

SEMINÁŘ STUDENTŮ ÚFCH JH **2015**



KC AV ČR v Liblicích
4.- 6.5. 2015

Seminář studentů ÚFCH JH 2015

Sborník příspěvků

**ze studentské konference konané
4. - 6. května 2015
v Konferenčním centru AV ČR Liblicích**

Seminar of Students of JHI 2015

Collection of abstracts

**of all lectures given at the student conference
held on 4 -6 May 2015
in Conference Centre of the Academy of Sciences
of the Czech Republic in Liblice chateau**

Seminář studentů ÚFCH JH 2015
Sborník příspěvků ze studentské konference
konané 4. - 6. května 2015
v Konferenčním centru AV ČR Liblicích

Kolektiv autorů

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SEMINÁŘ STUDENTŮ ÚFCH JH 2015

PROGRAM 1. dne konference - **pondělí 4.5.2015**

Odjezd autobusem z parkoviště před ústavem ve 14:30 hodin.

Předpokládaný příjezd do Konferenčního centra AV ČR v zámku
v Liblicích okolo 15:30 hodiny.

Čas	Předsedající	Přednášející	Název
15:30- 16:15	Registrace a ubytování účastníků konference - v recepci zámeckého hotelu		
16:15- 16:45	OBČERSTVENÍ PŘED ZAHÁJENÍM KONFERENCE (káva, nápoje, zákusek - v 1. patře, na ochozu)		
16:55	Zahájení konference „Seminář studentů ÚFCH JH 2015“ - prezentace studentů z kategorie I. (4 práce)		
17:00	<u>Jan</u> <u>Přech</u>	Kristýna KANTNEROVÁ (diplomantka, školitel J. Ludvík) kat I	ORTHOPHTHALALDEHYDE – ELECTROCHEMICAL REDUCTION, HYDRATION AND REACTIVITY WITH NUCLEOPHILES
17:20		Jan BOHUSLAV (bakalář, školitel P.Jandak) kat I	NANOMORFOLOGIE A ELEKTROCHEMIE ELEKTRODY PŘIPRAVENÉ Z HOPG A NANODESTIČEK SMĚSNÉHO HYDROXIDU NI/CO
17:40		Andrej ANTALÍK (diplomant, školitel J. Pittner) kat I	DENSITY MATRIX RENORMALIZATION GROUP CALCULATIONS AND ENTANGLEMENT OPTIMIZATION IN QUANTUM CHEMISTRY
18:00		Jaroslava ŘÁHOVÁ (diplomantka, školitel O. Frank) kat I	GRAPHENE WRINKLES
18:20	Ukončení prvního dne konference VEČEŘE v RESTAURACI - začátek v 18:45		

PROGRAM 2. dne konference - úterý 5.5.2015

Čas	Předsedající	Přednášející	Název
8:25	Zahájení druhého dne konference - pokračují prezentace studentů kategorie I a II.		
8:30	<u>Tomáš</u> <u>Chum</u>	Vít SVOBODA (diplomant, školitel O.Votava) kat I	VYSOCE ROZLIŠENÁ OVERTONOVÁ SPEKTROSKOPIE ATMOSFÉRICKY RELEVANTNÍCH MOLEKUL
8:50		Vojtěch HRDLIČKA (diplomant, školitel T. Navrátil) kat I	THE USE OF SELF-ASSEMBLED MONOLAYER OF THIOLATED CALIX[4]ARENE ON POLYCRYSTALLINE GOLD ELECTRODE SURFACE
9:10		Lukáš ŠIMAŇOK (bakalář, školitel J. Rathouský a R. Žouželka) kat I	PŘÍPRAVA NANOČÁSTIC OXIDU STŘÍBRNÉHO V SEMIORGANICKÉM PROSTŘEDÍ A JEJICH APLIKACE NA KULTURY PLÍSNÍ
9:30	PŘESTÁVKA NA KÁVU (1.patro, ochoz)		
10:00	<u>Alan</u> <u>Liška</u>	Tereza VLASÁKOVÁ (diplomantka, školitel Z. Zelinger) kat I	MICROMECHANICAL SENSOR AND LASER PHOTOACOUSTIC SPECTROSCOPY IN GASES
10:20		Taťána SUPÍŇKOVÁ (I. ročník PGS, školitel M. Kočířik a P. Hrabánek) kat I	SYNTHESIS OF ZEOLITE SSZ-16 LAYERS ON POROUS SUPPORTS
10:40		Lukáš PEČÍNKA (I. ročník PGS, školitel Z. Zelinger) kat I	QUASI-RANDOM SAMPLING FOR ESTIMATING UNCERTAINTIES AND SENSITIVITY OF NUMERICAL MODELS: CASE STUDIES IN COMBUSTION CHEMISTRY AND LASER ABLATION PHYSICS
11:00	PŘESTÁVKA		
11:20	<u>Jana</u> <u>Janošcová</u>	Věra KŘÍŽOVÁ (I. ročník PGS, školitel M. Polášek) kat I	LABORATORY MODELLING OF THE ENERGETIC ION PRECIPITATION IN THE IONOSPHERE OF TITAN
11:40		Jakub LANG (I. ročník PGS, školitel J. Pittner) kat I	EXPLICITLY CORRELATED COUPLED CLUSTER CALCULATIONS WITH INCOMPLETE MODEL SPACE AND OPEN SHELL TRIPLE CORRECTIONS
12:00		Alan LIŠKA (II. ročník PGS, školitel J. Ludvík) kat II	STEREOELECTROCHEMISTRY OF ISOMERIC NITRO- AND NITROSOCALIX[4]ARENES
12:20	PŘESTÁVKA NA OBĚD (podává se v restauraci od 12:30)		
14:30	<u>Magda</u> <u>Zlámalová</u>	Valeryia KASNERYK (I. ročník PGS, školitel M. Opanasenko) kat I	GERMANOSILICATE PRECURSORS OF ITH, ITR, IWR AND UOV ZEOLITES FOR ADOR PROCESS
14:50		Joel D.DAZIE (III. ročník PGS, školitel J. Ludvík) kat II	ELECTROCHEMICAL AND SPECTROPHOTOMETRIC STUDY OF REACTIVITY OF ORTHOPHTHALALDEHYDE WITH ALIPHATIC AMINES

