN LOCALISATION IN LIVING CELLS

Mgr. Tomáš Chum

Mgr. Marek Cebecauer, Ph.D.

Communication of cells with their environment requires surface expression of a palette of receptors. These are synthesized in the endoplasmic reticulum (ER) and need to be transported to the surface. This process, so-called protein sorting, is regulated by specific tags which are not fully understood yet. The length of receptor transmembrane segment is well-established sorting tag but does not apply to all surface receptors. In our previous work, we found that posttranslational lipid modification of proteins, palmitoylation, can serve as a secondary determinant for protein sorting to the surface. We demonstrate exclusive dependence of LAT protein surface expression on palmitoylation but also improved surface expression of artificial palmitoylated receptors in living cells (Chum et al. 2016).

To find out why LAT protein strongly depends on palmitoylation and surface expression of other receptors less, we have performed MD simulation of LAT transmembrane segment. The analysis suggests the presence of two kinks in the α-helix which is the prevalent structure of transmembrane segments of most surface receptors in mammals. The kinks are caused by the presence of two rigid amino acids, prolines, in the helix. The kinks can influence the length of the transmembrane segment and therefore protein sorting. New experiments were designed to test the impact of altered geometry on LAT surface expression. First, kink-forming prolines were mutated to helix-forming alanines in LAT proteins fused to fluorescent proteins. Then, mutant proteins were expressed in human T cells lacking native LAT and imaged using live-cell fluorescence microscopy. We demonstrate that N-terminal proline improves LAT surface expression, but the dominant effect of mutants is their targeting for degradation. Further studies are needed to better understand observed results.

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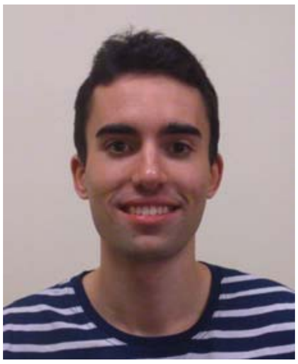

INVESTIGATING THE INTERACTION BETWEEN THE PRION PROTEIN AND MODEL MEMBRANES BY FLUORESCENCE CORRELATION SPECTROSCOPY

Mgr. EduardJeško

Mariana Amaro, Ph.D.

The aberrant aggregation and accumulation of the prion protein are responsible for the onset and progression of prion diseases, also known as transmissible spongiform encephalopathies. Prion diseases are characterized by early synaptic loss, astrocytosis, and progressive neuronal degeneration [1]. They appear to be caused by the intracerebral accumulation of an abnormal isoform of the cellular form of the prion protein, known as prion protein scrapie (PrPsc) [2].

Results from several studies suggest that the trigger mechanism of prion diseases appears to be the interaction between PrPsc and cellular membranes [3]. But the mode of interaction of such proteins with the membranes has not been elucidated yet.

In our work, the interaction between a Prion protein residue (PrP106−126) and model membranes called Giant Unilamellar Vesicles (GUV) is investigated. Several studies have shown that this residue exhibits some of the pathogenic and physicochemical properties of PrPsc [4]. It is protease resistant, forms fibrils and is neurotoxic.

We have been investigating this interaction using Z-scan Fluorescence Correlation Spectroscopy. This is a “state-of-the-art” technique, which allows monitoring the prion protein mobility at a single molecule level. The interactions with various lipid compositions of the GUVs have been tested, focusing mainly on sphingomyelin and negatively charged lipids such as phosphoserines, phosphoglycerols, and gangliosides. The data gathered so far indicates a potential role of the lipid sphingomyelin in the regulation of the interaction of PrP106−126 with the model membranes, which might be of importance for the pathological behavior of the protein.

In addition, zeta-potential measurements were performed in order to better understand the electrostatic properties of the charged model membranes.

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IN-SITU SPECTROSCOPY METHODS TOWARDS BETTER UNDERSTANDING OF STRESS AND CHARGE TRANSFER MECHANISMS IN 2D-3D SYSTEMS

Martin Jindra

Mgr. Otakar Frank Ph.D

Monolayer graphene, in spite of its exceptional properties, cannot act as a standalone element in mechanical applications because of its small bending rigidity. The role of substrate has to be always considered. Consequently, the mechanism of stress transfer between graphene and its support is one of the most important problems to be solved for a successful utilization of graphene in composite materials [1]. One option of graphene usage is to use it as nanofillier in materials based on polymeric matrix. The stress transfer efficiency is evaluated in situ by Raman spectroscopy during uniaxial loading through the cantilever beam technique [2]. The model composites were prepared by hot pressing graphene grown by CVD (Chemical Vapour Deposition) onto PMMA (Polymethylmethacrylate) bars. The stress transfer efficiency of more than ~40% is a promising results considering there is no additional encapsulation of the sample [2].

An important, yet not very studied question related to stress transfer between graphene and its environment is how the charge in the monolayer and at the interface influences their mutual interaction. The simultaneous mechanical loading and charging will be conducted by means of microdroplet spectroelectrochemistry on the cantilever beams. However, several technological issues have to be overcome first to reach repeatable and meaningful results.

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EXPERIMENTAL STUDY OF CHEMICAL EVOLUTION OF BIOMOLECULES UNDER EARLY EARTH CONDITIONS

Mgr. Antonín Knížek

prof. RNDr. Svatopluk Civiš, CSc.
RNDr. Martin Ferus, Ph.D.

Our recent experiments suggest a novel idea that neutral planetary atmosphere containing a mixture of neutral volcanic-type gasses (CO_2, N_2, H_2O) can be converted over acidic mineral catalysts upon irradiation by a soft UV-radiation into a relatively reactive mixture of reducing gases (CH_4, CO), which can be further reprocessed by high-energy chemistry. The resulting mixture (CH_4, CO + N_2) represents a common reducing atmosphere related e.g. to the chemistry of Titan, the largest moon of Saturn, as well as a possible representation of the secondary atmosphere of our planet. Also, photocatalytic reduction of CO_2-rich atmosphere can explain the abiotic origin of methane on current Mars or other terrestrial planets. In our subsequent experiments, corresponding equimolar model mixture of $CH_4 : CO : N_2$ in presence of water vapour was subjected to reprocessing by high-power laser plasma simulating an asteroid impact – one of a series of impact events which the young Earth experienced during the first 600 million years of her history. Upon delivery of in total 3250 J of laser shock-wave energy into the sample, formation of organic molecules closely related to prebiotic chemistry was observed. Among those are the nucleic acid bases of RNA (adenine, uracil, guanine and cytosine), glycine and urea. For the first time, a complete scenario of one pot HCN-based synthesis of all the canonical nucleobases, the simplest amino acid glycine and urea is presented.

