

MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Dr. Páll Þórðarson

Lærdómar náttúrunnar: Sjálfsmsett efni og nanótæki

(Nanobiotechnology and bio-organic chemistry)

Staður (Place): Stofa VR-158, Háskóli Íslands, Hjarðarhaga 2-4.

Dagsetning (Date): Fimmtudagur 17. júlí 2008.

Tími (Time): 11:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Í þessum fyrirlestri mun Dr. Páll Þórðarson, efnafræðingur við New South Wales Háskólan í Sydney, Ástralíu fjalla um nýustu rannsóknir sínar á sviði sjálfsmsettra efna og nanótæki. Áhersla verður lögð á tvö verkefni, annars vegar lífráfnanótækni sem ganga fyrir sólarorku (Chem. Commun. 2007) og hins vegar hönnun nýrra sjálfsmsettra gefna sem eru viðkvæm fyrir neikvæðum jónum s.s. klóríði og brómíði (J. Am. Chem. Soc. 2007) sem gæti haft mikilvægt notagildi fyrir lyfjagöf, sér í lagi gegn krabbameini.

(Our research interests are in the broad areas of nanobiotechnology and bio-organic chemistry. The approach we have taken is the bio-mimetic one, i.e. to look to Nature for inspiration for solving the challenges ahead, especially as Nature provides us with many functional examples of nanotechnology in action.

<http://www.chem.unsw.edu.au/research/groups/thordarson/>

Málstofustjóri: Bjarni Ásgeirsson/ bjarni@raunvis.hi.is

MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Meistaraprófsfyrirlestur

Sunna Ólafsdóttir Wallevik

Rannsóknir á stellingajafnvægi setinna silacyclohexan afleiða
(Conformational behavior of substituted silacyclohexanes)

Staður (Place): Stofa VR-158, Háskóli Íslands, Hjarðarhaga 2-4.

Dagsetning (Date): Mánudagur 25. ágúst 2008.

Tími (Time): 16:45.

Fyrirlesturinn verður á íslensku (The talk will be given in Icelandic).

Útdráttur: Valdar ein- og 1,1-tvísættar silacyclohexan afleiður voru smíðaðar í þeim tilgangi að rannsaka sameindarbyggingu áslægra og þverlægra stólforma þeirra og jafnframt að ákvarða varmafræðilegt jafnvægi þeirra á milli. Lagt var upp með að rannsaka þessar afleiður með beygju rafeindageisla í gasham (GED), hitastigsháðri Raman titringsrófagreiningu og lághita kjarnarófs mælingum (DNMR). Þegar möguleiki var á, voru niðurstöður tilrauna bornar saman við spágildi skammtafræðilegra reikninga (QC) og við niðurstöður samsvarandi cyclohexan afleiða. Þessar rannsóknir verða kynntar ásamt efnasmíðum og greiningu stellingajafnvægis á fleiri nýstárlegum kísilinnihaldandi efnasamböndum.

Summary: Conformational behavior of substituted silacyclohexanes. A selection of mono- and 1,1-disubstituted silacyclohexanes were synthesized with the main aim of investigating the molecular structure of their axial and equatorial chair conformers as well as the thermodynamic equilibrium between these species. The new compounds were intended for investigations by means of gas electron diffraction (GED), dynamic nuclear magnetic resonance (DNMR) and temperature dependent Raman spectroscopy. Comparisons with available quantum chemical calculations (QC) along with results for analogous cyclohexane derivatives were also made. These investigations will be discussed as well as the synthesis and conformational investigation of some other novel silicon containing compounds.

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Meistaraprófsfyrirlestur

Erlendur Jónsson

Theoretical studies of the excited states of HCl

(Kennilegir reikningar á örvuðum ástöndum HCl)

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.

Dagsetning (Date): Miðvikudagur 27. ágúst 2008.

Tími (Time): 16:45.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Summary:

The HCl molecule is a very popular molecule for spectroscopic studies. At the Science Institute of the University of Iceland, HCl has been studied for a few years with the REMPI (resonance enhanced multiphoton ionization) technique. This technique enables the study of previously unknown excited states.

Parallel to that research are the *ab-initio* calculations, where potentials of the excited states are calculated. From the potentials it's possible to find the spectroscopic parameters of each excited state. Several excited states of the HCl molecule have been calculated.

The capability to do useful calculations for excited states of molecules is fairly recent. The method, which is used here, is the equation of motions (EOM) formulations for the coupled cluster methods (CC).

Útdráttur:

HCl sameindin er vinsæl í rannsóknum með litrófsgreiningu. Sameindin hefur verið rannsökuð í nokkurn tíma við Raunvísindastofnun Háskólans með REMPI aðferðinni (Resonance Enhanced Multiphoton Ionization). Þessi aðferð gerir kleift að rannsaka áður óþekkt örvuð ástönd sameindarinnar.

Samhliða þessum rannsóknum eru *ab-initio* útreikningar, þar sem hægt er að reikna mættisferla örvuðu ástandanna. Út frá þessum mættisferlum er hægt að reikna litrófsfasta hvers ástands fyrir sig. Nokkur örvuð ástönd HCl sameindarinnar hafa verið reiknuð.

Getan til að beita útreikningum á örvuð ástönd sameinda er fremur nýleg. Aðferðin sem hér er beitt er equations of motion (EOM), sem er stækkun á coupled cluster (CC) aðferðinni.

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Meistaraprófsfyrirlestur

Ragnar Björnsson

Theoretical studies of silicon-containing six-membered rings

(Kennilegir reikningar á kísilinnihaldandi sexhringjum)

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.

Dagsetning (Date): Föstudagur 29. ágúst 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Útdráttur: Skammtafræðilegir reikningar á einsetnum og 1,1-tvísætum 1-silacyclohexanafleiðum voru framkvæmdir með það fyrir augum að ná samræmi milli kennilegra reikninga og tilraunaniðurstaðna fyrir stellingajafnvægi milli áslægrar og þverlægrar stellingar. Ný kynslóð DFT aðferða getur spáð fyrir um orkumun stellinga mun nákvæmar en áður, skv. samanburði við coupled cluster reikninga og tilraunaniðurstöður. Áhrif kísilviðbótar inn í cyclohexanhringinn voru rannsökuð og spáð var fyrir um stellingajafnvægi margra mismunandi kísilinnihaldandi sexhringja, sem sumir hafa aldrei verið rannsakaðir áður. Stellingajafnvægi kísilinnihaldandi sexhringja er töluvert frábrugðið því sem þekkt er fyrir cyclohexan og aðra heterohringi og bendir til þess að við eigum enn talsvert eftir í land með að skilja stellingajafnvægi einfaldra lífrænna sameinda.