15:10		Jana JANOŠCOVÁ (II. ročník PGS, školitel P. Sazama) kat II	SYNTHESIS OF MICRO-MESOPOROUS NANOCARBON MATERIALS WITH DEFINED STRUCTURE
15:30		Jakub VIŠŇÁK (III. ročník PGS, školitel J. Pittner) kat II	QUANTUM ALGORITHMS FOR MANY-BODY SYSTEMS – SIMULATION FOR FEW-BODY STARTING PROBLEMS
15:50	PŘESTÁVKA NA KÁVU (1.patro, ochoz)		
16:20	PREZENTACE STUDENTŮ Z MIMOSOUTĚŽNÍ KATEGORIE "ŠTŘEDOŠKOLÁCI"		
		Květa STEJSKALOVÁ (organizátor popularizačních a vzdělávacích aktivit ústavu) krátce představí stáže studentů Biskupského gymnázia ze Žďáru n. Sázavou v projektu MŠMT "Přírodní a technické obory-výzva pro budoucnost" realizované ve školním roce 2014/2015 v laboratořích našeho ústavu a FZÚ.	
16:25	<u>Květa</u> <u>STEJSKALOVÁ</u>	Anna WASSERBAUEROVÁ a Ondřej J. DOLEŽAL (školitel V.Svoboda)	Stáž na téma " Vysoce rozlišená spektroskopie atmosféricky relevantních molekul v molekulových paprscích "
16:35		Petra TOMICZKOVÁ (školitelka M. Zlámalová)	Stáž na téma " Moderní fyzikálně chemické metody při přípravě elektrochemických senzorů a jejich charakterizaci "
16:45		Radim LIPKA a Dan MUŽÁTKO (školitel M. Kocourek, FZÚ AVČR)	Stáž na téma " Příprava tenkých vrstev pulsní laserovou depozicí a jejich charakterizace "
17:00	Mimokonferenční prezentace (pro zájemce)	<u>Květa</u> <u>STEJSKALOVÁ</u>	Představení vzdělávacích a popularizačních aktivit našeho ústavu v projektu Otevřená věda IV (AV ČR), POSPOLU (MŠMT) a Tři nástroje (ÚFCH JH) v roce 2014/2015, opět něco málo o novinkách - letošní akce v harmonogramu EXPERIMENTUJI, TEDY JSEM 2015 a zapojení našich studentů do výukových programů ÚFCH JH (realizace a tvorby)
18:00	UKONČENÍ DRUHÉHO DNE KONFERENCE <u>VEČEŘE V RESTAURACI OD 18:15 HODIN</u>		

PROGRAM 3. dne konference - středa 6.5.2015

Čas	Předsedající	Přednášející	Název
8:55	Zahájení třetího dne semináře - pokračují prezentace studentů kategorie II.		
9:00	<u>Jakub</u> <u>Višňák</u>	Magda ZLÁMALOVÁ (III. ročník PGS, školitel P. Janda) kat II	CHARACTERIZATION OF GRAPHITE ELECTRODES MODIFIED BY METHYLENE BLUE- POLYMER
9:20		Tomáš CHUM (III. ročník PGS, školitel M. Cebecauer) kat II	THE ROLE OF PALMITOYLATION AND TRANSMEMBRANE DOMAIN IN SORTING OF TRANSMEMBRANE ADAPTOR PROTEINS
9:40		Jan PŘECH (III. ročník PGS, školitel J. Čejka) kat II	POSTSYNTHESIS INTRODUCTION OF TITANIUM INTO ZEOLITE BASED EPOXIDATION CATALYSTS
10:00	Ukončeny prezentace studentů kategorie II. (7 prací)		
10:20	PŘESTÁVKA NA KÁVU (1.patro, ochoz)		

**11:00 - SLAVNOSTNÍ VYHLÁŠENÍ VÝSLEDKŮ
SOUTĚŽNÍ KONFERENCE - V KONFERENCEČNÍM SÁLE**

OBĚD V RESTAURACI od 11:45 hodin
Odjezd do Prahy - autobusem z parkoviště u zámku ve 13:30

(Návrat do Prahy k budově ÚFCH JH ca v 14:30 hodin.)



Seznam prezentujících studentů (25)

Kategorie I (13)

Diplomanti a zájemci z řad bakalářů (8)

Antalík Andrej (diplomant Přf UK, školitel J. Pittner)
Bohuslav Jan (bakalář, VŠCHT, stáž u P.Jandy)
Hrdlička Vojtěch (diplomant Přf UK, školitel T. Navrátil)
Kantnerová Kristýna (diplomantka, VŠCHT, školitel J. Ludvík)
Řáhová Jaroslava (diplomantka Přf UK, školitel O. Frank)
Svoboda Vít (diplomant, FCHI VŠCHT, školitel O. Votava)
Šimaňok Lukáš (bakalář, VŠCHT, stáž u J.Rathouského a R.Žouželky)
Vlasáková Tereza (diplomantka VŠB-TU Ostrava, školitel Z.Zelinger)

Studenti 1. ročníku PGS (5)

Kasneryk Valeryia (školitel M. Opanasenko)
Křížová Věra (školitel M. Polášek)
Lang Jakub (školitel J. Pittner)
Pečinka Lukáš (školitel Z. Zelinger)
Supíňková Taťána (školitel M. Kočířík a P. Hrabánek)

Hodnotící komise:

Elena del Corro
Juraj Fedor
Jiří Pittner
Petr Sazama

Kategorie II (7)

Studenti 2. ročníku PGS (2)

Liška Alan (školitel J. Ludvík)
Janošcová Jana (školitel P. Sazama)

Studenti 3. ročníku PGS (5)

Dazie Joel Donkeng (školitel J.Ludvík)
Chum Tomáš (školitel :Cebecauer)
Přech Jan (školitel J. Čejka)
Višňák Jakub (školitel J. Pittner)
Zlámalová Magda (školitel P. Janda)

Mimosoutěžní kategorie:

Středoškolští stážisté (5)

Tomiczková Petra (stáž u M. Zlámalové)
Doležal Ondřej J. a Wasserbauerová Anna (stáž u V.Svobody)
Lipka Radim a Mužátko Dan (stáž u T. Kocourka, FZÚ AV ČR)

5 žáků Biskupského gymnázia ze Žďáru nad Sázavou absolvuje své roční stáže v rámci projektu školy "Přírodní a technické obory-výzva pro budoucnost" (v EU programu OPVK, řešitel: kraj Vysočina) v laboratořích ÚFCH JH nebo FZÚ.