Keywords: Origin of life, nucleic acid bases, photocatalytic reduction of carbon dioxide, methane, FTIR spectroscopy

PREPARATION AND CHARACTERIZATION OF CD4 GLYCOPROTEIN MUTANTS FOR FUNCTIONAL AND IMAGING ANALYSIS ON T-CELLS

Hugo Kocek

Marek Cebecauer, PhD

CD4 glycoprotein functions as a receptor on a subset of white blood cells called T-cells. It is important for the development of T-cells and their activation. CD4 also serves as a receptor for the HIV virus. The CD4 molecule contains several potential dimerization motifs in its structure but their function remains unclear.

The goal of this project is to create CD4 variants with specific mutations in these putative dimerization motifs and determine their impact on the receptor membrane organization and oligomerization state. The mutant variants were prepared using **DNA recombination techniques** and further characterized by **DNA sequencing** (*to determine successful mutagenesis at the level of the gene*), **fluorescent confocal microscopy** (*to determine their cell surface expression*) and **Western blotting method** (*to determine the appropriate size of the mutant proteins and potential dimeric state*). All prepared variants exhibited the correct size and were expressed in cells.

These were pre-requisites for the future analysis of membrane organization of CD4 variants using super-resolution imaging and their oligomerization state by fluorescence techniques. We will also verify their capacity to function as a receptor for the HIV virus.

ŠTÚDIUM MOLEKÚL A KLASTROV HEXAFLUOROPROPYLÉN OXIDU (HFPO)

Bc. Dominika Kollárová

doc. Michal Fárník, Ph.D., DSc.
Mgr. Juraj Fedor, Ph.D.
Ing. Andriy Pysaněnko, Ph.D

Hexafluoropropylén oxid (HFPO) je fluorovaný plyn C_3F_6O, ktorý sa používa na syntézu rôznych fluorovaných látok a slúži ako prekurzor v polymerizácií podporovanej plazmou na výrobu nízko dielektrických fluorokarbonových tenkých vrstiev s rôznorodým technickým využitím. Vďaka jeho vlastnostiam sa začalo uvažovať, či by sa mohol využiť i inde, napríklad ako náhrada vo vysokonapäťových spínačoch za fluorid sírový (SF_6), ktorý sa radí medzi skleníkové plyny. Na to sme ale museli preskúmať ako sa HFPO chová.

Preto sme na Oddelení dynamiky molekúl a klastrov študovali jeho interakciu s elektrónmi. Molekuly HFPO sme skúmali elektrónovým záchytom a elektrónovou ionizáciou. Boli sme schopní určiť fragmenty, ktoré pri procese elektrónovým záchytom vznikajú a absolútny účinný prierez pre jednotlivé rozpadové kanály. Následne sme pomocou pozitívnej (70 eV) a negatívnej ionizácie (0 – 15 eV) sledovali fragmentáciu klastrov pri koexpanzii molekúl HFPO s héliom a pick-up experimente molekúl HFPO na argónových klastroch.

V mojej prednáške vám predstavím výsledky z oboch experimentov, ktoré boli spracované do formy diplomovej práce pre Vysokú školu chemicko-technologickú v Prahe. Kde najdôležitejším výsledkom pri štúdiu samostatných molekúl HFPO bol jeho účinný prierez ~ 4140 eV.pm^2 a fragment F$^-$, ktorý bol najintenzívnejší z jednotlivých rozpadových kanálov s účinným prierezom ~ 1140 eV.pm^2. Na výsledkoch z elektrónovej ionizácie zase môžeme vidieť, že pri 70 eV dochádzalo k menšej fragmentácií ako pri 0 – 15 eV, pričom pôvodné veľkosti klastrov odpovedali v oboch prípadoch N ~ 10. Ďalej vidíme opakujúce sa trendy poklesu intenzity pravdepodobnosti vzniku jednotlivých sérií s rastúcim n, pričom v argónových klastroch dochádzalo k lepšej stabilizácii jednotlivých sérií.

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A COMBINED SIFT-MS AND PTR-MS STUDY OF PROTON TRANSFER FROM H_3O^+ TO GLYOXAL

Mgr. Michal Lacko

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

Glyoxal ($C_2H_2O_2$) is a reaction intermediate in several biological and environmental processes. Possibility to accurately detect presence of this molecule can help to solve several questions in atmospheric chemistry (Volkamer 2001) or to describe photocatalytic reduction of carbon dioxide (Shkrob 2012). Modern detection techniques based on a chemical ionization facilitate sensitive and real-time measurement of concentrations of organic species. However, to accurately determine a concentration of a molecule, we have to understand ion chemistry occurring during the detection process. In my lecture, I would like to express differences between the ion chemistry in two experimental SCI-MS techniques, the SIFT-MS and the PTR-MS, which may be used for detection of glyoxal in real time.

The experimental results show significant differences between the two mentioned experimental techniques based on the different ion chemistry. For both techniques we observed humidity dependent formation of protonated molecules and their fragmentation into protonated formaldehyde. Humidity dependence has however opposite character for both techniques: for the SIFT-MS fragmentation is increasing with humidity whilst in PTR-MS is fragmentation suppressed by humidity. To clarify the ion chemistry, we provided series of experiments involving change of kinetic energy of regent ions, concentration of carrier gas, type of carrier gas and concentration of water.

Change of the He carrier gas concentration in SIFT-MS showed significant change of branching ratios between the protonated glyoxal and protonated formaldehyde, pointing to the importance of three body processes. The same effect was insignificant in the PTR-MS, however, dependence on the change of carrier gas type expressed importance of the collision energy. Additionally, effect of association processes was studied according to presence of atomic or molecular gas in the PTR-MS.