Summary: Monosubstituted silacyclohexanes were studied by theoretical methods with the intent of reproducing experimental results of the energy difference between the axial and equatorial conformers. Density functional theory as well as post Hartree-Fock methods were utilized. Recent density functionals were found to be capable of reproducing highly accurate coupled cluster calculated electronic energy differences, as well as experimentally obtained free energy and enthalpy differences.

The effect of silicon substitution in the cyclohexane ring was investigated and the conformational properties of a number of silacyclohexanes, that have not been investigated experimentally or theoretically yet, were predicted. The remarkably different conformational properties of silacyclohexanes compared to cyclohexanes and other heterocycles indicate that we do not yet fully understand conformational behaviour of simple organic molecules.

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

The *Vibrio salmonicida* genome project

Nils Peder Willassen

Dept. of Molecular Biotechnology, Institute of Medical Biology,
University of Tromsø, Norway.

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.

Dagsetning (Date): Föstudagur 5. september 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Summary: Six years ago we initiated a project with the intention to provide sequences from a psychrophilic microorganism in order to explore cold adapted features of enzymes. *Vibrio salmonicida*, a psychrophilic and moderate halophilic pathogen, which is the causative agent of cold-water vibriosis in marine aquaculture, was selected as source.

The project developed soon into a whole genome sequencing project and further into a functional genome project were one of our aims is to understand environmental adaptation at a molecular level.

In the talk I will give an overview of the project and give some examples of subprojects we are currently running to achieve our goals.

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Meistaraprófsfyrirlestur

Ester Eyjólfsdóttir

Títanasiloxan komplexar: Smíðar, greiningar og hvörf.

Synthesis, analysis and reactions of novel titanasiloxane complexes.

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 12. september 2008.
Tími (Time): 12:30.
Fyrirlesturinn verður á íslensku (The talk will be given in Icelandic).

Ágrip: Þekkt er frá fyrri rannsóknum að í hvarfi milli $\text{Cp}^{\text{xpm}}\text{Ti}(\mu\text{-O})_3[\text{tBuSi-CH}_2]_3$ ($\text{Cp}^* = \text{C}_5\text{Me}_4(p\text{-C}_6\text{H}_4\text{Me})$) og MeOH í CDCl_3 myndaðist tvíliða þar sem Ti-Cp^{xpm} tengið hafði rofnað og títanatómin tengst í staðinn metanóli og tveimur brúandi metoxy hópum hvort.

Í þessu verkefni var fylgst var með framgangi hvarfa $\text{Cp}^*\text{Ti}(\mu\text{-O})_3[\text{tBuSi-CH}_2]_3$ (**1**) við alkóhólin MeOH, EtOH, ¹PrOH, ¹BuOH og PhOH með reglulegum NMR mælingum í CDCl_3 . Einnig voru gerðar tilraunir með aðra leysa og var bösunum NaOMe og NaOH bætt úti hvörf við MeOH í von um að hvarfhraði myndi aukast, en þessi hvörf gerast gífurlega hægt. Greint verður frá niðurstöðum þessarar tilrauna í fyrirlestrinum, auk þess sem tillaga að hvarfgangi verður sett fram. Einnig verður fjallað um smíði og greiningar á títanasiloxan átthring (**4**) sem myndaðist óvænt við hvarf siloxan sexhrings við Cp^*TiCl_3 , sem og myndefni hvarfs þessa sama átthrings við MeLi.

Abstract: A reaction between $\text{Cp}^{\text{xpm}}\text{Ti}(\mu\text{-O})_3[\text{tBuSi-CH}_2]_3$ ($\text{Cp}^* = \text{C}_5\text{Me}_4(p\text{-C}_6\text{H}_4\text{Me})$) and MeOH in CDCl_3 had previously been shown to yield a dimer where the Ti-Cp^{xpm} bond had dissociated and the titanium centers were instead connected to two bridging methoxy groups and a methanol group each.

In this project the reactions between $\text{Cp}^*\text{Ti}(\mu\text{-O})_3[\text{tBuSi-CH}_2]_3$ (**1**) and the alcohols MeOH, EtOH, ¹PrOH, ¹BuOH and PhOH in CDCl_3 were monitored by NMR spectroscopy. Experiments where other solvent systems were employed were carried out, and the bases NaOMe and NaOH added to reactions with MeOH in order to increase the reaction rate, since these reactions are extremely slow. The results from these experiments will be discussed in this presentation, and a mechanism proposed. The synthesis and analysis of an eight-membered titanasiloxane ring (**4**) will also be discussed, but it formed unexpectedly in a reaction between a six-membered siloxane ring and Cp^*TiCl_3 . The product from a reaction of **4** and MeLi will be described.

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Meistaraprófsfyrirlestur

Guðjón Andri Gylfason

Bestun aðferða við einangrun og greiningu himnufleka úr þarmaþekju Atlantshafsporsks (*Gadus morhua*), með áherslu á alkalískan fosfatasa.

Optimization of methods for isolation and analysis of lipid rafts from Atlantic cod (*Gadus morhua*) intestinal enterocytes, with alkaline phosphatase as a focus point.

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 19. september 2008.
Tími (Time): 12:30.
Fyrirlesturinn verður á íslensku (The talk will be given in Icelandic).

Ágrip: Himnuflekar eru þétt þökkuð svæði innan frumuhimnunnar, rík af kólesteróli og glýkósphingólípíðum. Einangrun þeirra hefur, eftir því sem við best vitum, ekki verið framkvæmd áður í geislauggum (*Actionoerygi*). Fyrsta markmiðið var að einangra og auðkenna burstalagshimnur og himnufleka úr þarmaþekjufrumum Atlantshafsporsks til að staðfesta tilvist þeirra. Ólíkar aðferðir sem þörfuðust bestunar sýndu allar aukningu í magni merkiensíma, bæði í burstalagshimnum og himnuflekum, auk þess sem kólesteról/prótein hlutfall var hátt innan himnuflekanna. Framkvæmdar voru ³¹P-NMR mælingar á fosfólípíðum sem gáfu upplýsingar um hátt fosfatidylkólínhlutfall í burstalagshimnum en hins vegar hátt hlutfall sphingómýelíns í himnuflekum. Próteinmengjafræðilegar upplýsingar fengust með notkun massagreina (MALDI eða LC-ESI) á trypsinmeltum próteinsýnum og hafa nokkur einkennandi prótein verið auðkennd í himnuflekunum s.s. aminópeptíðasi N, beta actin og villin 2. Samantekið sýndu allar mælingarnar þekkt einkenni himnufleka og tilvist þeirra því verið staðfest innan burstalagshimna þarmaþekjufrumna Atlantshafsporsks (*Gadus morhua*).