Do projektu je ústav zapojen v rámci různých programů svého vzdělávacího a popularizačního projektu Tři nástroje.





DENSITY MATRIX RENORMALIZATION GROUP CALCULATIONS AND ENTANGLEMENT OPTIMIZATION IN QUANTUM CHEMISTRY

Bc. Andrej Antalík

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

The DMRG method was originally developed in condensed matter physics, but in the last decade proved itself to be a very powerful computational method also in quantum chemistry. It is especially suited for systems with strongly correlated electrons that cannot be properly described by the Hartree-Fock wave function (single Slater determinant). Such systems require a multi-reference treatment, and DMRG is the most recent method of this type.

The key ingredient of the DMRG method related to its multicomponent subsystem wave function representation is entanglement, which in fact determines the complexity of the computation. Since the quantum chemical Hamiltonian is non-local (it contains interactions between all orbitals), there is no natural ordering of orbitals in the DMRG procedure and for efficient usage of the QC-DMRG method, the ordering optimization based on the entanglement analysis should be performed.

We applied the DMRG method with entanglement optimization to computation of singlet excited states of titan dioxide and its clusters (dimer, trimer). These due to the strongly correlated *d*-electrons represent interesting and complex electronic systems, suitable for testing of the DMRG performance.

References:

Szalay, S.; Pfeffer, M.; Murg, V.; Barcza, G.; Verstraete, F.; Schneider, R.; Legeza, Ö., arXiv:1412.5829 [physics.chem-ph]

Bererdo, E.; Hu H.-S.; Kowalski, K.; Zwijnenburg, M.A., *J. Chem. Phys.* **2013**, 139, 064313.



NANOMORFOLOGIE A ELEKTROCHEMIE ELEKTRODY PŘIPRAVENÉ Z HOPG A NANODESTIČEK SMĚSNÉHO HYDROXIDU Ni/Co

Jan Bohuslav

Ing. Pavel Janda, CSc.

RNDr. Hana Tarábková, PhD.

S rozvojem alternativních zdrojů energie je třeba vyvíjet zařízení pro její ukládání, která by nabídla vysoký specifický výkon a kapacitu. Velká pozornost je věnována elektrochemickým superkondenzátorům, které k ukládání náboje využívají elektrostatické nabíjení i Faradaické reakce.

Mezi materiály pro elektrody slibující nejlepší vlastnosti patří směsné hydroxidy kobaltu a niklu. Mimořádně vysoké specifické kapacity bylo dosaženo s využitím vrstevnatého směsného hydroxidu a grafitu.[1] Silnější vrstva tohoto materiálu ale vykazuje relativně vysoký odpor a zpomaluje tedy reakci.[2]

V této práci se věnujeme elektrodě vytvořené spin-coatingem suspenze delaminovaného směsného hydroxidu na HOPG. Touto metodou vznikají velmi tenké vrstvy umožňující rychlé Faradaické reakce. Elektrochemické reakce byly studovány pomocí cyklické voltametrie. Nanomorfologie a její změna během reakce byla sledována mikroskopem atomárních sil. Výsledky byly porovnány s daty získanými pro hydroxid nikelnatý a hydroxid kobaltnatý.

Reference:

[1] Z. A. Hu, Y. L. Xie, Y. X. Wang, H. Y. Wu, Y. Y. Yang and Z. Y. Zhang, *Electrochim. Acta*, 2009, **54**, 2737–2741.

[2] G. Wang, L. Zhang, J. Zhang, *Chem. Soc. Rev.*, 2012, **41**, 797–828



ELECTROCHEMICAL AND SPECTROPHOTOMETRIC STUDY OF REACTIVITY OF ORTHOPHTHALALDEHYDE WITH ALIPHATIC AMINES

Mgr. Joel DONKENG DAZIE
Prof. RNDr. Jiří LUDVÍK, CSc.

Orthophthalaldehyde (OPA) is used for several decades in two main applications: a) as a "pre-column" derivatization agent in fluorescent determination of amino acids (AAs) [1]; b) in hospitals for disinfection of surgery instruments made from plastics [2]. The second above mentioned application is most probably based on the reaction of OPA with primary amine substituents or other nucleophilic centers in nucleic acids, causing cross-linking and change of their tertiary structure and resulting in decomposition of the cell. In literature related to the disinfection procedure we can find many protocols that differ in composition and in recommended time of use. The reason is that this application has been developed empirically because the detailed mechanism of reaction of OPA with amines and other nucleophiles is not completely elucidated. Although the recent studies were focused on the reaction of OPA with ammonia [3], as the simplest amine, due to simultaneous multiple equilibria the identification of intermediates and products was very difficult. OPA is very slowly soluble in water, but in acetonitrile it dissolves quickly. Therefore the stock solution could be prepared in these two ways. It was found that there is a significant difference in reaction pattern with amines, when using aqueous or non-aqueous stock solution of OPA, respectively. Although the antecedent hydration of OPA was many times reported [4], the dialdehydic form was always considered as the species reacting with amines (generally with nucleophiles). However, the experiments showed that the hydrated OPA reacts with amines directly, whereas the non-hydrated OPA undergoes hydration reaction prior the reaction with amines. This difference is observable also spectrophotometrically. The hydration is pH-dependent: the hydration rate increases with higher pH. The changing course of the reactions of a) OPA with water and b) hydrated/unhydrated OPA with amines under various conditions was evaluated, discussed and the results were mutually compared. For this investigation DC- and DP-polarography, together with cyclic voltammetry were used. The experiments were performed in aqueous buffered solutions of different pH, in non-aqueous acetonitrile and in mixed acetonitrile/H₂O media. Simultaneously, the reactions were followed by UV/Vis spectrophotometry in order to distinguish heterogeneous and homogeneous principle of investigation and to compare the observed kinetics.