As a conclusion, for the SIFT-MS we observed significant dependence on secondary processes, mainly triggered by humidity. In PTR-MS is the chemistry controlled by a collision induced dissociation of protonated molecule.

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ALFA OXYGEN FOR SELECTIVE OXIDATION OF HYDROCARBONS OVER BINUCLEAR TRANSITION METAL ION STRUCTURES IN ZEOLITES. FTIR SPECTROSCOPY STUDY.

Mariia Lemishka

Mgr. Jiří Dědeček, CSc. DSc.

Zeolites (microporous crystalline aluminosilicates) represent very important group of heterogeneous catalysts applied both in acid and redox catalyzed reactions. Fe-containing zeolites are exceptional due to their ability to decompose N_2O and form unique type of oxygen (so called α-oxygen) [1]. This highly reactive oxygen form is able to selectively oxidize methane to methanol [2]. However, Fe species active in the formation of α-oxygen are difficult to be prepared and unstable. Our *ab initio* calculations suggest that binuclear structures of bare divalent cations (Co^{2+}, Ni^{2+}, Mn^{2+}) should decompose N_2O and form active oxygen. The aim of this study was preparation of the binuclear Co^{2+}, Ni^{2+}, Mn^{2+} structures in zeolite of the ferrierite structure and testing their activity in N_2O decomposition, active oxygen formation and selective oxidation of hydrocarbons.

FTIR study of perturbed skeletal vibrations of the zeolite showed formation of bare cations in extra-framework cationic sites of dehydrated ferrierites and confirmed the formation of their binuclear structures at high metal ion loadings as well as decomposition of N_2O and formation of α-oxygen over these structures. Analysis of C-O and C-H vibrations confirmed that methane is selectively oxidized by active oxygen form stabilyzed on cation.

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ELECTROCHEMICAL METHODS FOR DETERMINATION OF HOMOVANILLIC, VANILLYLMANDELIC, AND 5-HYDROXYINDOLE-3-ACETIC ACIDS IN HUMAN URINE

RNDr. Anna Makrlíková

Assoc. Prof. Ing. Tomáš Navrátil, Ph.D.

Homovanillic (HVA), vanillylmandelic (VMA), and 5-hydroxyindole-3-acetic (5-HIAA) acids are tumor biomarkers excreted in urine. HVA and VMA are major end products of catecholamine metabolism; 5-HIAA is a breakdown product of serotonin. Abnormally high urinary levels of these biomarkers can predict neuroblastoma, pheochromocytoma, and carcinoid tumors [1,2]. In this contribution, our results on voltammetric and/or amperometric determination of these biomarkers will be presented.

First part of this research was devoted to the determination of the biomarkers using differential pulse voltammetry at screen-printed carbon electrodes (SPCEs) in an optimum medium of Britton-Robinson buffer (BRB) (0.04 $\text{mol}\cdot\text{l}^{-1}$, pH 3.0). The obtained limits of detection (*LOD*s) were 0.24, 0.06, and 0.12 $\mu\text{mol}\cdot\text{l}^{-1}$ for HVA, VMA, and 5-HIAA, respectively. Furthermore, application of this method for the determination of HVA and VMA in their mixture [2] will be presented.

Afterwards, determination of these tumor biomarkers using flow injection analysis with amperometric detection (FIA-AD) at SPCEs in BRB (0.04 $\text{mol}\cdot\text{l}^{-1}$, pH 2.0) will be reported, with *LOD*s: 0.065 $\mu\text{mol}\cdot\text{l}^{-1}$ for HVA, 0.053 $\mu\text{mol}\cdot\text{l}^{-1}$ for VMA, and 0.033 $\mu\text{mol}\cdot\text{l}^{-1}$ for 5-HIAA.

Finally, determination of HVA, VMA, and 5-HIAA in human urine using HPLC-ED at a glassy carbon electrode in a “wall-jet” arrangement after solid phase extraction will be demonstrated, with *LOD*s: 2.5 $\mu\text{mol}\cdot\text{l}^{-1}$ (HVA), 2.6 $\mu\text{mol}\cdot\text{l}^{-1}$ (VMA), and 0.85 $\mu\text{mol}\cdot\text{l}^{-1}$ (5-HIAA).

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Acknowledgements:

This research was supported by the Grant Agency of the Czech Republic (the Czech Science Foundation) (Project No. 17-03868S) and by the Grant Agency of the Charles University (Project No. GAUK734216).

SURFACE SENSITIVITY OF PHOTO-ELECTROCHEMICAL WATER OXIDATION ON TIO_2 (ANATASE) SINGLE CRYSTALS

Ing. Roman Nebel

Doc. Ing. Petr Krtil, CSc.

The photo-electrochemical water splitting represents one of the key processes needed for successful utilization of renewable energy sources for distributed generation, storage and use of energy[1]. The research related to the electrochemical and photo-electrochemical splitting of water is primarily motivated by electricity storage in hydrogen. The overall process itself, however, is limited by the kinetically sluggish oxygen evolution reaction (OER). Fundamental understanding of the behavior of stable oxygen evolving photoanodes is, therefore, of great interest.

A comparison of the photocurrent data for both surface orientations obtained both in acid and alkaline media clearly outlines the role of the surface chemistry in the photo-electrochemical water oxidation. Regardless of the surface orientation the onset of the water oxidation related photocurrent shifts to more positive potentials. This behavior reflects the effect of the surface protonation/deprotonation reactions on the overall photo-electrochemical activity of the anatase. The observed difference between the behavior of the (100) and (101) surface can be related to the differences in the actual surface structures. The shift in the photocurrent onset also reflects the difference in the double layer structure on the solution side of the interphase namely to orientation of the water molecules in the double layer which is reflected in the difference of the photocurrent onsets in systems containing ions supporting or suppressing the formation of the hydrogen bonds between water molecules. The observed experimental trends will be explained in relation to the relative stability of the different surface structure which may be formed at the anatase surface under operando conditions.

