



The International Conference  
**Simulations of Functional Materials (SFM'22)**

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January 20-22, 2022, Poznań, Poland

**Editors:**

Jarosław S. Kłos, Grzegorz Musiał, Jolanta Latosińska, Magdalena Latosińska  
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# **The International Conference Simulations of Functional Materials (SFM'22) January 20-22, 2022, Poznań, Poland**

The International Conference "Simulations of Functional Materials" (SFM'22) in a hybrid form (on-site and on-line via MS Teams) will take place in a beautiful palace in Ciężen (Poland, approx. 82 km east of Poznań, convenient access via the A2 motorway) January 20-22, 2022.

The Conference will provide an international forum for the presentation and discussion of novel scientific ideas in the fields of broadly understood Simulations of Functional Materials, i.e. polymers, magnets (including molecular magnets), and others. The language of speeches and discussions at the Conference will be English.

The conference proceedings will be published in Computational Methods in Science and Technology (see Abstracts & Papers tab for details).

The meeting is organized by the Functional Materials Physics Division, the Faculty of Physics, Adam Mickiewicz University, Poznań.



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Szymon Krakowski  
Jakub Zaręba



# SCHEDULE

**THURSDAY, 01/20/2022**

**14:00 - 15:00**

LUNCH

**OPENING SESSION,  
CHAIRMEN J. S. KŁOS AND G. MUSIAŁ**

**15:15**

Opening lecture

MULTIFUNCTIONAL NANOMATERIALS FOR BIOMEDICAL APPLICATIONS

S. Jurga

*Nanobiomedical Centre, Adam Mickiewicz University,*

*Wszechnicy Piastowskiej 3, 61-614 Poznan, Poland*

**MAGNETIC NANOSTRUCTURES AND NANOPARTICLES,  
CHAIRMAN P. TOMCZAK**

**15:30**

POSSIBILITY OF MAGNETIC VORTICES IN A KEKULENE-LIKE MOLECULE

B. V. Costa

*Laboratório De Simulação, Departamento De Física, Icx,*

*Universidade Federal De Minas Gerais, 31720-901 Belo Horizonte, Minas Gerais, Brazil*

**16:00**

MAGNETIC NANOPARTICLES IN A THIN ELASTIC FILM AS A SENSOR OF MECHANICAL DEFORMATIONS - THE THEORETICAL CONCEPT

A. Drzewiński

*Institute of Physics, University of Zielona Gora, Prof. Szafrana 4A, 65-516 Zielona Góra, Poland*

**16:30 - 17:00**

COFEE BREAK

**APPLICATIONS OF MOLECULAR DYNAMICS IN MEDICINE,  
CHAIRMAN M. BARANOWSKI**

**17:00**

MOLECULAR DYNAMICS SIMULATIONS OF LIPID BILAYERS IN THE VICINITY OF CHOSEN  
SYNOVIAL FLUID COMPONENTS

N. Kruszewska

*Institute of Mathematics And Physics, Bydgoszcz University of Science and Technology,  
Kaliskiego 7, Pl-85796 Bydgoszcz, Poland*

**17:30**

THE STRUCTURAL AND ENERGETICAL CONSEQUENCES OF CHITOSAN DEACETYLATION  
DEGREE ON ITS AFFINITY TO COLLAGEN

P. Bełdowski

*Institute of Mathematics & Physics, Bydgoszcz University of Science & Technology,  
85-796 Bydgoszcz, Poland*

**18:30 - 19.00**

WELCOME DINNER

**19:00**

MUSIC CONCERT



**FRIDAY, 01/21/2022**

**8:00 - 9:00**

BREAKFAST

**STRUCTURE AND DYNAMICS OF COMPLEX POLYMER SYSTEMS I,  
CHAIRMAN M. BANASZAK**

**9:00**

DYNAMICS IN COMPLEX MACROMOLECULAR SYSTEMS

A. Sikorski

*Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland*

**9:30**

DYNAMIC LATTICE LIQUID MODEL USED IN THE MAPPING AND ANALYSIS OF SHAPE-  
MEMORY POLY(CARBONATE-UREA-URETHANE)S SYNTHESIS

