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Lodz University of Technology

2nd Workshop on Progress in Bio- and Nanotechnology

BioNanoWorkshop2015

Lodz, Poland, 28-29 September 2015, www.bionanoworkshop2015.pl

Book of Abstracts

28-29 September 2015
Lodz, Poland

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Preface

The Workshop is organized on an occasion of initializing of research activity of the BioNanoPark laboratories which constitute a new department of Technopark Lodz.

Lodz University of Technology (TUL) is a shareholder of Technopark Lodz, and the BioNanoPark project was elaborated at TUL on a basis of earlier project of the European Centre of Bio- and Nanotechnology (ECBNT). An initiative of the ECBNT project was formulated several years ago by Rector of TUL, Prof. Stanislaw Bielecki; Prof. Krzysztof Matyjaszewski chaired International Advisory Board and Prof. Jacek Ulanski coordinated work of researchers from almost all departments of TUL involved in preparation of the project.

One of the sessions of the Workshop, "*In memoriam* of Tadeusz Pakula", is dedicated to Professor Tadeusz Pakula in memory of the 10th anniversary of his premature passing away. The *Dynamic Liqiud Lattice* algorithm, developed by Professor Pakula, has inspired Dr. Jaroslaw Jung and other researchers at TUL to design the massively-parallel simulator ARUZ, which is a core of the Laboratory of Molecular Simulation, perhaps the most unique part of the BioNanoPark.

Organizers:

Lodz University of Technology
Technopark Lodz

Scientific Advisory Committee:

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Kamil Krysiak (Lodz University of Technology)
Joanna Jagas (Technopark Lodz)
Jolanta Wawrzyniak-Zientarska (Lodz University of Technology)

Location

On the first day (28.09.2015) Workshop will take place at:
Technopark Lodz Ltd.
93-465 Lodz, 114/116 Dubois Street, Poland
phone: (+4842) 684 44 44, fax: (+4842) 684 50 00

On the second day (29.09.2015) Workshop will take place at:
Lodz University of Technology, Faculty of Chemistry
building A27, 2nd floor, room CH-1
90-924 Lodz, 116 Zeromskiego Street, Poland
phone: (+4842) 631 32 05, fax: (+4842) 631 32 18

Workshop programme

Monday 28.09. (Technopark Lodz)

08:00 – 08:30 Registration

08:30 – 09:00 Opening (*J. Ulanski, S. Bielecki, B. Wasilewski, K. Matyjaszewski, representatives of local authorities*)

Session 1: ECBNT & BioNanoPark

09:00 – 10:40 Chairman: **J. Ulanski**

- 09:00 – 09:25 **K. Matyjaszewski**: *Densely grafted copolymers as molecular bottlebrushes*
- 09:25 – 09:50 **A. Pron**: *Rational design of organic semiconductors - tuning the electronic properties from n-type, through ambipolarity to p-type via functionalization*
- 09:50 – 10:15 **S. Bielecki**: *Molecular and engineering aspects of synthesis and application of bacterial nanocellulose*
- 10:15 – 10:40 **P. Ulanski**: *Nanomaterials for medicine synthesized by radiation- and sonochemical techniques*

10:40 – 11:05 coffee break

11:05 – 12:45 Chairman: **E. Vandamme**

- 11:05 – 11:30 **R. Wohlgemuth**: *Novel paths to metabolite manufacturing for molecular medicine and biotechnology*
- 11:30 – 11:55 **M. Koziolkiewicz**: *Natural and synthetic compounds as regulators of type 2 diabetes-related signaling pathways*
- 11:55 – 12:20 **P. Paneth**: *Isotopic fractionation - from basic science to application*
- 12:20 – 12:45 **J. Ulanski**: *Zone-casting: from anisotropic conducting composites to organic field effect transistors*

12:45 – 15:00 lunch, visiting laboratories and ARUZ in BioNanoPark (speakers and participants from outside Lodz)

Session 2: „*Pro memoriam* Tadeusz Pakula"

15:00 – 17:05 Chairman: **K. Matyjaszewski**

- 15:00 – 15:25 **K. Halagan**: *DLL algorithm as a universal tool for studies of complex systems*
- 15:25 – 15:50 **R. Kielbik**: *ARUZ - Hardware Implementation of DLL Algorithm*
- 15:50 – 16:15 **E. Jamro**: *The algorithms implemented in FPGA-accelerated systems*
- 16:15 – 16:40 **J. K. Jeszka**: *DLL simulations of star polymers prepared using ATRP method*
- 16:40 – 17:05 **G. Floudas**: *How different is water crystallization from polymer crystallization under confinement?*

17:05 – 17:30 coffee break

17:30 – 18:45 Chairman: **G. Wegner**

- 17:30 – 17:55 **I. Szleifer**: *Protein adsorption on pH responsive nanogels: non-trivial coupling between chemical equilibrium, physical interactions and molecular organization under nanoconfinement*

- 17:55 – 18:20 **D. Vlassopoulos**: *From polymeric to colloidal stars: tailoring the flow of soft matter at molecular scale*
- 18:20 – 18:45 **G. Fytas**: *Polymer-tethered colloidal assemblies enable robust phononic band gaps*

20:00 official dinner

Tuesday 29.09 (Lodz University of Technology)

Session 3 : Partnering

08:30 – 10:35 Chairman: **S. Bielecki**

- 08:30 – 08:55 **C. Griesinger**: *Making use of polymers for NMR & Interference with aggregation of polymers for Neuroprotection*
- 08:55 – 09:20 **H-J. Butt**: *Nanostructuring surfaces to control wetting*
- 09:20 – 09:45 **S. Slomkowski**: *Polymer colloidal crystals and related materials*
- 09:45 – 10:10 **M. Klapper**: *Biocompatible nanoparticles with a polypeptide shell by emulsion polymerisation*
- 10:10 – 10:35 **L. Wozniak**: *From DNA microarrays to Gestational Diabetes Mellitus*