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CHARACTERIZATION OF PRISTINE AND Si–MODIFIED Zr SURFACE BY ATOMIC FORCE MICROSCOPY AND ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

Ing. Michal Novák

Mgr. Magdaléna Hromadová, Ph.D.

Due to excellent corrosion resistance zirconium alloys are being used as a cladding material for the nuclear fission fuel. The main disadvantage of such materials is fast redox reaction with water, which leads to oxidation of base material and hydrogen evolution reaction (HER) [1]. Hydrogen can damage the cladding due to the zirconium hydride formation or can be released into the reactor space [2]. New materials are being developed to improve corrosion resistance of the cladding [3]. With this objective in mind we proposed Si modified Zr surface (SiZr) that could slow-down both HER and oxidation of the base Zr material. SiZr surfaces were prepared by DC magnetron sputtering from Si and Zr targets (1:1 ratio) at well-polished pure Zr pellets.

The aim of this work was to evaluate effect of HER on modified SiZr surface structure. As a reference, diamond paste polished (D3) and emery paper polished (5000) Zr surfaces were also studied. Surface topography of such samples was evaluated using the atomic force microscopy (AFM). Hydrogen evolution reaction was studied by electrochemical impedance spectroscopy (EIS). Spectra were evaluated by using equivalent circuit $R_{el}(CPE_{dl}R_{ct})$ containing constant phase element (CPE_{dl}), which provides parameter n related to fractal dimension (D_f) of the surface and thus enabling direct comparison of n obtained from EIS with AFM data by utilizing equation $n = 1/(D_f-1)$ [4].

Parameter D_f from AFM measurements at D3 and 5000 zirconium surfaces showed the expected trend as the values increased with increasing roughness of the abrasive. Fractal dimension of SiZr surface was comparable with the value at emery paper polished (5000) Zr surface. For pristine Zr surfaces the n values calculated from AFM-determined D_f are in a good agreement with n values obtained from EIS spectra. However values of n from EIS spectra were lower at SiZr surfaces than the calculated n based on AFM image analysis. These results suggest that in this case double layer distribution is not simply related to the surface structure. The electrode surface is heterogeneous and composed of the Si and Zr atoms, which leads to lower overall HER kinetics. AFM measurements prior and after HER indicate insignificant effect of HER on SiZr surface structure.

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THE STUDY OF THE INFLUENCE OF GAMMA RADIATION ON THE BIOGENIC MOLECULES' FORMATION

Ing. Adam Pastorek

prof. RNDr. Svatopluk Civiš, CSc.

It is a well-known fact that theories firstly brought by Oparin [1] became insanely famous in a short time after being proven by experiments of Miller and Urey in 1952 [2]. After those, many experiments have been performed in next years, with different energy sources and with different primordial soup mixtures. However, only brief amount of experiments and even lesser amount of theories have been developed through time with emphasis on possible role of ionizing radiation during early-life formation on Earth. See also [3, 4].

In my presentation I will focus on the available calculations of possible early Earth's radiation fields, new theories about the influence of gamma radiation and radiation generally on the origin of life on Earth, and the comparison of my experiments with already existing data from thermolyses.

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RUTHENIUM AND IRIDIUM PYROCHLORES WITH DIFFERENT LANTHANIDES AS CATALYSTS FOR OXYGEN EVOLUTION REACTION (OER)

Rebecca Pittkowski, M.Sc.
doc. Ing. Petr Krtil, CSc.

The electrocatalytic oxygen evolution reaction (OER) represents a process limiting widespread storage of renewable electricity in hydrogen. Catalysis of the OER is difficult to optimize due to the well-known scaling relation restriction.[1] An alternative to a search for a catalyst breaking this restriction[2,3] is to improve the current state-of-the-art catalyst's feasibility. In such an effort, one may aim at either optimizing the surface orientation or reducing the costly catalyst components. Here the later approach is outlined on the benchmark oxygen evolving systems for acid media, based on oxides of ruthenium and iridium. A decrease of noble metal content can conveniently be achieved if one moves from tetragonal oxides of rutile type (typical for RuO_2 and IrO_2) to cubic pyrochlores of the $A_2B_2O_7$ type. In this arrangement, one may expect the surface structure to deviate just moderately from those of rutile or perovskite investigated previously.

The flexible pyrochlore structure allows for different combinations of A-site and B-site cations. The smaller cation typically resides in the B-site. For catalytically active Ru or Ir occupying B-sites, the A-sites can be occupied by many lanthanides. These rare earth elements are subject to the effect of lanthanide contraction, differing in ionic radius. Hence, different lanthanide cations change the unit cell parameter and, consequently, the metal-to-metal distance between the transition metal cations. This again influences the position of the catalyst's d-band center.

This work presents synthesis, characterization, and OER activity of a range of ruthenium and iridium pyrochlores incorporating different Lanthanides (Yb, Gd, Nd). The catalysts were synthesized *via* spray-freeze freeze-dry approach. The phase pure materials, however, require prolonged annealing at temperatures above 1000°C. The obtained catalysts were characterized by XRD, SEM and EDX, and EXAFS. Differences in unit cell parameter can clearly be seen from the shift of reflection in the XRD patterns. The catalytic activity of the oxides towards OER is related to the experimental distances of the transition metal cations.

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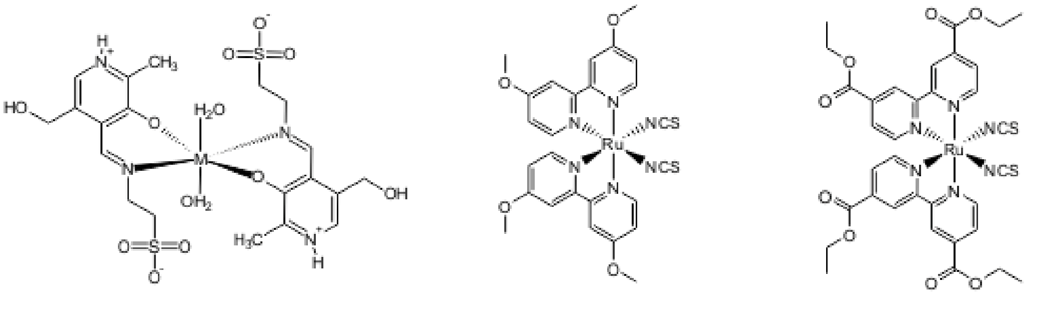
VIBRATIONAL SPECTRA OF TRANSITION METAL COMPLEXES: AN ANHARMONIC APPROACH

Ing. Martin Pižl

Ing. Stanislav Záliš, CSc.