Abstract: Membrane lipid rafts are glycosphingolipid/cholesterol-enriched membrane microdomains in the plasma membrane. To the best of our knowledge, no studies have been performed on lipid rafts from brush border membrane (BBM) in ray-finned fishes (*Actionoerygi*). Our aim was to isolate and characterize the BBM and lipid rafts from Atlantic cod (*Gadus morhua*) intestinal enterocytes to confirm their existence. All methods were first optimized and then used to show the enrichment of marker enzymes in both BBM and lipid rafts and high cholesterol/protein ratio in the lipid raft fraction. We also performed lipid analysis with ³¹P-NMR, which gave relative high content of phosphatidylcholine in the BBM but on the other hand high content of sphingomyelin in the lipid raft fraction. Proteomics studies were performed by MALDI or LC-ESI mass spectrometry from trypsin digested protein samples and various proteins have been associated with our lipid raft preparation such as aminopeptidase-N, beta-actin, and villin 2. In summary, the selected membrane fraction showed the characteristics of lipid rafts and their existence has, therefore, been confirmed in the intestinal BBM enterocytes from Atlantic cod (*Gadus morhua*).

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Puru Jena

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Nano Materials for Hydrogen Storage

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 26. september 2008.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given in English).

Abstract: The limited supply of fossil fuels, its adverse effect on the environment, and growing worldwide demand for energy has necessitated the search for new and clean sources of energy. The possibility of using hydrogen to meet this growing energy need has rekindled interest in the study of safe, efficient, and economical storage of hydrogen. The current methods for storing hydrogen as a compressed gas or liquid are not suitable for practical applications. An alternate method for hydrogen storage involves metal hydrides. Although conventional intermetallic hydrides can store hydrogen reversibly at around room temperature, the relative weight of stored hydrogen in these materials is rather low (1 – 3 wt %) and do not meet the requirements of the transportation industry (~10 wt %). For this the host materials have to consist of light elements such as Li, Be, B, C, Na, Mg, and Al. Unfortunately, the bonding of hydrogen in these materials is rather strong (covalent or ionic) and the thermodynamics and kinetics are poor. Ways must, therefore, be found to weaken the hydrogen bond strength so that host materials composed of light elements can be used as effective hydrogen storage materials.

This talk will discuss how the novel properties of materials at the nanoscale can improve the thermodynamics and kinetics of hydrogen. In particular, I will discuss how carbon based nanostructures such as nanotubes and fullerenes can be used as catalysts to improve the hydrogen uptake and release in complex light metal hydrides such as sodium alanate. I will also discuss how carbon nanotubes and fullerenes can be functionalized with metal and B atoms to adsorb hydrogen in a novel quasi-molecular form and how such a bonding can improve the kinetics and thermodynamics of hydrogen sorption. The results, based upon density functional theory and quantum molecular dynamics, provide a fundamental understanding of the interaction of molecular hydrogen with hosts consisting of light elements. It is hoped that the understanding gained here can be useful in designing better materials for hydrogen storage. Results will be compared with available experimental data.

MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Meistaraprófsfyrirlestur

Jón Bergmann Maronsson

Theoretical Calculations of Electrochemical Systems.

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): **Mánudagur** 29. september 2008.
Tími (Time): 16:45.
Fyrirlesturinn verður á ensku (The talk will be given in English).

Summary: Even though electrochemistry is an old and important branch of chemistry, the atomic level mechanism of the reactions, structure of the solid-liquid interface at the electrodes and the origin of overpotentials are not well understood.

Atomic scale information is hard to come by with experimental techniques and theoretical calculations on these complex systems pose challenges that scientists have only recently started to investigate.

A method for simulating an electrochemical cell will be presented and compared with other proposals for including the effect of an applied voltage in density functional theory calculations.

Calculations of the electron transfer between electrode surfaces and the binding of a water molecule as a function of applied voltage will be presented.

Extensions of the proposed simulation method to better reproduce the electrochemical cell will be discussed.

MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

Nils Peder Willassen

Dept. of Molecular Biotechnology, Institute of Medical Biology,
NorStruct & MabCent
Univ. of Tromsø, Norway

Marine bioprospecting - The MabCent-SFI initiative in Tromsø

Staður (Place): VR-II Stofa 257, Háskóli Íslands, Hjarðarhaga 2-4.
Breyttur staður - Please note new location.

Dagsetning (Date): **Priðjudagur**, 30. september 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Abstract:

MabCent-SFI is a centre for research based innovation hosted by the University of Tromsø. The centre focuses on bioactivities from Arctic and sub-Arctic organisms in search for compounds to be used in innovation- and commercialization projects.

MabCent-SFI integrates various disciplines and partnerships of academics at the University of Tromsø and expert SMEs, acting as a consortium. The consortium covers the pipeline from biology of marine resources/species through screening and research on bioactivities to commercialization.

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MÁLSTOFA efnafræðiskorar

Seminar - Dept. of Chemistry

E. Michael Danielsen

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Lipid raft organization and function in the small intestinal brush border.

Staður (Place): Stofa 158, Háskóli Íslands, VR-II, Hjarðarhaga 2-4.

Dagsetning (Date): Miðvikudagur, 8. október 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Abstract:

The apical cell surface of the small intestinal enterocyte functions as a selective filter facing the exterior: Thus, while acting as a permeability barrier to protect the organism from hazardous agents, it simultaneously needs to extract dietary nutrients from the environment. The accomplishment of this dual task requires a robust and stable, rather than dynamic, surface. Accordingly, a major part of the brush border membrane is made up by glycolipids organized in lipid raft microdomains (Danielsen and Hansen, 2003; Danielsen and Hansen, 2006). The divalent lectin galectin-4 has long been recognized as an abundant cross-linker of glycolipids and some of the major peptidases and glycosidases, enabling formation of detergent-resistant "superrafts". Furthermore, we have identified a group of lectin-like antibodies, so-called "anti-glycosyl" antibodies, of both IgA, IgM -and IgG classes, deposited at the luminal surface of the brush border. These antibodies, locally synthesized in the gut and raised against commensal bacteria, may have a protective function by preventing lectin-like pathogens from gaining access to the epithelium. Recently, intelectin was added to the list of lipid raft-associated brush border proteins. This trimeric D-galactosyl-specific lectin, expressed in goblet and Paneth cells and proposed to serve a protective role in the innate immune response to parasite infection, is identical to the lactoferrin receptor of the enterocyte brush border. Like galectin-4, intelectin was isolated from superrafts, indicating that also this lectin serves as an organizer and stabilizer of the brush border, preventing loss of digestive enzymes and protecting the glycolipid microdomains from pathogens.