10:35 – 11:00 coffee break

11:00 – 12:40 Chairman: **P. Paneth**

- 11:00 – 11:25 **Z. Klusek**: *Graphene in perspective of future innovative applications*
- 11:25 – 11:50 **R. Holyst**: *Nano-bio-machines against thermal noise and energy barriers*
- 11:50 – 12:15 **S. Jurga**: *Novel structures of block copolymers under spatial confinement*
- 12:15 – 12:40 **J. Szemraj**: *Analysis of antioxidative potential of proteins immobilized on nanoparticles. Study in vitro, in vivo*

12:40 – 13:00 closing remarks (*S. Bielecki, K. Matyjaszewski, J. Ulanski*)

13:00 – 14:30 lunch and end of Workshop

DENSELY GRAFTED COPOLYMERS AS MOLECULAR BOTTLEBRUSHES

Krzysztof Matyjaszewski

Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, Pennsylvania 15213

Atom transfer radical polymerization (ATRP) has been an excellent tool to control branching in well-defined polymers. Loosely branched comb polymers and densely grafted bottlebrushes were successfully prepared by ATRP in order to control their properties and fine tune them for specific applications.

[1] Burdynska, J.; Daniel, W.; Li, Y.; Robertson, B.; Sheiko, S. S.; Matyjaszewski, K., Molecular Bottlebrushes with Bimodal Length Distribution of Side Chains, *Macromolecules* **2015**, *48*, 4813-4822.
[2] Burdynska, J.; Li, Y.; Aggarwal, A. V.; Hoger, S.; Sheiko, S. S.; Matyjaszewski, K., Synthesis and Arm Dissociation in Molecular Stars with a Spoked Wheel Core and Bottlebrush Arms, *J. Am. Chem. Soc.* **2014**, *136*, 12762-12770.
[3] Stals, P. J. M.; Li, Y.; Burdynska, J.; Nicolay, R.; Nese, A.; Palmans, A. R. A.; Meijer, E. W.; Matyjaszewski, K.; Sheiko, S. S., How Far Can We Push Polymer Architectures?, *J. Am. Chem. Soc.* **2013**, *135*, 11421-11424.
[4] Sheiko, S. S.; Zhou, J.; Arnold, J.; Neugebauer, D.; Matyjaszewski, K.; Tsitsilianis, C.; Tsukruk, V. V.; Carrillo, J.-M. Y.; Dobrynin, A. V.; Rubinstein, M., Perfect mixing of immiscible macromolecules at fluid interfaces, *Nat. Mater.* **2013**, *12*, 735-740.
[5] Park, I.; Shirvanyants, D.; Nese, A.; Matyjaszewski, K.; Rubinstein, M.; Sheiko, S. S., Spontaneous and Specific Activation of Chemical Bonds in Macromolecular Fluids, *J. Am. Chem. Soc.* **2010**, *132*, 12487-12491.
[6] Sheiko, S. S.; Sumerlin, B. S.; Matyjaszewski, K., Cylindrical molecular brushes: Synthesis, characterization, and properties, *Prog. Polym. Sci.* **2008**, *33*, 759-785.
[7] Sheiko, S. S.; Sun, F. C.; Randall, A.; Shirvanyants, D.; Rubinstein, M.; Lee, H.-i.; Matyjaszewski, K., Adsorption-induced scission of carbon-carbon bonds, *Nature (London, United Kingdom)* **2006**, *440*, 191-194.

[8] Grigoriadis, C.; Nese, A.; Matyjaszewski, K.; Pakula, T.; Butt, H.-J.; Floudas, G., Dynamic Homogeneity by Architectural Design - Bottlebrush Polymers, *Macromol. Chem. Phys.* **2012**, *213*, 1311-1320.
[9] Pakula, T.; Koynov, K.; Boerner, H.; Huang, J.; Lee, H.-i.; Pietrasik, J.; Sumerlin, B.; Matyjaszewski, K., Effect of chain topology on the self-organization and the mechanical properties of poly(n-butyl acrylate)-b-polystyrene block copolymers, *Polymer* **2011**, *52*, 2576-2583.
[10] Gitsas, A.; Floudas, G.; Butt, H. J.; Pakula, T.; Matyjaszewski, K., Effects of Nanoscale Confinement and Pressure on the Dynamics of pODMA-b-ptBA-b-pODMA Triblock Copolymers, *Macromolecules* **2010**, *43*, 2453-2462.
[11] Berry, G. C.; Kahle, S.; Ohno, S.; Matyjaszewski, K.; Pakula, T., Viscoelastic and dielectric studies on comb- and brush-shaped poly(n-butyl acrylate), *Polymer* **2008**, *49*, 3533-3540.
[12] Pakula, T.; Zhang, Y.; Matyjaszewski, K.; Lee, H.-i.; Boerner, H.; Qin, S.; Berry, G. C., Molecular brushes as super-soft elastomers, *Polymer* **2006**, *47*, 7198-7206.
[13] Zhang, Y.; Costantini, N.; Mierzwa, M.; Pakula, T.; Neugebauer, D.; Matyjaszewski, K., Super soft elastomers as ionic conductors, *Polymer* **2004**, *45*, 6333-6339.

RATIONAL DESIGN OF ORGANIC SEMICONDUCTORS – TUNING THE ELECTRONIC PROPERTIES FROM N-TYPE, THROUGH AMBIPOLAR TO P-TYPE VIA FUNCTIONALIZATION

Kamil Kotwica, Renata Rybakiewicz, Piotr Bujak, Małgorzata Zagórska, Adam Proń

Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Two groups of solution processible organic semiconductors will be described, namely tetraalkoxydinapthophenazines obtained by appropriate functionalization of old, intractable and almost forgotten alizarine-type vat dyes and new arylene bisimides core- or N-functionalized with triarylamines. The effect of the substituent position on their self-assembly and the

resulting 2D and 3D supramolecular organizations will be discussed as well as their self-assembly. This will be competed by the description of their electrochemical, spectroscopic and spectroelectrochemical properties. The lecture will be completed by presentation of selected case of these new semiconductors applications in organic electronic devices such as light emitting diodes (LEDs) or field effect transistors (FETs).