References:

- [1] Roth, M. *Anal. Chem.* **1971**, 43, 880-882.
- [2] Simoes, M.; Simoes, L. *J. Basic Microbiol.* **2007**, 47, 230-242.
- [3] Kulla, E.; Zuman, P. *Org. Biomol. Chem.* **2008**, 6, 3771-3780.
- [4] Zuman, P.; Salem, N.; Kulla, E. *Electroanal.* **2009**, 21, 645-649.



THE USE OF SELF-ASSEMBLED MONOLAYER OF THIOLATED CALIX[4]ARENE ON POLYCRYSTALLINE GOLD ELECTRODE SURFACE

Bc. Vojtěch Hrdlička

Doc. Dr. Ing. Tomáš Navrátil

Although mercury electrodes are presumably the best choice for electroanalysis in the cathodic range, they provide only limited selectivity for certain analytes (e.g., nitrated aromatic compounds)¹. Solid electrodes modified with nano-baskets are possible alternative which offers improved selectivity and a much wider potential window for oxidizable analytes². In this study, the thiolated calix[4]arene³ (C[4]A) is used as polycrystalline gold electrode surface modifier.

Thiols rapidly chemisorb on the gold surface even in the absence of applied potential. Majority of the surface is usually covered in tens of seconds, total coverage takes up to a few hours. In our experiments, electrode was modified by dipping into 10^{-4} M thiol solution in DMF. Aliphatic undecanethiol was used for filling the gaps between the thiolated C[4]A molecules³. The C[4]A monolayer was stable in a wide range of potentials. Desorption potentials were pH dependent, cathodic desorption could be recorded only in basic solutions. The anodic desorption took place in the potential range of gold oxides formation.

The properties of the C[4]A monolayer were tested using electrochemically active compounds which are likely to fit inside the C[4]A cavity and possibly can form guest-host complexes: hydroquinone and various nitrated aromatic compounds. The premise of increased selectivity and/or sensitivity was met only partially. Obtained data suggest that the tested electrochemical processes do not take place inside the C[4]A cavity, probably due to its nonconductive properties⁴ and small lower gap of the basket, which does not allow even simple aromatic molecules or their parts to pass through. On the other hand, when the vacancies between the C[4]A molecules were not filled, substantially negative shift in the reduction potentials of nitrated aromatic, which can lead to increase of selectivity, could be recorded.

References

- [1] Prchal V., Vyskocil V., Danhel A., Barek J., Wang J.: Chem. Listy. **2011** 105, 217.
- [2] Mokhtari B., Pourabdollah K., Dalali N.: J. Incl. Phenom. Macro. **2011** 69, 1.
- [3] Sustrova B., Stulik K., Marecek V.: Int. J. Electrochem. Sc. **2013** 8, 4367.
- [4] Liska A., Vojtisek P., Fry A. J., Ludvik J.: J. Org. Chem. **2013** 78, 10651.



THE ROLE OF PALMITOYLATION AND TRANSMEMBRANE DOMAIN IN SORTING OF TRANSMEMBRANE ADAPTOR PROTEINS

Mgr. Tomáš Chum

Mgr. Marek Cebecauer, Ph.D.

Cells communicate with the surrounding environment via specific receptors at the surface. These are prevalently formed by integral membrane proteins or complexes. Their synthesis and insertion into the membrane take place deep inside the cell at the endoplasmic reticulum (ER). Following transport to the plasma membrane has to be effectively controlled by sorting system using specific determinants. Dominant hypothesis defines the length/hydrophobicity of the transmembrane domains (TMD) as primary sorting determinant. We were interested whether other signals may contribute to the effective protein sorting. Using a panel of mutant protein variants we have found that palmitoylation and proximal sequences can modulate sorting of proteins with TMDs of suboptimal length/hydrophobicity. We also demonstrate relationship between presence/absence of the intracellular domain and efficiency of the ER exit. Our observations go in hand with so called hydrophobic mismatch theory, but indicate a unique character of each TMD defined by its primary amino acid sequence. This has significant impact on exact localisation of membrane protein and, therefore, its function.



SYNTHESIS OF MICRO-MESOPOROUS NANOCARBON MATERIALS WITH DEFINED STRUCTURE

Ing. Jana Janošcová

Ing. Petr Sazama, Ph.D.

The microporous and mesoporous materials have received a great attention due to their many important applications. Porous nanocarbon materials have been applied in gas separation, water purification, catalyst supports, electrodes for electrochemical double layer capacitors, and fuel cells¹⁻³.

This study is focused on synthesis and structural analysis of micro-mesoporous nanocarbon materials with high surface area ($\approx 2000 \text{ m}^2 \cdot \text{g}^{-1}$), with defined architecture and dimensions of micro-mesoporous structure.

The main effort was to synthesis the nanocarbon materials using BEA and USY zeolites as hard templates, and the chemical vapour deposition with propylene as a carbon precursor. Synthesis of nanocarbon material was performed using carbonization of the zeolite in a propylene stream (5% vol. in He) from 750 to 850 °C for 1-3 h, followed by heating at 900 °C under helium atmosphere. The zeolite/carbon composite was treated 5 h with 5% HF solution, and the additional treatment was done with 42% HF solution for 1 h to remove the silica template. The final carbon material was isolated by centrifugation, filtration, and was dried in air at 120 °C for 12 h.

Structure of prepared nanocarbon materials was analysed using XRD, XPS, SEM, ¹³C MAS NMR and adsorption of N₂. We optimized the synthesis procedure for effective replication of the channel structure of USY zeolite into carbon. Prepared nanocarbon materials posses of high BET surface area (about $2\ 400 \text{ m}^2 \cdot \text{g}^{-1}$), with highly regular structure resembling organized layers of graphene.