Danielsen EM and Hansen GH (2003) Lipid Rafts in Epithelial Brush Borders: Atypical Membrane Microdomains With Specialized Functions. *Biochim Biophys Acta* 1617:1-9

Danielsen EM and Hansen GH (2006) Lipid Raft Organization and Function in Brush Borders of Epithelial Cells. *Mol Membr Biol* 23:71-79

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Proton conducting perovskites

Göran Wahnström

*Department of Applied Physics, Chalmers University of Technology,
SE-412 96 Göteborg, Sweden*

Staður (Place): Stofa 158, Háskóli Íslands, VR-II, Hjarðarhaga 2-4.

Dagsetning (Date): Föstudagur, 31. október 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Abstract:

There is currently a considerable interest in high-temperature proton conducting oxides. Certain perovskites, such as BaZrO_3 , appear to combine good thermal and mechanical stability with a reasonably high proton conductivity, which makes them potential candidates for a wide range of electrochemical applications. Due to their relatively simple structure they are also suitable for detailed theoretical investigations.

We will demonstrate how density-functional calculations can be combined with thermodynamic and kinetic modeling to assess several important macroscopic properties of this material. Firstly, we will show that the environmental conditions used during synthesis or processing of a sample (chemical potential of the substitutional dopants, oxygen partial pressure of the atmosphere, and temperature) may significantly affect the defect structure, which explains the large variation in available conductivity data. Secondly, we will present the elementary steps in the proton conduction, including the effect of quantization of the nuclear degrees of freedom. Thirdly, we will demonstrate that the presence of acceptor dopants - although necessary to achieve a high concentration of protonic defects - can result in a severe reduction of the proton mobility by acting as 'traps'.

Perhaps this means that the much longed-for improved solid-state proton conductors of tomorrow are more likely found among materials where hydrogen is an intrinsic part of the structure, rather than a minority defect.

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Nóbelsverðlaunin í efnafræði 2008

Birkir Þór Bragason

Tilraunastöð Háskóla Íslands í meinafræði að Keldum.

Staður (Place): Stofa 158, Háskóli Íslands, VR-II, Hjarðarhaga 2-4.

Dagsetning (Date): Föstudagur, 7. Nóvember 2008.

Tími (Time): 12:30.

Fyrirlesturinn verður á íslensku (The talk will be given in Icelandic)

Útdráttur:

Nóbelsverðlaunin í efnafræði 2008 skiptust jafnt á milli **Osamu**

Shimomura (Marine Biological Laboratory Woods Hole, MA;

Boston University Medical School Massachusetts), **Martin**

Chalfie (Columbia University New York) og **Roger Y. Tsien** (University

of California San Diego; Howard Hughes Medical Institute). Verðlaunin voru

veitt fyrir uppgötvun á grænu flúrpróteini (green fluorescent protein, GFP)

marglyttunnar *Aequorea victoria* auk rannsóknar og þróunarvinnu í kjölfarið

sem hafa gert GFP að mikilvægu "merkitæki" við margvíslegar rannsóknir í

lífvísindum. Í erindinu verður farið yfir sögu uppgötvunarinnar og fjallað

almennt um GFP og notagildi þess í rannsóknum.

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Ómar Gústafsson

Research Scientist Decode Genetics

Microchip Electrochromatography

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 14. nóvember 2008.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given in English).

Summary:

The objective of the work presented here was to explore microchip electrochromatography in terms of new integrated functionalities and new substrate materials. Here two different microchip designs for electrochromatography will be presented, each of them featuring a microfluidic network with a standard cross injector and a separation column with microfabricated pillars as support for a stationary phase. The fabrication techniques used will be briefly presented and results demonstrating the functionalities of the microchips will be presented. First, a silicon based microchip for electrochromatography is presented. All of the structures on the microchip are fabricated in silicon in a single etching step using deep reactive ion etching. The microchip features planar UV-transparent silicon oxide waveguides, a 1 mm long U-shaped detection for UV-absorbance measurements. A glass wafer is used to seal the microchip. An stationary phase is attached to the surface of the microchip and reversed phase electrochromatography is demonstrated by separating three neutral compounds. The latter microchip that is presented is a polymer based microchip. The microchip is fabricated by nanoimprint lithography. The microchip is sealed with a thin polymer layer that has been spun onto a glass wafer. Reversed phase electrochromatography separation of three fluorescently labeled amines is demonstrated where the underivatized polymer surface is used as a stationary phase. Laser induced fluorescence through the substrate is used for detection.

Málstofustjóri: Bjarni Ásgeirsson/ bjarni@raunvis.hi.is

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Peter Z. Qin

Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0744

Studying structure and dynamics of nucleic acids using a sequence-independent nitroxide probe

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Fimmtudagur 8. janúar 2009.
Tími (Time): 15:00.

Fyrirlesturinn verður á ensku (The talk will be given in English).

Abstract: In site-directed spin labeling (SDSL), a stable nitroxide radical is attached at a specific location within a macro-molecule, and structural and dynamic information at the labeling site is obtained via electron paramagnetic resonance (EPR) spectroscopy. Our work centers on a family of nitroxide probes, called the R5-series, which can be attached at a specific nucleotide of any given RNA and DNA in an efficient and cost-effective manner. I will present work on using the R5-probes for measuring nanometer distances as well as probing site-specific structural and dynamic features of DNA and RNA.

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MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Meistaraprófsfyrirlestur:

Andri Guðmundsson

Rúmvendnar efnasmíðar fjölsetinna bicyclo[4.4.0]dekanana og bicyclo[3.3.1]nónana

(Stereoselective synthesis of polysubstituted bicyclo[4.4.0]decanes and bicyclo[3.3.1]nonanes)

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Miðvikudagur 11. febrúar 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á íslensku (The talk will be given in Icelandic).