MOLECULAR AND ENGINEERING ASPECTS OF BACTERIAL NANOCELLULOSE SYNTHESIS AND APPLICATION

Marzena Jędrzejczak-Krzepkowska, Katarzyna Kubiak, Halina Kalinowska, Katarzyna Ludwicka, Teresa Pankiewicz, Marek Kołodziejczak, Stanislaw Bielecki

Institute of Technical Biochemistry, Lodz University of Technology, contact: stanislaw.bielecki@p.lodz.pl

Bacterial nanocellulose (BNC), synthesized by Gluconacetobacter xylinus is the natural biopolymer of the exceptionally high purity and outstanding biocompatibility with well-documented properties ensuing from its unique structure. BNC is being already investigated in our Institute in a wide range of industrial and medical applications. At present bacterial nanocellulose production technology and BNC based product, CelMat® wound dressing invented by us was successfully transferred to industry.

Both modern molecular tools based on – omics and technological approaches to improve the production efficiency and lowering costs of BNC biosynthesis and modifications are presented here. Based on genom of our Gluconacetobacter xylinus strain and comparative studies done with different cellulose producers, some mutants with changes in tpi, gene or clpP gene and further in two genes probably involved in yet unknown motility mechanism were obtained respectively. In all cases the differences in dynamisms of biosynthesis, both structural and mechanical properties of cellulose pellicles were observed.

To minimize costs of BNC biosynthesis, G. xylinus E25 was cultivated on media based on.enzymatic hydrolysates of sugar beet pulp,

apple pomace and wood cellulosic pulps as well as various fruit and vegetable juices and beers. The effect of culture medium composition and supplementation with either urea or ammonium phosphate on BNC yield was determined. The highest BNC yields in comparison with the Schramm-Hestrin medium and changes in water holding capacity were observed.

The novel methods of developing a stable 3D composite of bacterial nanocellulose and perforated metal or polymeric material, designed for tissues reconstruction is also presented. The products we managed to develop involve meshes for cranioplasty and herniorraphy. They are characterized by great mechanical strength, dependent on the strength of a material overgrown with BNC, the biocompatiblity and physical smoothness given by cellulose layer around the mesh.

NANOMATERIALS FOR MEDICINE SYNTHESIZED BY RADIATION- AND SONOCHEMICAL TECHNIQUES

Piotr Ulanski, Agnieszka Adamus, Renata Czechowska-Biskup, Sławomir Kadlubowski, Justyna Komasa, Bozena Rokita, Janusz M. Rosiak

Institute of Applied Radiation Chemistry, Faculty of Chemistry, Lodz University of Technology, Wroblewskiego 15, 93-590 Lodz, Poland, ulanskip@mitr.p.lodz.pl

Radiation chemistry and sonochemistry are convenient tools for synthesizing a variety of nanomaterials. Both these non-conventional synthetic approaches share common advantages. Since energy of ionizing radiation or ultrasound interacts directly with the substrates (including monomers and/or polymers), there is no need for any initiators and there is a good control of the amount and rate of generation of the reactive species (mostly radicals). Many radiation- and sonochemical syntheses can be performed in aqueous media. In this lecture a few examples will be presented, demonstrating the applicability of these two methods for synthesizing nanomaterials for medicine. These include: nanogels to be used as drug- or gene carriers, thermosensitive surfaces for cell layer engineering, and gold nanoparticles for potential applications in radiotherapy

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NOVEL PATHS TO METABOLITE MANUFACTURING FOR MOLECULAR MEDICINE AND BIOTECHNOLOGY

Roland Wohlgemuth

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Metabolites have traditionally contributed to many areas of biotechnology, healthcare and medicine, from analysis to manufacturing, from diagnostics to drug discovery and early development, metabolite production for preclinical and clinical studies to the active pharmaceutical ingredients in therapy. The understanding of biocatalytic systems in nature provides inspiration for the design of novel synthetic as well as analytical paths to and from metabolites. The integration of biological and chemical retroanalysis serves thereby as a useful guiding principle. Numerous metabolites for different applications in medicine and biotechnology have been synthesized by novel paths with high selectivity and molecular economy. Route selection, highly efficient expression of the required enzymes, stability of the intermediates and metabolites as well as engineering tools are among the key success factors. Miniaturized analytical methodologies are thereby essential for these synthetic developments, but also for applications in biotechnology. Building the analytical and synthetic frameworks from the systems perspective is an attractive option to provide key advances for medical diagnostics, engineering metabolic pathways in biotechnology and new therapies.

NATURAL AND SYTHETIC COMPOUNDS AS REGULATORS OF TYPE 2 DIABETES-RELATED SIGNALING PATHWAYS

Maria Koziołkiewicz, Edyta Gendaszewska-Darmach, Małgorzata Zakłos-Szyda, Anna Drzazga, Edyta Węgłowska

Institute of Technical Biochemistry, Lodz University of Technology, Stefanowskiego 4/10, 90-924 Lodz

Type 2 diabetes mellitus, which is usually a result of wrong dietary habits and reduced physical activity, represents 85-95% of all diabetes cases and among other diet-related diseases is the major cause of deaths. Pharmaceuticals currently available and widely used in T2D therapy have some undesirable side effects, so there is a need of search for better and less toxic agents. Among them are phytochemicals isolated from plants, fruits and vegetables. There is also evidence that some phospholipids as well as nucleotides can regulate signaling pathways responsible for metabolism of pancreatic cells and insulin secretion. Mechanisms and signaling pathways responsible for anti-diabetic activities of polyphenols, lysophospholipids and nucleotides studied in the Institute of Technical Biochemistry will be presented during the lecture.

