

**Belgian Physical Society meeting
ULB, May 21st 2008**

Parallel Session on Biophysics

Young Scientist Contest (11:20 – 12:20)

Evi Vinck

Universiteit Antwerpen, Department of Physics

Talk: Probing the electronic structure of transition-metal-ion complexes using EPR techniques

Parallel Session (15:20 – 17:15)

15:20 – 16:00

Dr. Michael Mertig – invited speaker

Max Bergmann Center of Biomaterials and Institute of Materials Science, Dresden University of Technology, Germany

Talk: Biomimetic materials synthesis: From DNA arrays to metallic super lattices

16:00 – 16:20

Dr. Francesca Cecchet

FUNDP Namur, Research Center in Matter and Radiation Physics

Talk: Probing (bio)organic layers adsorbed onto metal surfaces by sum-frequency generation

16:20 – 16:40

Ronald Thoelen

Universiteit Hasselt, Institute for Materials Research

Talk: Piezoelectric and Electrochemical Sensing of Small Molecules using Synthetic MIP-based Receptors

16:40 – 17:15

Prof. Dr. Enrico Carlon

Katholieke Universiteit Leuven, Institute for Theoretical Physics

Talk: Understanding hybridization in DNA Microarrays

Poster session (10:50 – 11:20, 14:50 – 15:20, 17:30 – 18:15)

K. Myriam Kroll

Katholieke Universiteit Leuven, Institute for Theoretical Physics

Poster: Modelling Background Intensities in Affymetrix Genechips

Jorg De Haeck

Katholieke Universiteit Leuven, Laboratory for Solid State Physics and Magnetism

Poster: Ge₉ nano building blocks

Filip Desmet - poster contest -

Universiteit Antwerpen, Department of Physics

Poster: Electron paramagnetic resonance investigation of the globin domain of the globin-coupled sensor of *Geobacter sulfurreducens*

Maria Ezhevskaya

Universiteit Antwerpen, Department of Physics

Poster: Dynamical, structural and functional aspects of neuroglobin

Maarten Gysemans

Katholieke Universiteit Leuven, Laboratory for Solid State Physics and Magnetism

Poster: Electrical and Structural properties of Insulin Amyloid Fibrils

Abstract EVI VINCK

Abstract for BPS General Scientific Meeting, ULB, May 21st

Probing the electronic structure of transition-metal-ion complexes using EPR techniques

E. Vinck,¹ S. Van Doorslaer,¹ D. M. Murphy,³ I.A. Fallis,³ S. Dewilde,² L. Moens,²

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Electron paramagnetic resonance (EPR) techniques form the ideal tool to analyze paramagnetic molecules. The potential of EPR techniques has increased enormously in the past years, due to the development of pulsed-EPR techniques, and due to recent advances in quantum-chemical computations. Therefore, many aspects of the technique remain largely unexplored. Especially the use of the HYSORE (*Hyperfine Sublevel Correlation*) technique, combined with spectral simulations is relatively new. In this work, we have tested the performance of the latter technique to analyze different paramagnetic transition-metal-ion complexes. The EPR analyses were compared with density functional theory (DFT) computations, which enhances the interpretation of the spectra. The techniques were applied to study the electronic structure of the cobalt Jacobsen catalyst, which is widely used in the pharmaceutical industry, for the hydrolytic kinetic resolution of terminal epoxides, an important step in the production of several medicines. Despite its widespread use, the active catalytic species is unknown. In this work, the structural changes that occur upon activation of the catalyst were mapped in detail, using EPR techniques. These analyses revealed the different molecules that are formed upon activation and allowed to probe their electronic structure. The analyses show the formation of a cobalt-bound phenoxyl radical, situated on the Jacobsen ligand. It is the first time that such a species is observed. In the second part of this work, it is shown how pulsed-EPR techniques can be applied to obtain information on both the electronic and geometrical structure of newly discovered globins, which are iron-containing proteins.