Útdráttur: Undanfarin ár hafa verið stundaðar nýsmíðar á fjölsetnum bicyclo[3.3.1]nónan og bicyclo[4.4.0]dekan efnasamböndum á Raunvísindastofnun Háskólans og lífvirkni þessara efnasambanda verið rannsökuð. Efnin hafa t.d. sýnt virkni gegn ýmsum tegundum krabbameins, sérstaklega þau bicycloefni sem hafa arómatíska sethópa. Aðferðirnar sem notaðar eru við nýsmíðar á þessum efnum eru fremur einfaldar og eru í eðli sínu mjög rúmvendnar. Bicyclo[3.3.1]nónan og bicyclo[4.4.0]dekan efnasamböndin eru mynduð með því að hvarfa α,β -ómettuð aldehyð og trikarbónýlefnið dimetýl 1,3-asetóndíkarboxylat við basískar aðstæður. Nokkur arómatísk α,β -ómettuð aldehyð voru nýmynduð í ágætum heimtum með Heck kúplunar hvarfi milli arýljodíða og 2-própenals. Chan-Lam kúplun var einnig notuð til að arýla 4-jodófenól með arýlbórsýru afleiðum. Þau arýljodíð sem fengust úr þeim hvörfum voru þá notuð til myndunar á nýstárlegum α,β -ómettuð arómatískum aldehyðum sem innihalda díarýl eter tengi. Öll nýmynduð aldehyð voru svo notuð ásamt nokkrum aðkeyptum aldehyðum til nýsmíða á nýstárlegum bicyclo[4.4.0]dekan afleiðum sem voru einangruð í meðalgóðum eða mjög góðum heimtum. Umfangsmiklar rannsóknir voru einnig gerðar til þess að þróa nothæfa aðferð við nýsmíðar á handhverfuhreinum bicyclo[3.3.1]nónan afleiðum með lífrænum hvötum. Niðurstöður þeirra rannsókna lofa góðu en aðferðir hafa ekki verið fullmótaðar.

Summary: For the past decade or so, synthesis of polysubstituted bicyclo[3.3.1]nonanes and bicyclo[4.4.0]decanes and research on the biological activity of such compounds has been conducted at the University of Iceland Science Institute (SI). These novel compounds have been tested against various types of cancer and results imply cytotoxic potential, especially those bicyclic compounds that bear an aromatic substituent. The synthetic pathways implemented at SI towards these bicyclo[3.3.1]nonanes and bicyclo[4.4.0]decanes are relatively simple and remarkably stereoselective. In both cases, these compounds are formed by reaction of an α,β -unsaturated aldehyde and dimethyl 1,3-acetonedicarboxylate under basic conditions. As precursors of bicyclo[4.4.0]decanes, various aromatic α,β -unsaturated aldehydes were synthesized in good yields using a Heck coupling reaction variant involving reactions of aryl iodides and acrolein. Chan-Lam coupling of arylboronic acid derivatives and 4-iodophenol was used to synthesize novel aryl iodides. The resulting aryl iodides were then reacted with acrolein under Heck reaction conditions, providing novel, ether-bonded, aromatic α,β -unsaturated aldehydes. These novel aldehydes, as well as aromatic aldehydes that were obtained from commercial providers, were then used in synthesis of novel bicyclo[4.4.0]decanes which were obtained in moderate to excellent yields. Extensive research on a viable synthetic pathway towards enantiomerically pure bicyclo[3.3.1]nonanes using asymmetric organocatalysis was also carried out showing some promise but has yet to be optimized.

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MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Johannes Voss

Risø laboratories / Technical University of Denmark (DTU)

Computational approaches to the prediction of the thermodynamic stabilities of crystal structures

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 6. mars 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Summary: Computational approaches to the prediction of the thermodynamic stabilities of crystal structures. The prediction of the energetically favorable configuration of the atomic coordinates at a given temperature is difficult for periodic systems in particular. I will present approaches and numerical results for systems where disorder is negligible, and lattice vibrations are the dominant source of entropy. I will show how symmetries can be taken advantage of to enhance the convergence of the search for equilibrium configurations, and how stabilities at finite temperatures can be assessed numerically. The example cases focus on complex metal hydrides, which are of interest as reversible hydrogen storage materials. These systems often exhibit large unit cells with many symmetrically inequivalent parameters and therefore mean a large effort for the calculation of their electronic structure.

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MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Adem Tekin, Ph.D.

Department of Physics, Technical University of Denmark (DTU)
and National Laboratory for Sustainable Energy (Risø)

Global optimizations applied to clusters and hydrogen storage materials

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 13. mars 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Summary: Global optimization techniques are widely applied to solve problems encountered in diverse research fields such as natural sciences, engineering, medicine, and economy. Genetic Algorithms (GA) and Simulated Annealing (SA) are two of the most robust, efficient, and well known stochastic global optimization approaches. The first part of my talk shows how GA was used to study the structure of Si clusters with up to 30 atoms. The second part of my talk focuses on SA geometry optimizations of Acetylene - Benzene clusters using fitted Acetylene - Acetylene, Acetylene - Benzene, and Benzene - Benzene dimer potentials. The final part of my talk describes both how global optimization methods can be used to predict the crystal structure and kinetics of hydrogen storage materials such as metal amines and borohydrides from Density Functional Theory.

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Nicolai Bork

Division for Fuel Cells and Solid State Chemistry
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Hydrogen - Hydrogen interaction in SrTiO₃ investigated by DFT

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 20. mars 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Summary:

Protonic membranes are currently receiving much attention due to the possible application in proton conducting fuel cells or for gas separation membranes. Solid oxide ceramics could be superior to polymeric and metallic membranes, but many fundamental properties of hydrogen in oxides is still poorly understood, making modelling difficult and experimental work less efficient. The interaction of hydrogen defects in the material is one of these.

We have performed DFT calculations on possible configurations of two hydrogen defects in a 2*2*2 (40 atoms) and 3*3*3 (135 atoms) SrTiO₃ supercell. The most stable configuration for two hydrogen in the system have been determined to be between 2.2 - 2.5 Å, stabilized by ca. 0.3 - 0.5 eV compared to isolated defects. Reasons for this apparently attractive interaction have been identified. Among the most important is the structural changes introduced by the hydrogen defect and the system symmetry.

The diffusional mechanism for the double defect have been investigated. We find that it is possible for the double defect to diffuse through the SrTiO₃ crystal without breaking up via several distinct reaction paths. The mobility have been calculated for a few of these and is compared to mobility of a single hydrogen defect. Major differences are observed, both regarding barrier heights and “transition state theory” prefactors.

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Gunnar Nyman

Professor of Physical Chemistry at Chalmers, Sweden.

A star is born - Adventures in interstellar chemistry

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 27. mars 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Abstract:

It has long been known that molecules exist in outer space. More recently it has become clear that molecules are important for star formation. There is therefore an interest to know how molecules form and how they are destroyed in interstellar space. As a result, a need for astrochemistry has turned up.

400 years ago Galileo Galilei turned his telescope to study the sky for the first time. To celebrate this, 2009 is the International year of Astronomy. I will give a general introduction relating to this before turning to a discussion of how chemical reaction rates can be calculated theoretically with emphasis on low temperature.