The studies were supported by grants from National Science Centre (Grants No. 3407/B/P01/2011/40, UMO-2011/01/B/NZ9/04699) and The National Centre for Research and Development (Grant No. PBS1/B8/7/2013).

ISOTOPIC FRACTIONATION – FROM BASIC SCIENCE TO APPLICATIONS

Kamila Klajman,[1,2] Piotr Paneth[2]

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Initial work on the theory of isotope effects originated from practical need for effective isotopic enrichment of uranium. Later, however, the effort has

been directed towards their use in understanding mechanisms of physical, chemical, and finally biological processes. With the advent of high-precision isotope-ratio mass spectrometry measurements of even very small isotope effects became possible. In order to interpret them theoretical predictions of their values started and matured to the point at which isotope effects on large systems, such as enzymatic reactions, can be now reliably calculated. Although some unresolved problems still remain generally we have quite good understanding of the basis of isotope effects. It is thus not surprising that the attention shifts slowly back to their practical applications. Isotopic fractionation, the consequence of isotope effects, has found its place in food authentication, environmental studies, rational drug design, and is moving to new areas such as medical diagnostics. This shift will be discussed from the personal perspective.

ZONE-CASTING: FROM ANISOTROPIC CONDUCTING COMPOSITES TO ORGANIC FIELD EFFECT TRANSISTORS

Jacek Ulanski

Department of Molecular Physics, Lodz University of Technology, 90-924 Lodz

Zone-casting technique of producing of highly anisotropic conducting polymer composites was developed in early 80-ies of XX century[1], as a modification of the reticulate doping method[2]. In recent years the zone-casting was rejuvenated and successfully applied in several laboratories to produce high performance organic field effect transistors[3-7]. In this work we present the last achievements in using the zone-casting for one-step production of bi-functional composites for flexible and ambipolar organic transistors.

This work was partially supported by Foundation for Polish Science (Grant Master 9./2014).

[1] L.Burda, A.Tracz, T.Pakula, J.Ulanski, M.Kryszewski, *J.Phys.D*, **16**, 1737 (1983).

[2] J.K. Jeszka, J. Ulanski and M. Kryszewski, *Nature*, **289**, 390 (1981).
[3] W. Pisula et al., *Adv. Mater*., **6**, 684 (2005).
[4] P. Miskiewicz et al., *Chem. Mater*., **18**, 4724 (2006).
[5] G. De Luca et al., *Adv. Funct. Mater*., **21**, 1279 (2011).
[6] I. Tszydel et al., *Adv. Funct. Mat*., **22**, 3840 (2012).
[7] T. Marszalek et al., *J. Mater. Chem. C*, **1**, 3190 (2013).

DLL ALGORITHM AS A UNIVERSAL TOOL FOR STUDIES OF COMPLEX SYSTEMS

Krzysztof Halagan, Piotr Polanowski, Jaroslaw Jung

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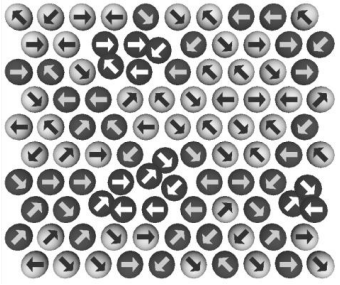
DLL algorithm (Dynamic Lattice Liquid) [1,2] was developed in 90s of the last century by prof. Tadeusz Pakula. The algorithm is based on the model of liquid molecular system considered as an assembly of structureless beads representing atoms or groups of atoms. Diffusive motion in this system is possible, even for completely occupied lattice, by cooperative moves – closed loops. In every time step all beads are attempting diffusion movement in parallel. The model satisfies the continuity and excluded volume condition. Its unique dynamic properties and parallel nature gave basis for the idea of massively-parallel simulator – ARUZ. DLL algorithm was already successfully applied for various non-equilibrium physical and chemical problems [e.g. 3-5] like diffusion limited aggregation, evolution of reaction front, linear and cyclic polymer chains dynamics, gelation process, polymer star formation, solvent dynamics in the neighborhood of brushed polymer chains, diffusion in crowded environments and spinodal decomposition in binary system.



[1] T. Pakula, J. Teichmann, *Mater. Res. Soc. Symp. Proc.* **455**, 211 (1997).
[2] T. Pakula, J. Teichmann, *J. Mol. Liq.* **86**, 109 (2000).
[3] P. Polanowski, A. Sikorski, *Soft Matter* **10**, 3597 (2014).
[4] P. Polanowski, J. K. Jeszka, K. Matyjaszewski, *Polymer* **55**, 2552 (2014).
[5] J. Saramak, K. Halagan, M. Kozanecki, P. Polanowski, *J. Mol. Model.* **20**, 2529 (2014)

ARUZ – HARDWARE IMPLEMENTATION OF DLL ALGORITHM

Rafał Kiełbik, Andrzej Napieralski

Lodz University of Technology, Department of Microelectronics and Computer Science

ARUZ is a parallel, digital data processing machine based on FPGA (Field Programmable Gate Array) devices. It is mainly composed of 3 000 DBoards (Daughter Boards) – printed circuits containing 9 FPGAs each. This gives the number of 27 000 configurable devices implemented in one structure, making it the biggest FPGA-based machine in the world. Every DBoard is connected to each of 6 DBoards from its nearest neighbourhood by means of dedicated cables allowing the data transfer at the rate of 8 GB/s (full duplex). Each FPGA can be independently configured in order to represent user-defined set of processing units. All of this makes ARUZ an ideal hardware for implementation of DLL (Dynamic Lattice Liquid) and any other algorithm, in which the fast, local interaction among many simple elements is crucial. In case of DLL, ARUZ is able to perform the analysis of over 1.3 million nodes, making about 1 500 simulation steps per second and consuming less than 100 kW of electric power. Bearing in mind all these numbers, ARUZ can be considered to be the biggest, fastest and most efficient chemical simulator in the world.