Abstract Dr. MICHAEL MERTIG – invited talk -

Biomimetic materials synthesis: From DNA arrays to metallic super lattices

Michael Mertig

*Max Bergmann Center of Biomaterials and Institute of Materials Science,
Dresden University of Technology, Germany*

Modern principles for the controlled bottom-up assembly of advanced nanostructures by making use of the unique molecular recognition and self-assembly capabilities of biomolecules will be discussed. Fundamental issues of biomolecular templating will be addressed to demonstrate the advantage of using biomolecules in an engineering context for future technological applications, including (i) site-specific integration of DNA duplexes into microelectronic systems, (ii) manipulation of DNA by molecular motors, (iii) assembly of artificially designed biomolecular structures with the aim to tailor the complexity of desired biomolecular templates, and (iv) growth of metallic clusters at biomolecular structures promoted and controlled by the template itself with the goal to transform the template into a stable, artificial nanostructure.

We will discuss the multifunctional use of selective properties intrinsic to biomolecules and important for a controlled bottom-up processing for two particular examples: engineering of nano-scaled electronic circuits when DNA is used as the biomolecular template, and growth of metallic super lattices on bacterial surface layer proteins.

Abstract Dr. FRANCESCA CECCHET – contributed talk -

Abstract for BPS General Scientific Meeting, ULB, May 21st

**Probing (bio)organic layers adsorbed onto metal surfaces
by sum-frequency generation spectroscopy (SFG)**

Francesca Cecchet, Dan Lis, Alaa Addin Mani, Yves Caudano, Paul A. Thiry,
André Peremans

*Research Center in Matter and Radiation Physics
FUNDP – University of Namur, Belgium*

As the surface properties depend on the chemical nature, on the structural organization and on the physico-chemical interactions within the outermost thin layer, there is a great technological interest in understanding, controlling and tailoring these characteristics in order to generate materials with well-defined properties and functions. In particular, organic monolayers, chemisorbed or physisorbed onto substrates, are extensively used for providing the material surface with precise physico-chemical properties.

In the present work, ordered monolayers of thiols prepared by the self-assembly technique (SAM), and of lipids obtained by the Langmuir-Blodgett method (LB), have been studied by sum frequency generation spectroscopy (SFG). This study is focused on the determination of the molecular orientation (i.e. the tilt angle and the twist angle of the axis and of the plane of the molecular groups, respectively) and on the analysis of the physico-chemical and biological interactions occurring within the layers or with outer target molecules.

Abstract RONALD THOELLEN – contributed talk -

Abstract for BPS General Scientific Meeting, ULB, May 21st

Piezoelectric and Electrochemical Sensing of Small Molecules using Synthetic MIP-based Receptor

R. Thoelen¹, J. Alenus¹, F. Horemans¹, J. Duchateau¹,
L. Lutsen², D. Vanderzande^{1,2}, T.J. Cleij¹, and P. Wagner¹

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The urge of detecting small molecules for biomedical, environmental and chemical purposes is huge. By mimicking the selectivity and sensitivity of biological systems, synthetic materials with imprinted nanocavities can act as highly selective tailor-made artificial receptors. Implementing these materials in a piezoelectric or electrochemical sensing device can offer fast and straightforward detection together with high sensitivity and device miniaturization. L-nicotine, a major addictive substance in cigarettes and histamine, a biomedical relevant neurotransmitter are used as target molecules. The highly selective imprinting material is made by adding the target molecule to a polymer matrix of polymethacrylic acid (PMAA) and hardening this solution with UV. Subsequently, microparticles of the imprinted polymer were immobilized on thin films of the conjugated polymer OC₁C₁₀-PPV. Using this technique L-nicotine and histamine could be detected in the submicromolar range and the sensor could distinguish L-nicotine from the resembling molecule L-cotinine, which differs only one oxygen atom.