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MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Bjarki Stefánsson

Sérfræðingur á Lífefnafræðideild Raunvísindastofnunar Háskóla Íslands.

Protein Phosphatase 6 Subunits and Effects on NF- κ B Signaling

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 3. apríl 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Protein Ser/Thr phosphatases (PPP) comprise a family that includes type-2 PP2A, PP4 and PP6, each with essential functions. PP6 is an essential phosphatase conserved among eukaryotes and known as Sit4 in *Saccharomyces cerevisiae* (yeast). Sit4 phosphatase function depends on regulatory subunits or SAP (Sit4 Associated Protein) proteins which contain a SAPS domain. To study the regulation and function of PP6, potential regulatory subunits of PP6 were identified based on sequence similarity to the yeast SAP proteins. Three human SAPS domain proteins were found and named PP6R1, PP6R2 and PP6R3. PP6R1 and PP6R2 co-precipitated endogenous PP6, but not PP2A or PP4, showing specificity for recognition of PPP phosphatases. The SAPS domain of PP6R1 alone was sufficient for association with PP6 and this predicts that the conserved sequence motifs in the SAPS domain account for specificity among PPP. Using mass spectrometry, three ankyrin repeat proteins were identified that stably associate with PP6R1. Immunoprecipitation of an ankyrin repeat subunit (PP6-ARS-A) showed specific association with PP6 and PP6R1 compared to PP2A and PP4. Previous results showed that PP6R1 associates with I κ B ϵ , a protein involved in NF- κ B signaling. Knockdown of PP6 or PP6R1 but not PP6R3 with siRNA significantly enhanced degradation of endogenous I κ B ϵ in response to Tumor Necrosis Factor-alpha (TNF α). This demonstrates that different SAPS domain subunits for PP6 have specific effects. Knockdown of PP6R1 and PP6-ARS-A produced equivalent enhancement of I κ B ϵ degradation. The results suggest that PP6 functions as a heterotrimer, composed of the PP6 catalytic subunit bound to a SAPS domain subunit (PP6R1) that associates with PP6-ARS-A. It is proposed that the function and specificity of PP6 will be determined by the specific combination of SAPS and PP6-ARS subunits in different heterotrimers.

MÁLSTOFA efnafræðiskorar

Seminar - Department of Chemistry

Hrönn Ólína Jörundsdóttir, Ph.D.

Verkefnastjóri / Project Manager

Matvælarannsóknir Íslands –MATÍS/ Food Research, Innovation and Safety.
Reykjavík.

Mengun í íslensku lífríki Environmental pollution in Iceland

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 24. apríl 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Abstract. Environmental pollution is an increasing problem in the modern society. The spatial trend of several organic pollutants, e.g. PCB, the pesticide DDT and some of their metabolites, was investigated in the Nordic countries where guillemot was used as a monitoring matrix. The pollutants were analysed in eggs from Iceland, the Faroe Islands, Norway and Sweden (The Baltic Sea) for a spatial comparison. The results show that the biota in the North Atlantic is less contaminated compared to biota in the Baltic Sea, with some exceptions that need to be clarified. Polyfluorinated alkyl compounds, which are coming from e.g. outdoor clothes, were recently discovered in a considerable amount in the environment. These compounds were found in eggs from all locations and in some cases in higher amount in eggs from the North Atlantic compared to eggs from the highly contaminated Baltic Sea. Brominated flameretardants, used in e.g. electronics, were detected in all egg samples and there seems to be a pattern indicating their origin, either from N-America or Europe. A comparison of pollutants in different bird species was also conducted, i.e. Arctic tern (kría), eider (æðarfugl), guillemot (langvía), fulmar (fýll), lesser black-backed gull (sílamáfur), great black-backed gull (svartbakur) and great skua (skúmur). Eggs of great skua contained highest amount of pollutants, including PCB and the pesticide DDT, and it is important to investigate the physical condition of the great skua. The results are showing that a certain part of the pollutants detected in the North-Atlantic are carried with wind and sea-currents from source locations. Still, a considerable amount is present because of our own use of products containing these pollutants.

Útdráttur: Áhyggjur af umhverfismengun er vaxandi í heiminum, enda er styrkur mengandi efna í mörgum tilvikum að aukast. Skoðuð var þrávirk lífræn mengun á Norðurlöndunum, t.d. PCB og skordýraeitrið DDT ásamt niðurbrotsefnum þeirra, og voru þau mæld í langvíueggjum. Efnin voru mæld í eggjum frá Íslandi, Færeyjum, Noregi og Svíþjóð til að fá landfræðilegan samanburð.

Niðurstöður sýna að lífríki Norður Atlantshafsins er minna mengað en lífríki Eystrasaltsins, en þó reyndust ýmiss mengandi efni vera í svipuðum styrk á þessum svæðum og þarf að rannsaka nánar af hverju það stafar. Flúoreruð alkanefni, sem koma m.a. úr útivistarfátnaði, hafa nýlega fundist í umtalsverðu magni í náttúrunni mældust í langvíueggjum frá Íslandi, Færeyjum, Noregi og Svíþjóð og voru í einstaka tilfellum í hærri styrk í eggjum frá N-Atlantshafi en í Eystrasaltinu. Brómeruð eldvarnarefni, sem m.a. eru notuð í raftæki, voru allstaðar mælanleg og virðist vera hægt að greina mismunandi uppruna efnanna sem berast til Norður Atlantshafsins, annars vegar frá N-Ameríku og hins vegar frá Evrópu.

Einnig var gerður samanburður á magni mengandi efna í sjö íslenskum fuglategundum, þ.e. kríu, æðarfugli, langvíu, fýl, sílamáfi, svartbak og skúmi. Skúmurinn reyndist hafa umtalsvert háan styrk mengandi efna, m.a. PCB sambanda og skordýraeitursins DDT, og er mikilvægt að rannsaka heilsuástand skúmsins.

Ljóst er að hluti þeirrar mengunar sem mælist í íslensku lífríki berst með haf- og loftstraumum til Íslands en hins vegar er umtalsverður hluti tilkominn vegna notkunar Íslendinga á varningi sem inniheldur margvísleg mengandi efni.