THE ALGORITHMS IMPLEMENTED IN FPGA-ACCELERATED SYSTEMS

K. Wiatr, P. Russek, E. Jamro, A. Dąbrowska-Boruch, M. Wielgosz, M. Pietroń, S. Koryciak, M. Karwatowski

AGH University of Science and Technology, Dept. of Electronics / ACC Cyfronet AGH

Fifty years since the formulation of the Moore's law, more and more scientists predict that the exponential growth of computational speed is no longer possible. This holds as a transistor size has reached the atomic scale, and large supercomputing centres consume a tremendous amount of electric power. The increase in the processing performance and power savings may be obtained if the dedicated hardware for specific computational problems is employed. Field Programmable Gate Arrays (FPGAs) contain programmable logic which can be configured for selected computational tasks. FPGAs are best suited for the bit/byte manipulations, logic operations, and state-machines. They can be efficiently employed for data encryption (description), compression (decompression), string matching, and look-up table operations for example. However, the FPGA computational power is in most cases limited by IO bandwidth of a data transfer in these tasks. The FPGAs can be also employed for a reduced bit-width fixed point arithmetic, e.g. image processing. The FPGAs cannot compete with the CPUs and GPGPUs in typical floating-point operations. Nevertheless, FPGAs can be efficiently employed for sparse matrix and adaptive precision floating-point operations.

DLL SIMULATIONS OF STAR POLYMERS PREPARED USING ATRP METHOD

Jeremiasz Jeszka[1], Piotr Polanowski[2] and Krzysztof Matyjaszewski[3]

[1]*Department of Man-Made Fibres, Technical University of Lodz, 90-924 Lodz,*
[2]*Department of Molecular Physics, Technical University of Lodz, 90-924 Lodz,*
[3]*Department of Chemistry, Carnegie Mellon University, Pittsburgh, Pa 15213.*

Polymers of complex architecture, stars, brushes nanogels ect. find various practical applications. Atom transfer radical polymerisation (ATRP) method makes possible obtaining such materials in a convenient, one-pot method. During the polymerisation diffusion constants, molecular weight and polymer structure change dramatically so simulation method should take thermal moves of the reagents into account. Dynamic lattice liquid (DLL) method of Monte Carlo simulation proposed by T. Pakula is therefore most suitable. In this communication we present DLL simulations of ATRP synthesis of star polymers by suitable copolymerization of a monomer and bifunctional crosslinker. Two methods of star preparations were simulated: (i) arm-first, where the linear arms are grown first and then crosslinker is added to form star cores and (ii) core-first, where crosslinker forms cores at the beginning. The results of simulations are in good agreement with experimental data obtained in K. Matyjaszewski's group. In particular they show importance of dilution and full conversion of the crosslinker for the average number of arms of the obtained stars and possible gelation. The results can be used as a guidelines in the experiment.

HOW DIFFERENT IS WATER CRISTALLIZATION FROM POLYMER CRYSTALLIZATION UNDER CONFINEMENT?

G. Floudas

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(http://softmatter.physics.uoi.gr/)

The freezing mechanism of water under confinement can be fundamentally different from the bulk [1-4]. Despite fundamental importance, the lack of well-defined confining media precluded a systematic investigation. Herein we employ self-ordered nanoporous aluminum oxide (AAO) which contains arrays of discrete, parallel and cylindrical nanopores with uniform pore length and diameter to study the effect of confinement on water crystallization [5]. By varying different parameters such as pore size, temperature and cooling rate, the respective conditions under which the hexagonal form (I_h) and the less common form of cubic ice (I_c) could be

studied. We found a transition from heterogeneous nucleation of I_h to homogeneous nucleation of predominantly I_c with decreasing pore diameter. Furthermore, the monotropic $I_c \rightarrow I_h$ transition commonly observed upon heating is suppressed inside pores having diameters ≤ 35 nm. These findings lead to the phase diagram of water under confinement. It contains a predominant cubic form, a form known to exist only in the upper atmosphere**.** There are many similarities between the freezing of water and the crystallization of polymers under confinement.

***In collaboration with MPI-P: Y. Suzuki, H. Duran, M. Steinhart, and H.-J. Butt.**

[1] H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Nano Letters* **2011**, *11*,*1671*.
[2] Y. Suzuki, H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Soft Matter* **2013**, *9*, 2769.
[3] Y. Suzuki, H. Duran, W. Akram, M. Steinhart, G. Floudas, H.-J. Butt, *Soft Matter*, **2013**, *9*, 9189.
[4] Y. Suzuki, H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Macromolecules* **2014***, 47,* 1793.
[5] Y. Suzuki, H. Duran, M. Steinhart, M. Kappl, H.-J. Butt, G. Floudas*, Nano Letters* **2015**, *15*, 1987-1992.

PROTEIN ADSORPTION ON PH RESPONSIVE NANOGELS: NON-TRIVIAL COUPLING BETWEEN CHEMICAL EQUILIBRIUM, PHYSICAL INTERACTIONS AND MOLECULAR ORGANIZATION UNDER NANOCONFINEMENT

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The development of synthetic materials for biorelated applications requires exquisite control of the physical and chemical environment within the materials. In this talk we will discuss how charge within a hydrogel is controlled by bulk pH and ionic strength. The pH within hydrogels is very different from that of the bulk solution. The physical and chemical properties of pH-responsive gels are found to depend on the coupling between acid-base equilibrium, molecular organization and physical interactions. For example, the network's degree of protonation is not only determined by chemical composition of the bath solution but also by the ability of the polymeric structure to modify the local environment. This coupling results in swelling (or shrinking) that depends on the bath pH and salt concentration. We will discuss the gradients of protonation state and pH in hydrogel thin films that result from the inhomogeneous distribution of species within the film and how this effect has implications on the effective interactions between proteins and the film. The role of pH and ionic strength on protein adsorption and its implications to chromatography will be discussed. In particular the dramatic changes that we predict for different amino acids within the proteins when adsorbed in the hydrogel as compared to bulk solution. The theoretical predictions can be used as guidelines for the design of responsive gels in a variety of applications ranging from drug delivery systems to tissue engineering scaffolds and they provide for fundamental understanding on the non-trivial behavior of these gels. Moreover, our predictions demonstrate that the chemical state within soft materials may be dramatically different from that of the environment solutions in contact with them.