Vibrational properties are often used for characterization of coordination compounds. Harmonic approximation is a standard approach for description of vibrational properties like infrared or Raman spectra. On the other hand, anharmonic calculation is important for better understanding of spectra and detailed description of experimental data by calculated results. Vibrational second-order perturbation theory (VPT2) is widely used for estimation of anharmonic frequencies. All calculations were performed by Gaussian 16 program package.

In this study, we focused on anharmonic effects on Raman spectrum of Co (**1**), Ni (**2**) and Cu (**3**) complexes derived from vitamin B6. This work also contains application of anharmonic approach for estimating of diagonal and off-diagonal anharmonicities in 2DIR spectra of Ru complexes – [Ru(4,4'-di-R-2,2'-bipyridine)$_2$(NCS)$_2$] (R = OMe (**4**) and CO$_2$Et (**5**). Structures of complexes 1-5 are depicted on Fig.1.



M = Co (**1**), Ni (**2**) or Cu (**3**)

[Ru(MeObpy)$_2$(NCS)$_2$] (**4**)

[Ru(EtCOObpy)$_2$(NCS)$_2$] (**5**)

Figure 1 Structures of metal complexes

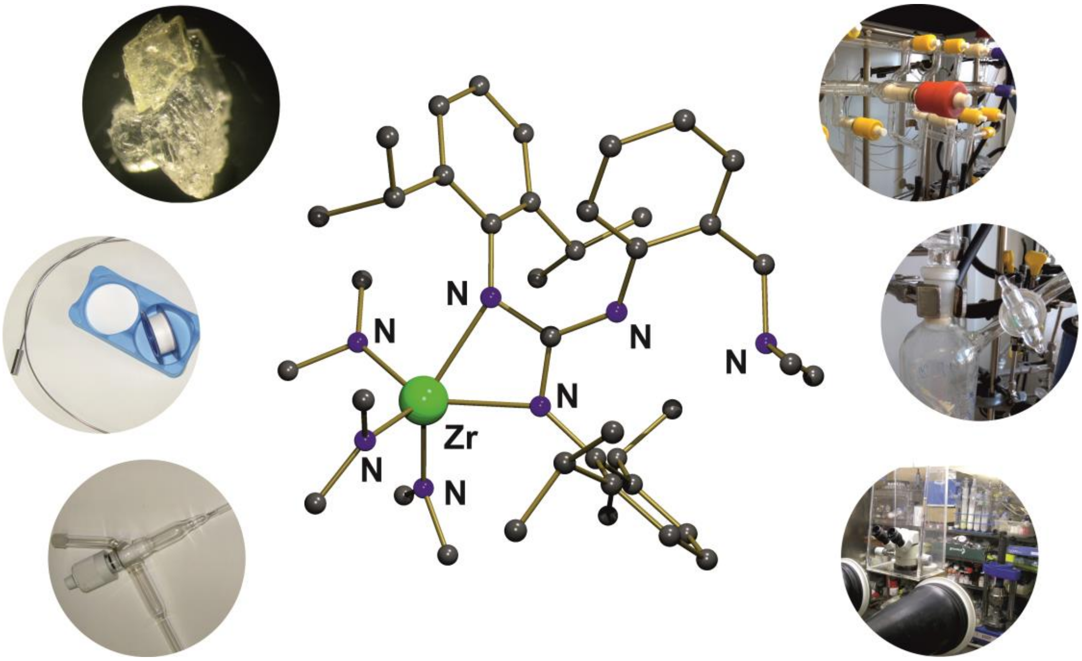
Acknowledgements This work was supported by Ministry of Education of the Czech Republic (grant LTC17052), by the Czech Science Foundation (grant 17-01137S) and the COST Action CM1405.

PŘÍPRAVA GUANIDINÁTOVÝCH KOMPLEXŮ ZIRKONIA

Kristýna Pokorná

Mgr. Michal Horáček, Ph.D.

Tato práce se zabývá přípravou a studiem vlastností sloučenin zirkonia obsahujících guanidinátový ligand mající ve svém strukturním motivu N-C(N)-N skelet. Cílem práce bylo především osvojení si technik experimentální práce v laboratoři při manipulaci s látkami citlivými na vzduch a vlhkost, které jsou v dnešní době již požadovaným standardem ve všech oborech chemie. V rámci této práce se podařilo připravit novou tris(dimethylamidovou) sloučeninu zirkonia obsahující guanidinátový ligand a rovněž lithnou sůl výchozího guanidinátového ligandu. Připravené sloučeniny byly charakterizovány pomocí spektroskopických technik nukleární magnetické rezonance a infra-červené spektroskopie.



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LOCAL PHOTOCURRENT CHARACTERIZATION OF GRAPHENE-SILICON SCHOTTKY JUNCTION

Mgr. Jaroslava Řáhová

Mgr. Otakar Frank, PhD.

Graphene and numerous other 2D materials (e.g. TMDCs like MoS_2) exhibit interesting electrical properties which are, however, significantly influenced by surrounding environment. Thus, interfacing of materials with different dimensionalities becomes increasingly relevant for many applications which can utilize the exceptional properties of low-dimensional materials on one hand, and build-up on the existing production know-how for bulk (3D) materials on the other. Numerous appealing possibilities are offered by such combinations. This work is focused on 2D-3D heterostructures composed of mechanically exfoliated single- and few-layer graphene in combination with n -doped crystalline silicon. Photovoltaic characteristics (PV) of this heterojunction were studied at nanoscale under different light conditions.