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MÁLSTOFA efnafræðiskorar
Seminar - Department of Chemistry

Flemming Besenbacher

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Interdisciplinary Nanoscience Center (iNANO)
University of Aarhus, DK-8000 Aarhus C, Denmark

Introduction to iNANO and dynamics of nanostructures on surfaces revealed by high-resolution, fast-scanning STM

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 8. maí 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Abstract

The rapidly expanding field of nanoscience and nanotechnology is cross-disciplinary by nature and involves physics, chemistry, biology, molecular biology and medicine. It is considered a very promising field, which is expected to give powerful impetus to a new industrial revolution. The Interdisciplinary Nanoscience Centre (iNANO) (www.inano.dk) was established in 2002, and the iNANO mission is based on the following three equally important pillars: Education, Research and Innovation. We have established a new bachelor and master educational programme in nanoscience that incorporates a broad spectrum of basic, advanced and specialized courses to provide students with a sufficiently broad basis to conduct interdisciplinary nanoscience research and at the same time obtain disciplinary depth and specialised skills in selected areas. I will give a brief introduction to the activities at iNANO.

I will thereafter give an overview of the research activities in my own research group. Scanning tunneling microscopy (STM) has since it was invented 25 years ago proven to be a fascinating and powerful technique in the field of surface science and nanotechnology. The fact that sets STM apart from most other surface sensitive techniques is its ability to resolve single atoms and molecules on surfaces and in certain cases to reveal the dynamics of surface processes and nanostructures by recording many sequential STM images using a fast-scanning, variable temperature STM. I will in particular demonstrate the capability of the STM to record time-resolved, high-resolution STM images, visualized in the form of STM movies (see www.phys.au.dk/spm), which can be used to obtain important new insight into the dynamics of surface processes and of nanostructures, such as surface diffusion of adatoms and molecules [1-3], diffusion of vacancies and molecules on oxide surfaces [4-6]. I will show how STM studies of MoS₂ nanoclusters supported on a gold substrate have led to a new and detailed atomic-scale insight into the variety of MoS₂ nanostructures that may form under conditions relevant to operation and sulfiding of hydrodesulfurization (HDS) catalysts

[7,8]. Finally, the self-assembly of Nucleic Acid (NA) base molecules on solid surfaces has been investigated since NA base molecules and DNA molecules are particularly interesting as promising building blocks for the bottom-up fabrication of functional supramolecular nanostructures on surfaces. I will discuss the fact that Guanine molecules form the so-called G-quartet structure on Au(111) that is stabilized by cooperative hydrogen bonds. Interestingly, cytosine molecules only form disordered structures by quenching the sample to low temperatures, which can be described as the formation of a 2D organic glass on Au(111) [9].

1. F. Besenbacher, Reports on Progress in Physics 59, 1737 (1996)
2. R. Otero *et al.*, Nature Materials 3, 779 (2004)
3. S. Weigelt *et al.*, Nature Materials 5, 112 (2006)
4. R. Schaub *et al.*, Science 299, 378 (2003); Science 303, 511 (2004)
5. S. Wendt *et al.*, Physical Review Letters 96, 066107 (2006)
6. D. Matthey *et al.*, Science 315, 1692 (2007)
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8. J.V. Lauritsen *et al.*, Nature Nanotechnology 2,1, 53-58 (2007)
9. R. Otero *et al.*, Science 319, 312-315 (2008)

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MÁLSTOFA efnafræðiskorar
Seminar - Department of Chemistry

HARALDUR GARÐARSSON

Meistaraprófsfyrirlestur—MS Thesis Lecture

Ç^f as a universal SNP probe

Staður (Place): Stofa VR-II 158, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 15. maí 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður á ensku (The talk will be given English).

Abstract

The fluorescent nucleoside (fluoroside) Ç^f is a cytosine-analogue that forms a stable base pair with deoxyguanosine in duplex DNA. Upon incorporation of the fluoroside into double stranded DNA, it retains most of its fluorescence. Furthermore, the fluorescent signal is different depending on the nucleotide that Ç^f is base-paired to, making it able to identify its base-pairing partner. These abilities make it a promising candidate for single nucleotide polymorphism (SNP) genotyping. A preliminary study showed that the flanking sequence, i.e. the nucleotides immediately flanking the 3' and 5' side of the fluoroside, affected the emission of Ç^f (Cekan P and Sigurdsson ST (2008), *Chem. Comm.*, 29, 3393-3395). We were therefore interested in examining the effects of all possible flanking sequences on the fluorescence intensity of Ç^f. We found that the flanking sequence does induce changes in the emission, but to a different degree depending on the flanking sequence in question. In fact there were three distinct levels of mismatch detection. First, in the majority of flanking sequences (10 of 16), Ç^f was capable of identifying its base-pairing partner. In the second category (3 of 16), Ç^f was able to discriminate the fully base paired duplex from the mismatches. In the last category (3 of 16), the fluoroside was not able to distinguish the fully base paired duplex from a mismatch. However in the sequences where distinction between all base-pairing partners was not possible, we were able to alter conditions, so that full discrimination was facilitated. The ability to use Ç^f in any flanking sequence makes it one of the most versatile SNP genotyping probes available today.

Ágrip

Flúrljómandi kirnisleifin (flúorósíð) C^f er afleiða deoxýsýtídíns og myndar stöðugt basa-par við gúanósín. Við innlimun flúorósíðsins í tvíþætta kjarnsýru (DNA), viðhelst megnið af flúrljómuninni. Að auki er hið flúrljómandi merki ólíkt eftir því við hvaða kirnisleif C^f er parað. Þannig getur C^f greint hvaða basi er á móttæða þættinum. Þessir eiginleikar gera flúorósíðið að mjög ákjósanlegum flúrljómandi hópi til að greina SNP (*e.* Single Nucleotide Polymorphism), sem eru einkirnis-stökkbreytingar sem geta valdið hinum ýmsu sjúkdómum. Fyrri rannsóknir á áhrifum hliðstæðra basa, þ.e. basa sitt hvorum megin við C^f , bentu til þess að þeir hafa áhrif á flúrljómun (Cekan P and Sigurdsson ST (2008), *Chem. Comm.*, 29, 3393 – 3395). Því var ákveðið að skoða áhrif allra mögulegra hliðstæðra basa á flúrljómun flúorósíðsins og 16 flúrljómandi fákirni smíðuð. Niðurstöðurnar sýndu að hliðstæðu basarnir hafa töluverð áhrif, en að mismiklu magni. Unnt var að greina áhrif hliðstæðra basa í þrjá flokka. Í fyrsta flokknum, og reyndar þeim stærsta (10 af 16), var hægt að greina nákvæmlega hvaða basi væri á móttæða þættinum. Í næsta, var unnt að greina rétta basa-pörun við G frá mispörun (3 af 16). Í þriðja flokknum gat C^f ekki greint réttu basa-pörunina frá mis-pörunu DNA (3 af 16). Aftur á móti var unnt, með því að breyta aðstæðum, greina á milli allra basa sem basa-paraðir voru við C^f , óháð hliðstæðum bösum. Því er unnt að nota C^f til þess að greina SNP, óháð hliðstæðum bösum.