FROM POLYMERIC TO COLLOIDAL STARS: TAILORING THE FLOW OF SOFT MATTER AT MOLECULAR SCALE

Dimitris Vlassopoulos

FORTH, Institute of Electronic Structure & Laser, and University of Crete, Department of Materials Science & Technology, Heraklion, Crete, Greece

Branching is known to influence the properties of entangled polymers. High level of branching results in hyperbranched or dendritic Cayley-tree polymers, which can be viewed as soft colloids. We attempt at systematically bridging the interesting gap between polymers and colloids by accessing highly functionalized well-characterized polymers and exploring their dynamic properties. We discuss two examples. (i) High- functionality star polymers can respond as soft colloids either in solution or in melt. In solution in particular, their (ultra)softness is responsible for a variety of new metastable states and transitions at high fractions in molecular or polymeric solvents. Here we focus on glass-liquid-gel transition in star-linear polymer mixtures. (ii) Dendronized polymers are a relatively new class of hyperbrached polymers, akin to bottlebrushes, which each branch being a dendrimer. By varying the molar mass of the backbone and the dendrimer generation it is possible to switch from polymeric to colloid-like response. Here, we focus on their entanglement-like dynamics.

Work in collaboration with M. Gauthier (Waterloo), K. Matyjaszewski (Carnegie-Mellon) and A. D. Schlüter (ETH Zurich).

POLYMER-TETHERED COLLOIDAL ASSEMBLIES ENABLE ROBUST PHONONIC BAND GAPS

George Fytas[1,2]

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Phononic crystals-composite materials in which a periodic distribution of elastic parameters facilitates control of the propagation of phonons- hold the promise to enable transformative material technologies in areas ranging from acoustic and thermal cloaking to thermoelectric devices. Realizing these opportunities requires strategies to deliberately “engineer” the band structure of materials in the frequency range of interest controlling phononic band gaps of Bragg-type, due to destructive interference of waves in periodic media, and hybridization-type (HG), resulting from the avoided

crossing of two bands of the same symmetry. Colloid and polymer science offers methods to create novel materials with varying size and shape of solid particles, and polymer architecture of grafted particles. Harnessing the anisotropic elasticity across the particle-polymer interface, we report a new type of HG. It utilizes the l=1 torsional resonances of the individual particles, localized in the core surface and conditioned by the densely tethered PS brushes that causes an interfacial anisotropy. Brillouin scattering and theoretical analysis confirm the robustness to disorder and the tunability of the resulting HG. Compared to hard sphere and core-shell colloid crystals, the unique phonon propagation in particle brush materials emphasizes a rich parameter-space for controlling new properties such as thermal and optomechanic response in hybrid materials. Materials chemistry plays a central role also in this development assessing the necessary material parameters at nanoscale thereby enabling tuning of the phononic band structure.

NMR SPECTROSCOPY AND POLYMERS: TOOLS AND OBJECT OF STUDY

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Polymer gels can be used to align small molecules in solution in order to reintroduce anisotropic parameters such as residual dipolar couplings and residual chemical shift anisotropies. In applications I will show that these parameters can be used to determine the conformation and configuration of small molecules down to concentrations in the mikromolar range. In a second part of the talk, modern NMR techniques will be used to describe the conformation and conformational transitions of biomolecules on the example of a sensory bacterial membrane protein. Finally, the potential of modulating the aggregation landscape of biopolymers with small molecules will be shown on the example of intrinsically disordered proteins (i.e. biopolymers) that are involved in neurodegeneration and type II diabetes mellitus.

NANOSTRUCTURING SURFACES TO CONTROL WETTING

Frank Schellenberger, Noemí Encinas, Periklis Papadopoulos, Doris Vollmer, Hans-Jürgen Butt

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Super liquid-repellency can be achieved by nano- and microstructuring a low energy surface in such a way, that protrusions entrap air under¬neath the liquid. To better understand how a drop advances and recedes on such a structured surface, we imaged the motion of a water drop on a superhydrophobic array of micropillars by laser scanning confocal microscopy. Commonly, super liquid-repellency is defined by a high apparent advancing contact angle and a low roll-off angle for a liquid droplet. These microscopic videos demonstrate that to define super liquid-repellency the apparent receding contact angle should be high. In addition, a high impalement pressure is required. By calculations we demonstrate that to achieve both, the features constituting the layer should be as small as possible. Therefore, two models for super liquid-repellent layers are theoretically analyzed: A superhydrophobic layer consisting of an array of cylindrical micropillars and a superamphiphobic layer of an array of pillars of spheres. For the cylindrical micropillars a simple expression for the apparent receding contact angle is derived. It is based on a force balance rather than a thermodynamic approach. The absolute size of surface features should be as small as possible, to maximize the impalement pressure.

POLYMER COLLOIDAL CRYSTALS AND RELATED MATERIALS

Stanislaw Slomkowski, Teresa Basinska, Monika Gosecka

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Polymer colloidal crystals constitute special class of polymer materials formed by assembly of nano- and microparticles. In last years, due to special

optical properties, these materials attracted attention of many researchers interested in a variety of sensors and elements of diagnostic devices. Recent development of synthesis of non-spherical particles (e.g. ellipsoidal ones) did open a possibility for preparation of their ordered assemblies analogous to liquid crystals.
The lecture will present progress in development of methods used for preparation of ordered assemblies of polymer colloidal crystal related materials and synthesis of nano- and microparticles with surface properties tailored in a way facilitating their spontaneous or induced assembly. Specific optical properties of polymer colloidal crystals will be discussed.
Last part of the lecture will be devoted to the already existing, under development and potential practical applications of polymer colloidal crystals for design and fabrication of chemo- and biosensors with special attention paid to the so-called "lab-on-the-chip" and "reagent free" diagnostic devices.