Abstract Prof. Dr. ENRICO CARLON – contributed talk -

Abstract for BPS General Scientific Meeting, ULB, May 21st

Understanding DNA hybridization in Microarrays

Enrico Carlon, Alessandro Ferrantini, Kyung-Myriam Kroll

Institute for Theoretical Physics, KULeuven, Celestijnenlaan 200D, B-3000 Leuven, Belgium

DNA microarrays are devices used in Molecular Biology laboratories to investigate the activity of thousands of genes simultaneously. Their functioning is based on the hybridization, ie the binding of complementary DNA strands, one attached to a solid surface and one in solution. In this talk some recent advances in the understanding of the physico-chemical properties of DNA hybridization in microarrays will be reviewed. A simple physical model based on an extended Langmuir isotherm will be presented [1]. The model is in good agreement with experimental data and provides a tool for microarray data analysis which has several advantages compared to traditional bioinformatics-based methods. A recently developed estimator of background noise level will also be briefly discussed [2].

[1] E. Carlon and T. Heim, *Physica A* **362**, 433 (2006)

[2] K.-M. Kroll, G. T. Barkema and E. Carlon, *Phys. Rev. E* (submitted);
<http://arxiv.org/abs/0712.3494>

Abstract MYRIAM KROLL – poster

Abstract for BPS General Scientific Meeting, ULB, May 21st

Modelling Background Intensities in Affymetrix Genechips

K.M. Kroll,¹ G. Barkema^{2,3}, E. Carlon¹

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³ *Lorentz-Institute for Theoretical Physics, Universiteit Leiden, The Netherlands*

A new physical model for the calculation of the background intensity in Affymetrix GeneChips is introduced [1]. We identify two major sources of background noise; the first is related to the sequence composition (CG-rich sequences are expected to have higher affinities for non-specific hybridization than e.g. AT-rich sequences). The second is due to local dependence of intensities from locations which are the physical neighbors of a specific spot on the chip. Both effects are incorporated in a background function whose free parameters are fixed via minimization on a training data set. In all data analyzed, the sequence specific parameters strongly correlate with empirically determined stacking free energies in solution. Moreover, we find an overall agreement with experimental background data. We show that our physics/physical-chemistry model globally performs better in calculating background intensities than approaches which are only based upon statistics. Thus, our model provides an interesting alternative method for background subtraction schemes in Affymetrix GeneChips.

[1] K.-M. Kroll, G. T. Barkema and E. Carlon, Phys. Rev. E (submitted);
<http://arxiv.org/abs/0712.3494>

Abstract JORG DE HAECK – poster -

Abstract for BPS General Scientific Meeting, ULB, May 21st

Ge₉ nano building blocks

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Recent progress in the chemical synthesis of nine-atom clusters and reports on cluster coupling, put the basis of the idea of a controlled stepwise growth of chains of [Ge₉]^x units. These units can be functionalized with organo-metal groups or doped with an interstitial atom, tailoring the chemical and physical properties of what can be conceived as a promising nano-scaled material. [1]

Here we present a combined experimental and theoretical study of Li doped Ge clusters, showing the existence of oligomers with up to five [Ge₉]^x units in the gas phase. [2] The Li atoms serve as a one electron donor, revealing the charge state of the oligomers. However, due to the isotopical nature of Ge, the exact composition could not be resolved. The implementation of a novel high resolution time-of-flight mass spectrometer will address this problem.

[1] J.M. Goicoechea, S.C. Sevov, J. Am. Chem. Soc. 128, 4155 (2006)

[2] X. Wang, Mass Spectrometric Study of Metal-doped Group IV Clusters, Ph.D. Thesis (2006)

Abstract FILIP DESMET – contest poster –

Abstract for BPS General Scientific Meeting, ULB, May 21st

Electron paramagnetic resonance investigation of the globin domain of the globin-coupled sensor of *Geobacter sulfurreducens*