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MÁLSTOFA efnafræðiskorar
Seminar - Department of Chemistry

Meistaraprófsfyrirlestur–MS Thesis Lecture

Jón Steinar G. Mýrdal

**Theoretical Studies of Aluminum Based Nano
Scale Materials for Hydrogen Storage**

(Kennilegar rannsóknir á álríkum nanóefnum fyrir
vetnisgeymslu)

Staður (Place):	Stofa VR-II 157, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date):	Föstudagur 22. maí 2009.
Tími (Time):	12:30-13:30.

Abstract

Hydrogen is, for many reasons, an appealing energy carrier. The main problem for using hydrogen as fuel in mobile application is the onboard storage. Many studies have been done on so called metal hydrides for the purpose of storing hydrogen. For a metal hydride system to fulfill its task of being a good hydrogen storage it needs to release the hydrogen close to 100°C and the gravimetric portion of hydrogen in the system should be high, at least 6 wt%. Former studies done in the H. Jónsson group showed that hydrogen binds more strongly to Mg, compared to large crystalline MgH_2 , if the Mg is in nano scale clusters. Unfortunately, for Mg the hydrogen binding energy is already too large for the MgH_2 crystal. These results have motivated us to look at the hydrogen binding in nano scale Al clusters, since the alane crystal (AlH_3) is thermodynamically unstable at room temperatures but has a very high gravimetric portion of hydrogen, 10.1 wt%. We have studied the stability and structure of nano scaled aluminum and aluminum hydride clusters with plane wave based density functional theory (DFT). The structures of Al_nH_{3n} clusters are surprisingly open and all aluminum atoms are connected through a hydrogen bridging bonds. These bridging bonds make

the clusters very open and floppy. The binding energy of hydrogen in the aluminum hydride clusters has been calculated for clusters with 2 to 30 Al atoms. As for MgH_2 , the binding energy is larger for small clusters of AlH_3 than for the crystalline material. A model has been fitted to our data, to predict the binding energies of hydrogen for even larger clusters. By comparing the stabilities of the pure aluminum clusters to the stability of aluminum hydride clusters, one sees that the reason for the increase in binding energy is due to the fact that the pure aluminum clusters destabilize more than the aluminum hydride clusters with decreasing size.

Ágrip

Vetni er fyrir margar sakir ákjósanlegur orkuberi. Helsta vandamál við að nota vetni sem eldsneyti í farartækjum er geymsla þess um borð. Málmhýdríð hafa mikið verið rannsökuð sem hugsanlegar vetnisgeymslur. Til þess að málmhýdríð uppfylli skilyrði sín sem góðvetnisgeymsla þarf það að losa vetnið við um $100^\circ C$ og massahlutfall vetnisins í kerfinu þarf að vera hátt, í það minnsta 6 wt%. Fyrri rannsóknir sem gerðar hafa verið í rannsóknarhópi Hannesar Jónssonar hafa sýnt

að vetni bindst fastar í Mg, í samanburði viðstóra kristalla, ef Mg er í nanóstærðar

klösum. Svo óheppilega vill þó til að fyrir Mg bindst vetni of fast í MgH_2 kristalnum

og er þessi aukna binding því óhagstæð. Þessar niðurstöður hafa veitt okkur innblástur fyrir því að skoða bindingu vetnis í nanóstærðar ál klösum, þar sem alane kristallinn (AlH_3) er varmafræðilega óstöðugur við herbergishita en hefur mjög hátt massahlutfall vetnis, 10.1 wt%

Við höfum rannsakað stöðugleika og atóm byggingu á nanó stærðar ál og álhýdríð

klösum með plan bylgju byggðri þéttifellafræði (DFT). Það kemur á óvart hversu opin atóm bygging Al_nH_{3n} klasanna er, en í henni eru öll ál atómin tengd með brúuðum vetnistengjum. Þessi brúuðu vetnistengi gera það að verkum að álhýdríðklasarnir eru mjög opnir og sveigjanlegir. Bindiorka vetnis í álhýdríð klösum hefur verið reiknuð fyrir klasa með 2-30 atómum. Líkt og fyrir Mg þá er bindiorkan hærri fyrir smáa klasa af áli heldur en fyrir kristalinn. Líkan, byggt á reiknuðum gögnum, hefur verið notað til þess að spá fyrir um bindiorku vetnis í ennþá stærri klösum. Með því að bera saman stöðuleika hreinna ál klasa við stöðugleika álhýdríðklasa sést að ástæða vaxtar bindiorkunnar er uppruninn frá því að hreint ál missir stöðugleika mun hraðar en álhýdríð þegar klasarnir minnka.

MÁLSTOFA efnafræðiskorar
Seminar - Department of Chemistry

Jón Tryggvi Njarðarson

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Natural Products and New Synthetic Methods

Staður (Place): Stofa VR-II **157**, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 5. júní 2009.
Tími (Time): 12:30.
Fyrirlesturinn verður fluttur á ensku/ The talk will be given in English.

Abstract:

Our research group is focused on the development of new useful synthetic methods and the total synthesis of complex natural products with appealing biological functions. Two case studies, representing each one of these research areas, will be presented along with a preview of other ongoing programs.

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MÁLSTOFA efnafræðiskorar
Seminar - Department of Chemistry

Auður Magnúsdóttir, PhD

Department of Biochemistry and Biophysics
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A novel fold and speculations on holoenzyme assembly: Insights from structural studies of the Protein Phosphatase 2A system

Staður (Place): Stofa VR-II 157, Háskóli Íslands, Hjarðarhaga 2-4.
Dagsetning (Date): Föstudagur 26. júní 2009.
Tími (Time): 12:30-13:30.
Fyrirlesturinn verður fluttur á ensku/ The talk will be given in **English**.

Abstract:

PP2A is a major phosphatase in the cell that participates in multiple cell signaling pathways. It is a heterotrimer of a core dimer and variable regulatory subunits. Details of its structure, function and regulation are slowly emerging. By using X-ray crystallography we have solved the structure of two regulators of PP2A; PTPA and B56 γ . PTPA is a highly conserved enzyme that plays a crucial role in PP2A activity but whose biochemical function is still unclear. PTPA has a novel all α helical fold that can now be described as well as a putative peptide binding site for interaction with the catalytic subunit of PP2A. B56 γ is a PP2A regulatory subunit linked to cancer and we have solved the structure of B56 γ in its free form. This is particularly valuable in light of the recent structures of the PP2A holoenzyme and core dimer and allows for speculations about the holoenzyme assembly.