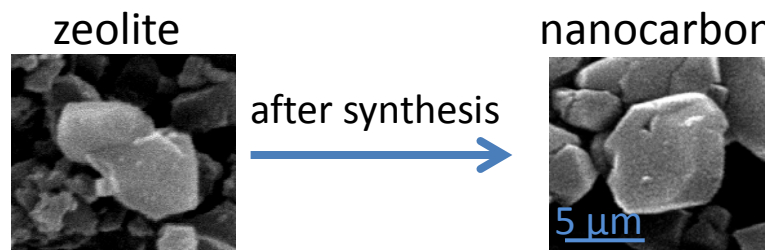


Fig.1 Schematic illustration of synthesis of porous nanocarbon materials using USY zeolite

References:

1. Kyotani, T.; Ma, Z.; Tomita, A.; *Carbon* **2003**, 41, 1451-1459.
2. Lee, J.; Kim, J.; Hyeon, T., *Adv. Mater.* **2006**, 18, 2073–2094.
3. Xu H. et al., *Journal of Catalysis* **2011**, 281, 263–272.



ORTHOPHTHALALDEHYDE – ELECTROCHEMICAL REDUCTION, HYDRATION AND REACTIVITY WITH NUCLEOPHILES

Bc. Kristýna Kantnerová

prof. RNDr. Jiří Ludvík, CSc.

Orthophthalaldehyde (OPA) is used in amino acid determination in combination with HPLC [1] and in medicine as disinfecting agent [2]. Both these methods have been developed only empirically, in literature we can find many protocols that differ in composition and in recommended time of use. The applications are based on reactions of OPA with nucleophiles (mostly amines) however the mechanism is not known (neither in aqueous nor in non-aqueous solutions) [3].

Last years my activity was focused to the role of hydration of OPA and reactivity of OPA with eight aliphatic amino acids. All these reactions were performed in buffered aqueous media to mimic the intracellular conditions. Nevertheless, the non-aqueous conditions in the cell (membranes, liposoms etc.) should be also taken into account.

In order to find the differences in OPA behavior in aqueous and non-aqueous solutions an electrochemical study was made (cyclic voltammetry, preparative electrolysis and coulometry) concerning OPA reduction in aqueous buffer solutions and in non-aqueous acetonitrile. The results were compared and completed by UV-vis spectra.

In slightly basic aqueous solutions OPA is reduced in two irreversible two-electron steps which are strongly suppressed by OPA hydration (dependent on pH). In non-aqueous acetonitrile, the reduction occurs in two one-electron steps and colored radical intermediates are formed. These processes were characterized with *in-situ* UV-Vis spectroelectrochemistry.

In addition to this, the role of oxygen was followed. It was found out that in non-aqueous acetonitrile in the presence of oxygen an electrocatalytic reduction of OPA most probably takes place at more positive potentials than without the presence of oxygen.

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GERMANOSILICATE PRECURSORS OF ITH, ITR, IWR AND UOV ZEOLITES FOR ADOR PROCESS

Valeryia Kasneryk

Maksym Opanasenko, Ph.D.

Recently, the ADOR strategy was developed for the synthesis of new zeolites [1]. It includes following steps: a) **Assembly** – synthesis of initial 3D zeolite; b) fabrication of lamellar 2D material from parent 3D zeolite – **Disassembly**; c) post-synthetic modification resulting in the **Organization** of layers; and finally d) **Reassembly** – condensation of 2D layers to produce new 3D-material. Presence of germanium-rich double four-member rings (D4Rs) in the framework of germanosilicates, such as ITH, ITR, IWR and UOV, makes them perspective starting materials for ADOR process.

The tunable disassembly of Ge-rich zeolites UOV, ITR, ITH and IWR was performed under mild conditions [2]. Chemical composition of the parent zeolite, acid concentration, temperature and duration of hydrolysis were found to be the critical factors controlling the disassembly degree of mentioned zeolites. However, partial distraction of the layers was observed in the case of ITH and IWR zeolites.

Controllable hydrolysis of zeolite UOV followed by calcination of obtained precursor allowed to produce new zeolite, that was confirmed by the theoretical simulations.

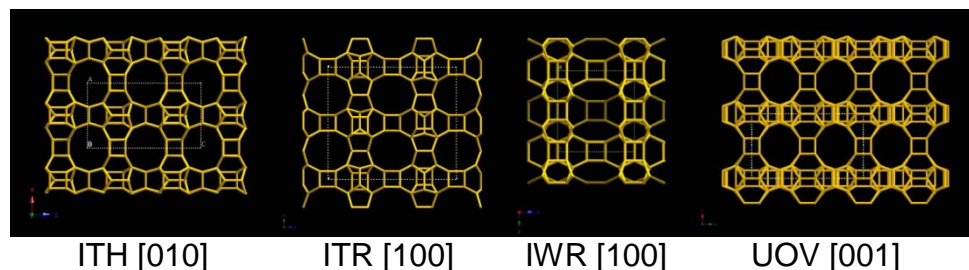


Fig. Structure of zeolites in different projections

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LABORATORY MODELLING OF THE ENERGETIC ION PRECIPITATION IN THE IONOSPHERE OF TITAN

Mgr. Věra Křížová

Mgr. Miroslav Polášek, Ph.D.

Saturn's magnetosphere produces a plasma consisting of H^+ , H_2^+ and so-called water group ions (H_3O^+ , H_2O^+ , OH^+ , and O^+). These ions are the products of ionization of neutrals, which takes place in the inner and middle magnetosphere. [1] The plasma is quite rapid, varying from $\sim 30 \text{ km}\cdot\text{s}^{-1}$ near Enceladus at $4 R_S$ to $170 \text{ km}\cdot\text{s}^{-1}$ near Titan at $20 R_S$. [1] Cassini CAPS spectrometer detected a precipitation of O^+ ions with energies of 1 – 4 keV on Titan. [2] It has been speculated [3] that a low percentage of O^+ flux is converted to O^- ions. These ions may play a part in Titan's negative ion chemistry, which is, however, rather poorly understood. [4, 5] The plasma ions subsequently induce ionization and fragmentation of the Titan's atmospheric constituents, namely N_2 , CH_4 , C_2H_2 , C_2H_4 , HCN , HC_3N , etc. [6]

The main aim of our study is to determine ionization cross sections and the extent of fragmentation of the above mentioned atmospheric constituents on Titan by simulating the collisions of high energy water ions ($\sim \text{keV}$), both positively and negatively charged, with gases typical for Titan's atmosphere. For that purpose, a modified sector type mass spectrometer was used. There is a small quadrupole mass analyser with a collision chamber attached to the instrument between the magnetic and the electrostatic analyser. The projectile ions are produced in an electron impact ion source and mass selected by the magnetic analyser. As they fly through the analyser, they reach the collision chamber, where they eventually collide with a molecule of a neutral gas. The secondary ions produced by such collisions are then analysed by the quadrupole mass analyser.