Flakes of the studied 2D materials of various thickness were prepared by exfoliation on polydimethylsiloxane (PDMS) substrate, followed by oriented transfer onto the final bulk, freshly etched Si substrate (3D material). Electrical properties of the thus formed 2D/3D heterostructures were studied mainly by methods based on the principles of Atomic Force Microscopy: local photocurrents were studied by conductive AFM (CAFM), as well as using I-V sweeps, and changes in surface potential (i.e., work function) were acquired using Kelvin Probe Force Microscopy.

From CAFM, the fill factor (FF) and open-circuit potential (VOC) can be safely determined, however, the short-circuit current (JSC) values can be compared only for a particular tip, otherwise JSC needs to be normalized. The PV characteristics of p-Gr/n-Si Schottky junction shows strong dependance on light conditions as well as on the overall quality of 2D/3D contact within individual graphene flakes. The parameters of solar cell efficiency further also differ according to the number of graphene layers and level of graphene doping. Connection between aging of heterostructure and changes in photovoltaic properties is briefly discussed.

Even though the quantitative information provided by the local PV characterization methods has its limits, we have shown such methods to be very useful for revealing details invisible to macroscopic measurement.

ORGANOMETALLIC COMPOUNDS IN THE CONTEXT OF DNA STRAND BREAK INDUCTION DURING IRRADIATION

Dan Reimitz

Mgr. Jaroslav Kočišek, Ph.D.

It was shown, that the presence of cisplatin increase radiation sensitivity of plasmid DNA [1]. Cisplatin also shows a synergy with ionizing radiation during concomitant chemoradiotherapy *in vivo* [2]. One of the possible explanations of this, so far not yet explained phenomena, can be hidden in the reactions of DNA with low energy electrons (LEE), which are the most abundant secondary species generated by an interaction of ionizing radiation with living matter. LEE can induce strand-breaks in DNA, even if their energy is below the ionization thresholds, via the dissociative electron attachment (DEA) process [3]. Cisplatin has a much higher cross section for electron capture than DNA constituents. Molecule of cisplatin can capture an electron, create a transient anion, and then the extra electron can be transferred to the bounded DNA and cause a strand break via DEA process.

To test, if this process has a relevant contribution to the reported synergy [1], we compare the abundance of strand-breaks in DNA and DNA-cisplatin complex after the irradiation by γ rays of ^{60}Co source [4], as well as by protons. We investigate not just the effect of cisplatin, but also other organometallic compounds such as RAPTA-C and titanocene complexes [5]. DNA plasmids pBR322 are irradiated in buffer with different scavenging capacity to distinguish effect of oxidative hydroxyl radicals and electrons. Induced single and double strand breaks are analyzed using agarose gel electrophoresis. Our results show, that cisplatin can increase the number of single strand breaks (SSB) during irradiation, for the experimental conditions specified in [4], other compounds are under investigation. The abundance of double strand breaks (DSB) induced in plasmid DNA for these conditions is more than ten times lower than that of SSBs. This low abundance is not easily quantified and reproduced by the agarose gel electrophoresis. So besides experiments with plasmid DNA, we are working on the implementation of technique to study shorter DNA oligomers using DNA origami templates [6], which will allow us much better evaluation of DBSs. This technique enables to test specific sections of DNA and an evaluation of how much the synergy differs for different DNA bases.

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STUDIUM VLIVU ZVOLENÝCH LÉČIV NA MODELU LIPIDOVÉ VRSTVY SLZNÉHO FILMU LIDSKÉHO OKA

Mgr. Kamila Riedlová

Dr. habil. Lukasz Cwiklik, Ph.D.

Slzný film je tenká vrstva na povrchu lidské rohovky. Lipidová část (TFLL) této vrstvy na nejsvrchnějším rozhraní má funkci ve snižování povrchového napětí slzného filmu. Což jednak pomáhá při opětovném rozprostření slzného filmu po mrknutí oka a jednak při předcházení evaporaci slz. Slzný film a TFLL jsou také vůbec první struktury na povrchu oka, které se setkávají s oftalmologickými léčivy – např. při léčbě suchého oka. Mechanismus funkce těchto léčiv je stále nejasný. Cílem mé práce je proto porozumět interakci vybraných oftalmologických léčiv s modelovými systémy napodobujícími slzný film lidského oka a TFLL na molekulární úrovni. Ke studiu používám zejména hrubozrnné (*coarse-grained)* simulace molekulové dynamiky a pro vybrané menší subsystémy k získání detailnějšího popisu budou využívány i atomistické simulace (*all-atom*). Hrubozrnné simulace doplňují souběžně probíhající experimentální měření využívající fluorescenční mikroskopie.

CHLORACE HYDROSILANŮ S POUŽITÍM KATALYZÁTORU B(C$_6$F$_5$)$_3$

Adam Šimarek

Mgr. Jiří Pinkas, Ph.D.

Chlorsilany a jejich deriváty jsou velmi významné látky pro polymerní průmysl. Jejich polymerací vzniká, dnes hojně používaný, silikon. Vázáním odlišných skupin na řetězce monomerů se dají upravit vlastnosti vzniklého polymeru. Postupem z této práce možná bude možné navázat na monomer i skupiny jinou cestou nenavazatelné, a tak vytvořit zcela nové silikony.

Při výzkumu katalytické silylace alkoholů v laboratoři organokovové chemie [1] se objevila anomálie v případě silylace trifenylmethanolu. Při této reakci se místo silanu aktivoval trifenylmethanol, bylo tedy nutné prozkoumat toto anomální chování vzniklého tritylového kationtu Ph_3C^+ i v jiných typech reakcí - konkrétně chloraci hydrosilanů.

Námi objevený postup spočívá v reakci tritylchloridu (halogenační činidlo) se substrátem (silanem). Tato soustava je katalyzována silnou Lewisovou kyselinou $B(C_6F_5)_3$ (viz. Schéma). Zajímavým faktem je, že rychlost reakcí s přibývajícími stupni chlorace klesá (minuty/hodiny/dny), dá se tak dosáhnout vysoké selektivity reakce. To je zvláště výhodné pro přípravu hydridochlorsilanů a hydridodichlorsilanů ze sekundárních a primárních silanů.