Filip Desmet¹, Liesbet Thijs², Hassane El Mkami³, Graham Smith⁴, Sylvia Dewilde², Luc Moens²,
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We present the results of our electron paramagnetic resonance (EPR) investigation of the globin-coupled sensor (GCS) of the bacterium *Geobacter sulfurreducens*. These GCSs are multi-domain heme proteins that combine a heme-containing globin domain with a signal-transduction domain. Gaseous ligands such as O₂, CO and NO can bind to the heme iron atom in the globin domain. This ligand binding triggers a signal-transduction cascade that results in the activation of the second domain, however at present little is known about this mechanism. We have used X- and Q-band pulsed and continuous wave EPR in combination with different optical techniques to investigate the ferric and NO-ligated ferrous forms of the globin-domain of GsGCS. The UV/Vis absorption, resonance Raman and CW-EPR spectra of ferric GsGCS showed unambiguously that this protein exhibits a bis-histidine coordination of the heme iron. We used an in-house developed pulsed EPR strategy to determine the orientation of the axial imidazole ligands of the heme iron. This method involves spectral simulations of the experimental HYSCORE and pulsed ENDOR spectra. The resulting structural parameters will be confronted to preliminary XRD results on the protein. The NO-bound form of GsGCS was studied with CW EPR. Interestingly, this study shows that binding of nitric oxide breaks the bond between the heme iron atom and the evolutionary conserved proximal histidine, which is reflected in the NO-binding kinetics.

Abstract MARIA EZHEVSKAYA – poster –

Abstract for BPS General Scientific Meeting, ULB, May 21st

Dynamical, structural and functional aspects of neuroglobin

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The vertebrate neuroglobins were discovered already 8 years ago, but their functions are still not known. Several interesting hypotheses have been put forward. The observed ability of human neuroglobin (NGB) to form a disulfide bridge and its related change in oxygen affinity led to the assumption that NGB regulates oxygen release in hypoxia conditions. In the disulfide bridge, a Cys located on the flexible CD loop is involved. This flexible loop is found in many globins and has been suggested to modulate the function and accessibility of the heme region. Furthermore, some studies indicate that NGB would give protection against ROS (reactive oxygen species).

In this work, we attempt to elucidate some of the above points using EPR. Three NGB variants with an MTSSL spin label attached at one of the three native Cys are constructed using site-directed mutagenesis. In the first step, the mobility of the spin label is studied for these different sites. The experimental correlation times are confronted with theoretical predictions based on the PDB structure of NGB and using the rotamer library approach developed by G. Jeschke and co-workers. In a second set of experiments, the distance between the spin label and the heme iron (Fe(III)) are determined via determination of T1 and T2 using saturation recovery, time-dependent CW EPR and two-pulse ESEEM. In a last part, the reaction of neuroglobin with ROS are followed by CW EPR (use of both spin trapping agents and freeze quenching). The results will be related to the protein's possible functions.

Abstract for BPS General Scientific Meeting, ULB, May 21st

Electrical and Structural properties of Insulin Amyloid Fibrils

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Recent research has focussed on new methods for the production of microelectronic devices to meet the requirements of miniaturization. A promising strategy is the bottom-up assembly of electronic devices on a biological template [1]. In this study, we investigated amyloid fibrils polymerized from insulin. In order to study deposition patterns of Ag nanoparticles immobilized along insulin-derived amyloid fibrils, we rely on atomic force microscopy (AFM). We have studied the substructure of fibrils polymerised from normal insulin and from the insulin B-chain only [2]. A broad range of substructures can be observed on the normal fibrils, while the B-chain fibrils display a much narrower height distribution. The formation of Ag particles on the insulin template is done by electroless plating. The fibrils are incubated with Ag nitrate, immobilized on an oxidized silicon substrate, and reduced with sodium borohydride. This procedure yields nearly continuously metallized fibrils. The metallized fibrils are deposited on contacts which are predefined with optical lithography in order to measure their electrical properties.

[1] E. Braun, Y. Eichen, U. Sivan, G. Ben-Yoseph, Nature 391(1998), p. 775.

[2] G. Devlin, T. Knowles, A. Squires, E. MacPhee J. Mol. Biol. 360 (2006), p. 407.