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EXPLICITLY CORRELATED COUPLED CLUSTER CALCULATIONS WITH INCOMPLETE MODEL SPACE AND OPEN SHELL TRIPLE CORRECTIONS

Mgr. Jakub Lang

Doc. Mgr. Jiří Pittner Dr. rer. nat.

The single reference coupled cluster (CC) method is one of the most popular methods in quantum chemistry, however its description of systems with high static correlation is rather poor. For example black box coupled cluster methods such as CCSD and CCSD(T) are unable to properly calculate activation barrier of two transition states during the isomerization of bicyclo[1.1.0]butane to buta-1,3-diene. In these cases, use of multireference methods, which correctly describe static correlation, is necessary.

Unfortunately, to accurately describe the static correlation we need to use model (active) space spanned by all reference determinants, which can substantially prolong calculations and/or cause intruder state problems. However, this can be bypassed using the C-condition incomplete model space approach developed in my group and extensively researched for standard multireference CC methods.

Additionally, open shell triple corrections allows us to use single excited determinants and describe systems when single excited determinants play considerably big role.

Furthermore, explicitly correlated methods are able to converge to CBS much faster and gives almost same results as methods with bigger basis sets and can rapidly speed-up the convergence. Combining already mentioned methods with explicit correlation, we can achieve results comparable to experiments with much lesser computational demands.

In my lecture, I will present overview and theoretical details of these two approaches.

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STEREOELECTROCHEMISTRY OF ISOMERIC NITRO- AND NITROSOCALIX[4]ARENES

Mgr. Alan Liška

prof. RNDr. Jiří Ludvík, CSc.

Calixarene skeleton is a favorite framework in supramolecular chemistry [1], which is, however, not electroactive. Therefore, for any direct electrochemical studies it's essential to introduce a redox probe. Our project is focused mainly in nitro [1-5], if need by nitroso group [2]. Both of them – in the first step – are reversibly reduced in aprotic media by one electron to form a stable radical anion, e.g. (1) [3].



Calix[4]arenes can exist in four atropoisomers: *cone*-, *paco*-, *1,2*- and *1,3-alt*. To find the relation between conformation and electrochemical response (“*stereo-electrochemistry*”), several series of experiments have been done recently [2,4,5]. The main findings show that

- (a) simple electrochemical methods can reveal the dynamics of calixarene systems in the solutions independently on classically used techniques (NMR) and
- (b) the flexibility vs. rigidity of calixarene skeleton seems to be unpredictable on the basis of conformation or substitution knowledge itself.

The *m*- or *m/p*-polynitro-/nitroso-*cone*-calix[4]arenes are rigid like *p*-polynitro-*1,3-alt*-calix[4]arenes [2] but only the *p*-substituted *cone*-calix[4]arenes are flexible [4,5].

All the discussed compounds contain non-communicating redox centres, the reduction intermediates are polyradical polyanions [5]. As expected, the nitroso derivatives are reduced at less negative potentials than the nitro analogues [2].

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QUASI-RANDOM SAMPLING FOR ESTIMATING UNCERTAINTIES AND SENSITIVITY OF NUMERICAL MODELS: CASE STUDIES IN COMBUSTION CHEMISTRY AND LASER ABLATION PHYSICS

Ing. Lukáš Pečínka

prof. Ing. Zdeněk Zelinger, CSc.

Quasi-random sampling (QRS) is an efficient strategy for exploring multidimensional input parameter space of complex models and for the determination of variance based sensitivity indices through the application of response surface methods [1, 2].

In frame of this study QRS (also known as QMC – Quasi Monte Carlo) is used to estimate the global uncertainty and sensitivity of selected mathematical models. Analogous approach employing low-discrepancy (Sobol) sequence was used to support the modelling issues recently solved in the field of combustion chemistry (gas phase kinetics) and laser ablation physics (thermodynamics of condensed matter).

In the first case, chemical kinetics of elementary reaction steps for the case of high temperature oxidation of dimethyl ether (DME) in gaseous phase was considered. The most important reactions in premixed flat flames of dimethyl ether/air mixture were identified and their global sensitivity indices were quantified based on chemical kinetic modelling (Cantera software toolkit). The second case relates to uncertainties of predicted ablation curve determined from material (thermophysical) properties of lithium fluoride using one-dimensional thermomechanic model (XUV-ABLATOR code).

Open-source and cross-platform framework (set of specific purpose Python scripts) was developed to interface the original FORTRAN routine (XUV-ABLATOR) or C++ kernel (Cantera) and to enable efficient data manipulation and ensembles of calculations.

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POSTSYNTHESIS INTRODUCTION OF TITANIUM INTO ZEOLITE BASED EPOXIDATION CATALYSTS

Ing. Jan Přeč

Prof. Ing. Jiří Čejka, DrSc.

Titanosilicate zeolites are subject of interest as catalysts for epoxidation of C=C double bonds with hydrogen peroxide as oxidation agent. Surface area, diameter and topology of the channels and number and coordination state of titanium atoms are the basic parameters, determining the catalyst performance. The amount of Ti atoms, which can be incorporated into the framework, is limited to approximately 3% of all tetrahedral atoms in the best cases (TS-1). This means that the total amount of active sites remains much lower than in case of acidic aluminosilicate zeolites.

Our group has reported a method of postsynthesis titanium introduction during pillaring of layered TS-1 in order to suppress active phase dilution by the silica pillars. Addition of titanium into the pillaring mixture led to strong increase in activity of the catalyst. The yield of cyclooctene oxide over Ti-pillared TS-1 catalyst was 16.9% after 4 h contrary to pillared TS-1 without titanium addition (yield 3.5%)¹.