V budoucnu se pokusíme navázat na silany touto cestou i jiné skupiny (CN-, SCN-, Br-).

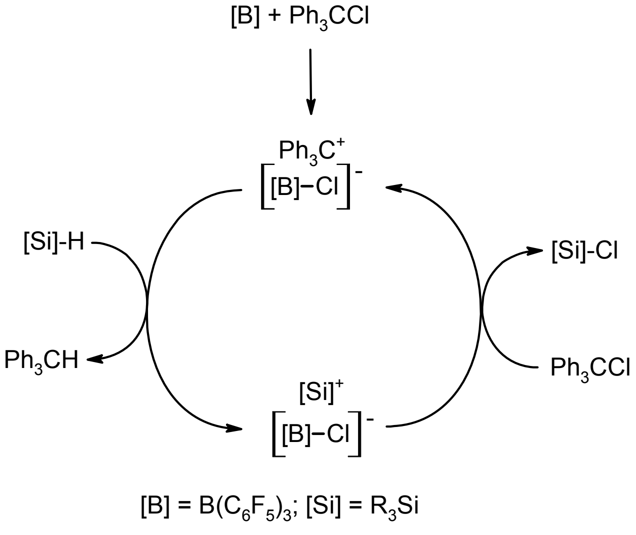

Schéma: Předpokládaný cyklus chlorace hydrosilanu katalyzovaný $B(C_6F_5)_3$

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PREPARATION OF PROAPOPTOTIC PROTEIN BAX

Kristián Skála

RNDr. Radek Šachl, Ph.D.

Protein Bax is a member of bcl-2 family proteins that can regulate the permeability of the outer mitochondrial membrane. Stress factors cause accumulation of Bax on the membrane and subsequent formation of oligomers that can form a pore. Cytochrom c is subsequently released from the mitochondria, which triggers a reaction cascade leading to the apoptosis of cells.

The main aim is for the first to recombinantly express and purify Bax protein and subsequently label mutated version of Bax with fluorescent probe. For the second to examine the impact of the lipid composition and the activator of Bax tBid on the oligomerization of Bax in model lipid bilayers. The project also aims to find out a possible relation between the oligomerization of Bax and formation of pores induced by this protein.

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DOXORUBICIN HYDROCHLORIDE AND ITS DETERMINATION IN A MICRO VOLUME CELL USING DIFFERENTIAL PULSE CATHODIC STRIPPING VOLTAMMETRY

Mgr. Štěpánka Skalová

Doc. Ing. Tomáš Navrátil, PhD.

Monitoring of anticancer drugs in a micro sample volume of body fluids increases patient chances to recover by optimized dosage treatment[1].

Our research is focused on determination of doxorubicin hydrochloride (Fig. 1) in 50 µL of analyzed sample using a newly developed micro-volume voltammetric cell (MVVC) described in ref.[2]. For these purposes, differential pulse cathodic stripping voltammetry and three-electrode system with a polished silver solid amalgam electrode as a working electrode have been used.

After the experimental condition optimization (Britton-Robinson buffer pH 6, potential of accumulation -300 mV, time of accumulation 90 s, initial potential -200 mV, final potential -800 mV, scan rate 20 mV s^{-1}, pulse width: 80 ms and pulse height -50 mV) the following results were found: limit of detection 3.9×10^{-7} mol L^{-1}, repeatability of measurement 3.73 % (DOX concentration of 0.4 µmol L^{-1}) and 3.22 % DOX concentration of 100 µmol L^{-1}), respectively.

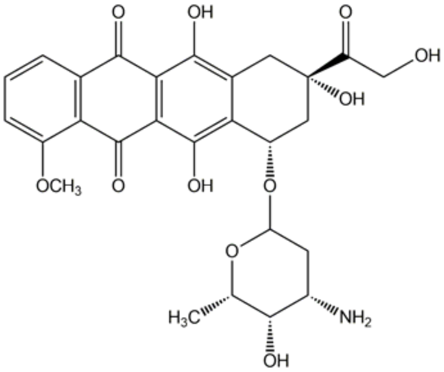

Fig. 1 Structural formula of doxorubicin hydrochloride

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SPATIALLY RESOLVED COVALENT FUNCTIONALIZATION PATTERNS ON GRAPHENE

Bc. Leoš Valenta

Ing. Petr Kovaříček, Ph.D.

Graphene is one of the most investigated 2D materials due to its unique properties,[1] which can be further adapted for a specific application, e.g. by covalent chemical functionalization.[2,3] As the more complex applications of graphene require spatially resolved patterns on the graphene monolayer, the recently used homogenous modification methods becomes obsolete.[4,5]

This work describes a new method of spatially resolved covalent functionalization using the Mitsunobu reaction on an oxygen plasma treated monolayer graphene. The hydroxyl groups in graphene are exchanged by the carboxylate anion when azodicarboxylate, triphenylphosphine and carboxylic acid are used. Using UV light and a photomask, the differences between the irradiated and non-irradiated areas emerge. The non-irradiated areas undergo the conventional Mitsunobu substitution. However, the action of light on the unmasked regions causes decomposition of the azodicarboxylate, which represents the crucial Mitsunobu reagent. Therefore, the unreacted triphenylphosphine remaining in the solution is employed in the reductive de-oxygenation leading to the restored structure of pristine graphene. In this manner, the spatially resolved patterns of the covalently functionalized and pristine graphene are prepared with micrometer resolution.

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PHOTOCATALYTIC ABATEMENT OF NO_X: NITROUS ACID AS EMERGING POLLUTANT

Mgr. Eva Vaněčková

Ing. Jiří Rathouský, CSc.

Heterogeneous photocatalysis on TiO_2 coatings is one the most efficient advanced oxidation processes for NOx abatement. According to the ISO and CEN standards for photocatalytic abatement, the activity of this process is determined solely by reduction in NO concentration. However, an environmentally responsible application of this process should recognise that minimizing the potential formation of harmful nitrogenous species, such as HNO_2, is at least as important as the activity itself. Here, two photocatalytic TiO_2 layers, one prepared by spin-coating and the other by magnetron sputtering, were tested for NO and NO_2 abatement. Under conditions simulating the real environment, the photocatalytic oxidation of NO and NO_2 was investigated at inlet concentrations of both 0.1 and 1.0 ppm. Our results show that the amount of HNO_2 produced was dependent on the structural properties of the photocatalytic coatings. The amount of HNO_2 formed on the coatings prepared by magnetron sputtering varied greatly from those formed on the spin-coated ones. Therefore, we propose that strategies for evaluating the photocatalytic air treatment should be more complex including the determination of all intermediates and final products; otherwise, the results can be misleading and open to misinterpretation.