K. Rolińska

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

*Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland*

**10:00**

FROM THE LCST TRANSITION TO AQUAMELTS: TYPE-II PHASE TRANSITIONS IN POLYMERS

J. U. Sommer

*Leibniz-Institute of Polymer Research Dresden and Tu Dresden, Hohe Strasse 6,  
D-01069 Dresden, Germany*

**10:30 - 11:00**

COFEE BREAK

**STRUCTURE AND DYNAMICS OF COMPLEX POLYMER SYSTEMS II,  
CHAIRMAN A. SIKORSKI**

**11:00**

DYNAMICS AND STRUCTURE OF OPPOSING POLYMER BRUSHES. A COMPUTER  
SIMULATION STUDY

K. Hałagan

*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology,  
Zeromskiego 116, 90-924 Lodz, Poland*

**11:30**

BINDING MECHANISMS IN DENDRIMER-SURFACTANT COMPLEXES

J. S. Kłós

*Department of Physics of Functional Materials, Faculty of Physics, Adam Mickiewicz University  
In Poznań, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*

**12:00**

SIMULATION MACHINES BUILT IN TAUR TECHNOLOGY: FEATURES AND EXAMPLES

J. Jung

*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology,  
Zeromskiego 116, 90-924 Lodz, Poland*

**12:30 - 14:30**

LUNCH

**MOLECULAR NANOMAGNETS AND JUNCTIONS,  
CHAIRMAN J. JUNG**

**14:30**

DESCRIPTION OF MOLECULAR NANOMAGNETS BY THE MULTIORBITAL HUBBARD MODEL  
WITH CORRELATED HOPPING

R. Lemański

*Institute of Low Temperature and Structure Research, Polish Academy of Sciences,  
Okólna 2, 50-422 Wrocław, Poland*

**15:00**

SIMULATIONS OF MOLECULAR NANOMAGNETS WITH VARIOUS METALLIC CORES AND TOPOLOGIES

M. Antkowiak

Department of Physics of Functional Materials, Faculty of Physics, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland

**15:30**

QUENCH DYNAMICS OF MAGNETIZATION IN QUANTUM IMPURITY SYSTEMS

K. Wrześniewski

Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland

**16:00 - 16:30**

COFEE BREAK

**SIMULATING AND PROBING MAGNETIC PROPERTIES AND SIMULATION OF HUMORAL IMMUNITY, CHAIRMAN M. ANTKOWIAK**

**16:30**

CONFIRMATION OF THE NEW BAXTER PHASE IN THE 3D ASHKIN-TELLER MODEL

G. Musiał

Faculty of Physics, Adam Mickiewicz University,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland

**17:00**

UNIVERSAL FMR PROCEDURE OF PROBING MAGNETIC PROPERTIES OF FERROMAGNETS

P. Tomczak

Faculty of Physics, Adam Mickiewicz University,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland

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**17:30**

ABOUT POSSIBLE UNEXPECTED CONSEQUENCES OF ONE UNINTENTIONAL SIMULATION

J. J. Langer

*Laboratory for Materials Physicochemistry and Nanotechnology, Faculty of Chemistry,  
Uniwersytetu Poznańskiego 8,*

*Department of Physics of Functional Materials, Faculty of Physics, Uniwersytetu Poznańskiego 2,  
Adam Mickiewicz University in Poznań, 61-614 Poznań, Poland*

**18:30**

DINNER

**SATURDAY, 01/22/2022**

8:00 - 9:00

BREAKFAST

**APPLICATIONS OF MD AND CST SIMULATIONS; FABRICS FOR DEFENSE,  
CHAIRMAN ANETA WOŹNIAK-BRASZAK**

**9:00**

FUNCTIONALIZATION OF FABRICS FOR DEFENSE, SECURITY, RESCUE AND HOUSEHOLD

J. J. Langer

*Laboratory for Materials Physicochemistry and Nanotechnology, Faculty of Chemistry,  
Uniwersytetu Poznańskiego 8,*

*Department of Physics of Functional Materials, Faculty of Physics, Uniwersytetu Poznańskiego 2,  
Adam Mickiewicz University in Poznań, 61-614 Poznań, Poland*