Extention of this method to Ti-IPC-1PI material (lammelar titanosilicate prepared from Ti-UTL (Si/Ti=100) by the top-down synthesis) provided even better results. The yield of cyclooctene oxide over Ti-pillared Ti-IPC-1TiPI catalyst was 23% after 2 h and the yield over Ti-IPC-1PI without titanium addition was 5.5% after 2 h.

Similarly, a very active Ti-SSZ-33 catalyst (yield of cyclooctene oxide 28% after 4 h) was prepared from deboronated SSZ-33 zeolite². The SSZ-33 material was treated with titanium (IV) butoxide or titanium (IV) chloride at conditions similar to the above pillaring procedures.

The results observed in the case of Ti-SSZ-33 lead us to a theory that an impregnation of the external surface of the layers occur during the pillaring with titanium addition. The resulting material possess high amount of well accessible and active Ti species and therefore in provides good performance during the catalytic epoxidation of bulky substrates.

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GRAPHENE WRINKLES

Bc. Jaroslava Řáhová

*Mgr. Otakar Frank, PhD.,
Prof. RNDr. Jan Jehlička, CSc.*

Graphene provides wide range of technical utilities. A lot is known about its electrical and optical properties, however, the electron structure of graphene may be influenced by mechanical deformation of the lattice. This can provide even wider range of possible applications of graphene. We measured graphene wrinkles induced by strain and observed their topography as well as their arrangement.

Graphene monolayers as well as few-layers graphene flakes were prepared by mechanical exfoliation on both unstrained and pre-strained (bent) PMMA substrates. Graphene flakes were detected with an optical microscope, the characterization of wrinkles was made mainly by Raman spectroscopy (to distinguish number of graphene layers) and Atomic Force Microscope. Parameters (full wavelength and amplitude) of graphene wrinkles were measured in Gwyddion programme and the obtained values analysed statistically in Wavemetrics Igor.

Strong linear relation between wavelength and amplitude of the thus formed wrinkles as well as the dependence of wavelength and amplitude values on the number of layers appear to be the most noticeable features. Upon comparison of wrinkles exfoliated on unstrained and pre-strained substrates, the pre-strained substrate induces formation of wrinkles with a narrower distribution (expressed as standard deviation) of wavelengths and amplitudes.



SYNTHESIS OF ZEOLITE SSZ-16 LAYERS ON POROUS SUPPORTS

Mgr. Tat'ana Supiňková

Ing. Pavel Hrabánek, Ph.D.

RNDr. Milan Kočířík, CSc.

Zeolites are stable microporous aluminosilicates that can be used as molecular sieves for separations of various gas mixtures. The framework structure of zeolite SSZ-16 consists of three-dimensional pore network with pore size of 0.34 nm x 0.36 nm. Small pore zeolite SSZ-16 is considered to be promising candidate for CO₂ capture from natural gas. The current aim of study is focused on the development of SSZ-16 layers that can be further up-scaled to prepare SSZ-16 composite membranes. SSZ-16 layers were synthesized on macroporous stainless steel supports coated by TiO₂ to suppress influence of support leaching during direct in situ hydrothermal crystallization. The syntheses were performed inside Teflon-lined stainless steel rotational autoclaves at 160 °C from 7 to 21 days. Before the crystallizations, the synthesis solutions were pre-aged at elevated temperature of 80 °C inside an oil bath for 7 days under vigorous stirring to promote the formation of nuclei. Molar ratio of synthesis solutions was varied to examine phase purity of the prepared layers measured by XRD. Morphology of prepared layers and crystal size coupled with support coverage were observed by SEM. The results showed that pure phase SSZ-16 layers were synthesized only in narrow molar compositions of pre-aged synthesis solutions. Crystallizations from diluted solutions led to amorphous phases or different zeolite phases (mordenite). The support coverage by SSZ-16 particles was increased with longer crystallization period.



VYSOCE ROZLIŠENÁ OVERTONOVÁ SPEKTROSKOPIE ATMOSFÉRICKY RELEVANTNÍCH MOLEKUL

Bc. Vít Svoboda

Mgr. Ondřej Votava, Ph. D.

Zemská atmosféra může být nahlížena jako ohromný fotochemický reaktor, kde energie nutná k překonání aktivační bariéry reakce je dodána pomocí fotonů. Nejčastěji se jedná o ultra-fialové (UV) fotony, jejichž energie je srovnatelná s vazebnou energií typické kolalenní vazby. Ovšem i méně energetické infračervené (IR) fotony mohou iniciovat reakční přeměnu. Toho je docíleno excitací vyšších vibračních stavů molekuly, které jsou energeticky blízké tranzitnímu stavu reakce. Pak hovoříme o tzv. vibračně iniciované fotochemii.

Tyto stavy můžeme studovat pomocí overtonové spektroskopie, kdy sledujeme přechody ze základního vibračního stavu do vyšších vibračních stavů, které doprovází změna vibračního kvantového čísla o více než jedničku. Pracujeme-li s vysokým rozlišením, můžeme získat overtoné rotačně-vibrační spektrum, ze kterého lze získat detailní informaci o struktuře molekuly blízké struktuře tranzitního stavu. Její znalost je důležitá pro studium vibračně iniciované fotochemie.

Proto bude představena komplexní metoda, jak overtonová spektra molekul měřit (vysoce rozlišená overtonová spektroskopie v supersonických expanzích) a následně analyzovat (metoda dvou teplotní analýzy kombinovaná s metodou kombinačních diferencí). Metoda bude demonstrována na dvojici atmosféricky relevantních molekul – kyselina mravenčí a metanolu. Bude ukázáno, že v obou případech je možné získat spolehlivá spektroskopická přiřazení, i přes velmi komplikovaná spektra těchto molekul. Výsledky pak mohou sloužit jako kvalitní experimentální data pro následné teoretické studie.

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PŘÍPRAVA NANOČÁSTIC OXIDU STŘÍBRNÉHO V SEMIORGANICKÉM PROSTŘEDÍ A JEJICH APLIKACE NA KULTURY PLÍSNÍ

Lukáš Šimaňok

Mgr. Radek Žouželka

V dnešní době jsou velmi rozvinuty metody syntézy nanočástic stříbra, kterých se hojně využívá jako biocidního prostředku. Tyto metody jsou založeny na redukci kationtů kovů pomocí redukčních činidel, což ovšem do výsledné směsi zanáší množství dalších eventuálně nežádoucích látek.