FRET REVEALS INTER-LEAFLET COUPLED NANODOMAINS IN LIPID BILAYERS OF GIANT UNILAMELLAR VESICLES

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Although it is widely accepted nowadays that plasma membranes are heterogeneous on the nanoscale, it is very little known about these nanoheterogeneities (=nanodomains). Here, combination of Monte Carlo simulations with Förster Resonance Energy Transfer (MC-FRET) was used to characterize these nanodomains in terms of sizes, concentrations and inter-leaflet organization. The emphasis was given on DOPC (1,2-dioleoyl-sn-glycero-3-phosphocholine), cholesterol and sphingomyelin bilayers enriched by oxidized phospholipids*1-palmitoyl-2-(5'-oxo-valeroyl)-sn-glycero-3-phosphocholine* and *1-palmitoyl-2-glutaryl-sn-glycero-3-phosphocholine*. Oxidized phospholipids (OxPls) are products of oxidative stress, but their exact role in living organisms is yet not clear.

The formation of nanodomains was probed by different donor-acceptor pairs (g-GM1/r-GM1, g-PGPE/r-GM1, g-POVPE/r-GM1 and CF-PEG-DSPE/Rh-PEG-DSPE) and the measured kinetics were further analyzed by four different models assuming anti-registered, registered, partially registered and independent nanodomains. It follows from the comparison of the models that the nanodomains are inter-leaflet coupled. Similar observations were reported for microscopically sized domains. Also, we have studied the influence of the distribution of nanodomain radii on the outcomes of the MC simulations.

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SYNTHESIS OF PT-MWW WITH CONTROLLABLE NANOPARTICLE SIZE

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Supported metal nanoparticles are widely used in many industrial processes as heterogeneous catalysts in water-gas shift, CO oxidation, or hydrogenations. The size of metal nanoparticles is a significant factor affecting the catalytic performance since smaller particles possess high surface/volume ratios [1]. It has been widely reported that the catalytic activity increases with decreasing size of metal particles with the best catalytic performance for catalysts with particle size below 5 nm [2]. So it is important to prepare controllable size of nanoparticles on supported materials.

Layered zeolite precursors consist of zeolite sheets kept by relatively weak and easily breakable non-covalent force. A two-step procedure of swelling and pillaring can tailor layered zeolites to hierarchical structures. This method seems suitable to introduce and encapsulate the metal nanoparticles within the interlayer space of zeolite during the swelling process followed by calcination. Corma et al. [3, 4] reported a strategy for encapsulation of subnanometric Pt clusters with a high stability during the transformation of a 2D zeolite into 3D zeolite.

Herein, we investigated the effect of the length of the surfactant used for the swelling process in relation to the size of Pt nanoparticles in the final zeolite. Pt nanoparticles were introduced during the swelling followed by calcination. The interlayer distances of swollen materials increases with the length of the surfactant from 1.06 nm ($C_{12}OH$) to 2.89 nm ($C_{18}OH$). During swelling, the Pt nanoparticles were intercalated to the interlayer space of MCM-22P. Calcination resulted in Pt-MWW materials showing similar morphologies, textural properties and Pt content despite the different initial distance of layers. As a result, the average size of Pt nanoparticles increased from 0.85 nm (MCM-22-C_{12}OH-Pt) to 2.04 nm (MCM-22-C_{18}OH-Pt) which is related to the length of the hydrocarbon chain of the surfactant used for the swelling process.

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OVERCOMING APPLICATION LIMITATIONS OF GERMANOSILICATE ZEOLITES: POST-SYNTHESIS TAILORING THE ACTIVE SITES

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In recent years, germanosilicate zeolites have attracted a lot of attention. Both theoretical and experimental studies have shown that germanium favor the crystallization of low-density frameworks containing D3R, D4R building units. This finding resulted in discovery of new germanate and germanosilicate large- and extra-large pore zeolites being attractive for catalytic conversion of bulky molecules.[1] However, a development of approaches allowing to decrease cost price of germanosilicate zeolites is required to make practical use of their attractive characteristics.[2]

In this work, we addressed a possibility and features of Ge recycling as a step of catalysts preparation. For the study we chose three germanosilicates differing in channel sizes: medium-pore ITH, large-pore IWW and extra-large pore UTL. We assess the influence of treatment conditions (e.g., time, acid concentration, temperature, liquid-to-solid ratio), zeolite topology, and crystal size on the extent of Ge recovery and textural properties of zeolites under investigation. Up to 88 % of Ge was recovered under optimized conditions by the treatment of parent germanosilicates in acidic environment (Table 1), followed by precipitation of leached germanium in oxide form.

Table 1. The influence of acid nature and concentration on the degermanation degree of IWW zeolite (T = 25 ^oC, τ = 12 h, 0.1 g zeolite / 20 ml solution)

Concentration, M	Recovered Ge, %	
	HCl	HNO_3
0	50	
0.1	55	76
1	76	84
4	86	88

Recovered GeO_2 was successfully used as a source of framework germanium in the repetitive synthesis of ITH, IWW and UTL zeolites demonstrating the possibility to perform full synthesis-recovery-synthesis cycle. Degermanation of Ge-poor ITH and IWW zeolites (Si/Ge > 4) was found accompanying with a significant increase in the concentration of silanol and germanol defects. This fact can be used for post-synthesis incorporation of heteroelements into germanosilicates to design functional materials with unusual zeolite topologies for application in catalysis or adsorption.

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SEMINÁŘ STUDENTŮ ÚFCH JH 2018

Sál Rudolfa Brdičky, ÚFCH JH, Praha

12.-13.6.2018