BIOCOMPATIBLE NANOPARTICLES WITH A POLYPEPTIDE SHELL BY EMULSION POLYMERISATION

Markus Klapper, Filiz Karagöz, Sapun H. Parekh, Robert Dorresteijn, Klaus Müllen,

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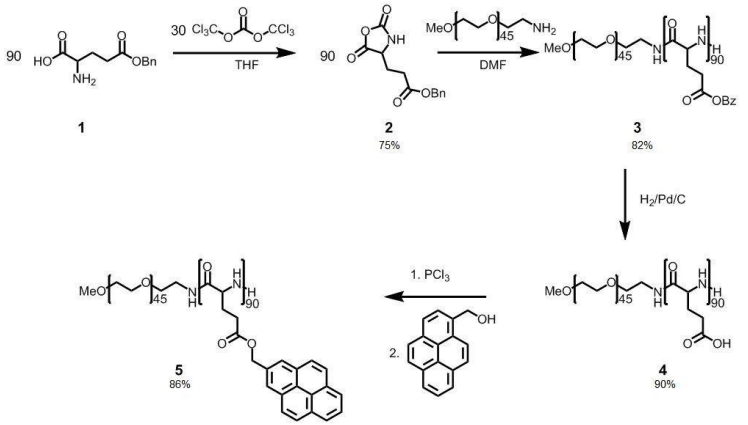
For nanoparticles that are used as intravascular drug delivery systems, aggregation resulting in carrier sizes >250 nm is a serious issue as those systems are removed from the blood stream by Kupffer cells.[4] Herein, we describe the synthesis of polylactide particles decorated by a polyglutamic acid corona by non-aqueous emulsion polymerization. While in many other approaches polypeptides are either after particle formation adsorbed or grafted herein we us a specially designed emulsifier to form a polypeptide shell.
A light sensitive PEG-*block*-poly((1-pyrenyl methyl) glutamate) (PEG-*b*-PGlu(Pyr)) copolymer *is synthesized a*nd used as emulsifier in a non-aqueous

emulsion polymerization of lactide which is required due to the moisture sensitivity of the polymerization catalysts. Poly(L-lactide) (PLLA) nanoparticles were synthesized via ring-opening polymerization of L-lactide with a moisture-sensitive catalyst in a non-aqueous emulsion consisting of acetonitrile, cyclohexane, and the PEG-*b*-PGlu(Pyr) copolymer as emulsifier. Upon UV irradiation, hydrophobic pyrenyl methylene units are cleaved from the block copolymer, resulting in a polarity reversal of the particle surface from hydrophobic to hydrophilic. The product particles have a fully hydrophilic and biocompatible PEG-*b*-PGlu shell and can be dispersed in water without aggregation. Furthermore, introducing MMP-3 cleavable peptide sequences in the nanoparticles allows for a full degradation of the particles when they are getting close to tumor cells. This offers the opportunity to selectively release drugs which have already been incorporated before during in the particle formation.
The particles consist exclusively of non-toxic biodegradable polymes (polylactide and polypeptide making them suitable candidates for medical applications in particular for cancer therapy.



[1] Polarity Reversal of Nanoparticle Surfaces by the Use of Light-Sensitive Polymeric Emulsifiers, R. Dorresteijn, R. Ragg, G. Rago, N. Billecke, M. Bonn, S. H. Parekh, G. Battagliarin, K. Peneva, M. Wagner, M. Klapper, K. Müllen, *Biomacromolecules* **2013**, 14, 1572–1577.

[2] Biocompatible Polylactide-block-Polypeptide-block-Polylactide Nanocarrier, R. Dorresteijn, N. Billecke, S. H. Parekh, M. Klapper, K.Müllen, *J. Pol. Sci, Part A: Pol. Chem* **2015**, 53, 200.

FROM DNA MICROARRAYS TO GESTATIONAL DIABETES MELLITUS MECHANISMS

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Gestational diabetes mellitus (GDM), defined as glucose intolerance with onset or first recognition during pregnancy, is the most prevalent metabolic disorder occurring during pregnancy that affects from 3% to 17% of all pregnancies, depending on racial and ethnic group as well as the diagnostic and screening criteria. GDM is associated with increased risk of adverse maternal and perinatal outcomes, including preeclampsia, preterm delivery, cesarean section, macrosomia, and respiratory distress syndrome, among other [1]. There is also an increased risk of complications after pregnancy such as the development of type 2 diabetes mellitus (T2DM) and cardiovascular disease in the mothers and developing obesity, metabolic syndrome, and T2DM in the children during childhood and adolescence. Although the precise mechanisms underlying GDM are still not completely understood, a close immune-metabolic relationship with inflammatory cytokines regulating metabolic homeostasis has been found [2].

[1] Wozniak LA, Cypryk K, Wojcik M. Molecular mechanisms of diabetes prevention by structurally diverse antioxidants (Chapter 25). In Nutritional and therapeutic interventions for diabetes and metabolic syndrome (Ed. Debasis Bagchi and Nair Sreejayan). Elsevier, 2012: 315-330.
[2] The elevated gene expression level of the A_{2B} adenosine receptor is associated with hyperglycemia in women with gestational diabetes mellitus.

Wójcik M, Zieleniak A, Mac-Marcjanek K, Wozniak LA, Cypryk K. *Dabetes/Metabolism Research and Reviews* **2014**; 30: 42-53.