U stříbrných iontů byly biocidní účinky zjištěny také, nicméně vyšší koncentrace poškozují i tkáně člověka. Z tohoto důvodu není vhodné používat dusičnan stříbrný, což je nejčastější zdroj stříbrných iontů, jakožto velmi dobře rozpustné soli, pro přímou aplikaci jako protekčního materiálu. Také je zde problém fotostability samotného dusičnanu, neboť roztok po aplikaci a interakci se světelným zářením tmavne a dochází k chemickým změnám.

Pokud chceme využít aktivity stříbrných iontů ve vodném prostředí, je zapotřebí sloučeniny, jejíž rozpustnost ve vodě je omezená. Zároveň chceme minimalizovat negativní změnu struktury ošetřovaného povrchu, na což jsou vhodné nanočástice a nanovrstvy.

Ve své práci se zabývám přípravou nanočástic oxidu stříbrného v prostředí voda-ethanol, kdy se jedná o fotochemickou reakci ve slabě zásaditém prostředí. Tyto syntézy jsou šetrné k životnímu prostředí, a produkty jsou velice stabilní v čase i při změnách teplot.

U takto připravených částic jsou následně zjišťovány biocidní vlastnosti na kulturách plísní, kdy jsou částice aplikovány jednak přímo do živné půdy před vystavením spor plísní, a jednak již přímo na půdu očkovanou kulturami plísní.

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QUANTUM ALGORITHMS FOR MANY-BODY SYSTEMS – SIMULATION FOR FEW-BODY STARTING PROBLEMS

Ing. Mgr. Jakub Višňák

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

The study presents (classical) computer simulations of quantum algorithms for hamiltonian eigenvalue estimation. Quantum algorithms allow for the efficient eigenvalue calculation (considering all possible multi-particle states within given set of one-particle functions – e.g. in the frame of Full CI method) in contrast with the classical ones where exponential scaling for the FCI method is unevitable [1,2].

For example, the Abrams-Lloyd algorithm applied to the Nuclear orbital-Molecular orbital method (NOMO,[3]) goes beyond the Born-Oppenheimer approximation and give us direct access to vibrational frequencies, anharmonicities and rotational constants.

The lecture presents results of NOMO/CI hamiltonian eigenvalue estimation by the Iterative Phase Estimation Algorithm (IPEA, part of the QCI [4]), simulated on a classical computer, as a demonstration of possibility to directly compute energy of rotationless vibrational 0-1 transition in several isotopomers of the hydrogen molecule (H_2 , HD, HT, ...) on (future) quantum computers.

In the second part, the possibility of applying the general formalism of NOMO/CI (coupled with quantum algorithm for FCI based on IPEA) to different bounded many-body quantum systems (e.g. atomic nuclei within the phenomenological mechanical approach) is studied.

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MICROMECHANICAL SENSOR AND LASER PHOTOACOUSTIC SPECTROSCOPY IN GASES

Bc. Tereza Vlasáková

Prof. Ing. Zdeněk Zelinger, CSc.

Laser photoacoustic spectroscopy (PAS) is a method that utilizes the sensing of the pressure waves that emerge upon the absorption of radiation by absorbing species. The use of the electret or condenser microphone as a pressure sensor has already reached its limit, and a new type of microphone – an optical microphone – has been suggested to increase the sensitivity of this method [1]. The movement of a micro-lever or a membrane is sensed via a reflected beam of light, which falls onto a position-sensing detector.

Our method utilizes a photoacoustic (PA) cell equipped with a microphone as well as a place for mounting the investigated elements. A discretely tunable CO₂ laser was used as a source of radiation energy for PAS experiments. Sensitivity testing of investigated sensing elements was performed with aid of concentration standards based on permeation method and a mixing arrangement in a flow regime.

Two types of sensing elements have been tested – four coupled silicon micro-levers and a multilayer graphene membrane – which have the potential to enhance this sensitivity further. Graphene sheets possess outstanding electromechanical properties and demonstrate impressive sensitivity as mass detectors. Their mechanical properties make them suitable for use as micro-/nano-levers or membranes, which could function as extremely sensitive pressure sensors.

To our knowledge, we have produced the first demonstration of the feasibility of using four coupled silicon micro-levers and graphene membranes in an optical microphone for PAS. New sensing Multi-Layer Graphene elements were later prepared according to slightly modified method [2] using different technique of attaching membrane to glass window. Further, we have studied the influence of surface metallization and construction changes on the sensitivity of these elements.

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CHARACTERIZATION OF GRAPHITE ELECTRODES MODIFIED BY METHYLENE BLUE-POLYMER

Mgr. Magda Zlámálová

Ing. Pavel Janda, CSc.

In recent years, hydrogen sulphide has been extensively studied as the human endogenous messenger molecule of gas with auspicious therapeutic effects ¹. It has a physiologic gasotransmitter function comparable to NO and CO ². Due to very low physiological concentrations and potential therapeutic concentrations, there has been increasing need for more appropriate analytical methods with emphasis on their sensitivity and selectivity.

Electropolymerization is an effective way of the electrode surface modification. Electrolytically synthesized polymers exhibit some unique behavior that the corresponding monomers not always display. The electrocatalytic activity of poly(methylene blue) (pMB) in the presence of some biologically active compounds has been reported in several studies ³⁻⁵.

This work deals with electrochemical study of methylene blue (MB) polymerization as well as characterization of deposited conductive film on basal plane highly oriented pyrolytic graphite (HOPG) and pencil-graphite electrode (PGE). Poly(methylene blue) modified electrodes (HOPG/pMB and PGE/pMB) have been prepared by potential cycling in basic aqueous electrolyte solution containing methylene blue monomer. It has been found that electrochemical properties and electrocatalytic activity of deposited film are greatly influenced by the type of electrode substrate. Developed electrodes have been further investigated as potential sensors for SH⁻ group containing compounds.

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