GRAPHENE IN PERSPECTIVE OF FUTURE INOVATIVE APPLICATIONS

Zbigniew Klusek, Maciej Rogala, Pawel Dabrowski, Igor Wlasny, Witold Kozlowski, Pawel Kowalczyk, Adam Busiakiewicz

University of Lodz, Department of Solid State Physics

We will focus on issues important in applications of graphene and graphene oxide (GO) in nanoelectronics and photonics. Particularly, interactions of graphene with metals, insulators and modification of graphene during doping processes will be briefly outlined. This is important when graphene is used in fabrication of metal-graphene contacts in electronic devices. We will also present recent achievements in graphene inkjet printing. This is one of the most promising and developmental technique used to manufacture flexible electronics, mainly for production of thin conductive graphene tracks on elastic polymer foils and textile surfaces. Finally, we concentrate on resistive switching (RS) phenomenon recently discovered in graphene oxide. RS shows a new way of non-volatile data storage in flexible solid state devices. The very recent studies proving that GO has a potential for application in ReRAM devices will be shown. Presentation is based on the world-wide literature and selected papers published by our group.

NANO-BIO-MACHINES AGAINST THERMAL NOISE AND ENERGY BARRIERS

Robert Holyst

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Nano-bio-machines cannot act against thermal noise. They rather utilize the noise in the directed motion. I will describe three nano-machines in my talk: nano-windmills driven by the flux of water; and kinesin motors driven by

thermal fluctuations with ATP used solely for detachment of kinesin motor domain from microtubules. Nanowindmills consisting of liquid crystalline, chiral molecules are spread over the surface of water, forming a monolayer. Evaporation of water spins the molecules, which acting in concerto rotate collectively. The rotations of nano-windmills are in the range of Hz and ceases at equilibrium between water and its vapour or at low temperature when transition to solid phase occurs. The increase of viscosity on approach to 2D liquid-solid phase transition slows down rotations to sub-Hz region. The power of this nano-machine is few orders of magnitude smaller than the power of thermal noise, yet their rotations are very stable. I will discuss the origin of this stability at the nanoscale. The dimeric motor protein kinesin-1 moves processively along microtubules against forces of up to 7 pN. The force corresponds to hydrodynamic drag in solution of viscosity 700 Pas. Here, I point to the crucial importance of diffusion of the tethered motor domain for the stepping of kinesin-1: small crowders in solution stop the motor at a viscosity of 5 mPas – corresponding to a hydrodynamic load in the sub-fN ($\sim 10^{-4}$ pN) range. This indicates that the scale-dependent, effective viscosity experienced by the tethered motor domain, which increases the energy barrier for diffusion, is a key factor determining kinesin's functionality. These results emphasize the role of diffusion in kinesin-1 stepping mechanism and the general importance of the viscosity scaling paradigm in nanomechanics.

[1] K.Sozański at al, Phys.Rev.Lett. 111, 228301 (2013).
[2] P.Nitoń et al, Nanoscale 5, 9732-9738 (2013).
[3] K.Sozanski et al, Phys.Rev.Lett. (submitted) (2015).
[4] T.Kalwarczyk et al, Nano Letters 11, 2157-2163 (2011).

NOVEL STRUCTURES OF BLOCK COPOLYMERS UNDER SPATIAL CONFINEMENT

Stefan Jurga [1,2], Jacek Jenczyk[1,2]

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Block copolymers (BCPs) due to their self-assembling nature into periodic nanostructures present potential applications in nanotechnology and nanobiomedicine. The key challenges of today's nanotechnogy are new fabrication techniques, for the large scale inexpensive production of nanodevices, which would be highly scalable. Top-down techniques, like lithography, have the limitations down to about 40 nm, smaller sizes can be achieved by bottom-up techniques, using e.g. block copolymers that self-assemble into well-ordered nanodomain morphologies. A spatial confinement of the bulk may provide thin films which due to various wall interactions of nanodomains and confinement-induced entropy loss can lead to different from bulk novel structures, characterized, e.g. by long-range order, single crystalline and dendritic forms, specific crystalline growth dynamics. A study of structure and dynamics in BCPs will be discussed with a special focus on PS-b-PEO di-block copolymer in the bulk and thin films on reconstructed sapphire substrate.

Financial support from the National Centre for Research and Development, contract number PBS1/A9/13/2012, is gratefully acknowledged.

ANALYSIS OF ANTIOXIDATIVE POTENTIAL OF PROTEINS IMMOBILIZED ON NANOPARTICLES.
STUDY *IN VITRO*, AND *IN VIVO*

Janusz Szemraj

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Oxygen free radicals and their reactive derivatives react readily with cellular components such as lipids, proteins and DNA. As a result of these interactions cell membranes are damaged, there is improper activity or inactivation of enzymes and genetic mutations may happen. The excess of free radicals and of their derivatives in the cells and tissues of the body causes multiple lesions. The enzymatic antioxidant barrier is built with enzymes with antioxidant activity. The main enzyme of the antioxidant is dismutase (SOD) and catalase. The aim of the presented study is the

elaboration of optimal model of antioxidative enzymes immobilization on silver and gold nanoparticles. The determination of how enzymes immobilization affect their biological activity (by binding RFT) and influences the process of wound treatment is yet another objective of the study. The comparison between silver and gold nanoparticles and their influence on enzyme activity will also be studied. Silver nanoparticles were investigated because of their antibacterial and antivirus activity. Some of limitations to use enzymes in clinic is to make them more stable, less immunogenic and toxic and to present a longer in vivo circulation life time. Experiments with catalase immobilizated on Au nanoparticles show that catalase is biologically active. Activity of catalase is smaller after the immobilization on NPs surface compared to reference sample (catalase solution in deionized water with the corresponding protein concentration as in the case of investigated NPs colloid). In the case of 13 nm AuNPs-CAT and 20 nm AuNPs-CAT after 10 days higher activity of catalase was observed compared to reference sample. The highest protein activity exhibits samples with NPs size about 13 nm AuNPs-CAT) among all tested samples.

Index of lecturers

Notes

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