**9:30**

THERMAL CONDUCTIVITY OF ARGON NANOWIRE: A MOLECULAR DYNAMICS STUDY

K. V. Tretiakov

*Institute of Molecular Physics, Polish Academy of Sciences,  
M. Smoluchowskiego 17/19, 60-179 Poznań, Poland*

**10:00**

CST AS A SIMULATION TOOL FOR APPLIED PHYSICS

M. Baranowski

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

**10:30 - 11:00**

COFEE BREAK

**11:00**

POSTER SESSION

P-1

POLY(ETHYLENE OXIDE)-B-POLYSTYRENE BLOCK COPOLYMER STUDIED BY NMR, DSC, WAXS AND AFM

J. Zaręba

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-2

TUNABLE MICROWAVE MAGNETIC ELEMENTS RESONATOR SIMULATED IN CST

M. Baranowski

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-3

ELECTRON TRANSPORT IN NAPHTHALENE DIIMIDE DERIVATIVES

A. Selerowicz

*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology,  
Zeromskiego 116, 90-924 Łódź*

P-4

PRELIMINARY ESR AND VSM STUDIES ON MAGNETIC AND NON-MAGNETIC CORE SILICA GELS

R. Pietrzyk

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-5

STRUCTURE AND MOLECULAR DYNAMICS OF POLY(L-LACTIC ACID)/PINE WOOD  
BIO-BASED COMPOSITES

A. Woźniak-Braszak

*Functional Materials Physics Division, Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

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MANUFACTURING AND STRUCTURE OF POLY (VINYL CHLORIDE) COMPOSITES WITH  
A HYBRID CARBON FILLER CARBON FIBERS/CARBON NANOTUBES

K. Skórczewska

*Bydgoszcz University of Science and Technology, Faculty of Chemical Technology and  
Engineering, Seminaryjna 3, 85-326 Bydgoszcz, Poland*

P-7

EFFECT OF GRAPHENE ON PHYSICOCHEMICAL PROPERTIES OF POLY(VINYL CHLORIDE)  
NANOCOMPOSITE MATERIALS

R. Gwoździk-Bujakowski

*Functional Materials Physics Division, Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-8

STUDY OF THE STRUCTURE AND MOLECULAR DYNAMICS OF A PHARMACOLOGICALLY  
ACTIVE SUBSTANCE INCORPORATED INTO MESOPOROUS SILICA

M. Wachowiak

*Functional Materials Physics Division, Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-9

ENTROPY DRIVEN PHASE BEHAVIOR OF GRAFTED BLOCK COPOLYMERS SOLUTIONS

Sz. Krakowski

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-10

MONTE-CARLO SIMULATIONS IN THE DESIGN OF THE NEW INS SPECTROMETER AT FLNP  
JINR

M. Klepacka

Physics Faculty, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland

P-11

DOUBLE NETWORK OF TRUNCATED OCTAHEDRONS IN BLOCK COPOLYMERS SYSTEMS -  
MONTE CARLO STUDY

S. Wołoszczuk

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

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TOPOLOGICAL CHARGE SCALING A QUANTUM PHASE TRANSITION

P. Tomczak

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

P-13

FLUCTUATION THEOREMS IN NON-EQUILIBRIUM LATTICE MODELS

A. Napierała-Batygolska

*Faculty of Physics, Adam Mickiewicz University in Poznan,  
Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland*

**12:30**

SFM'22 Conference closing and lunch





## ABSTRACTS

THURSDAY, 01/20/2022

### Possibility of magnetic vortices in a Kekulene-like molecule

B.V. Costa, L.S. Menicucci

*Laboratório de Simulação, Departamento de Física, ICEx,  
Universidade Federal de Minas Gerais,  
31720-901 Belo Horizonte, Minas Gerais, Brazil*

F.C. Sá Barreto

*Departamento de Física e Matemática, Campus Alto Paraopeba,  
Universidade Federal de São João del Rei,  
36420-000, Ouro Branco, Minas Gerais, Brazil*

Nanostructures capable of supporting nonlinear structures are important in the nanodevices construction. It is important the structure to be simple and as smaller as possible. Having this in mind we have studied the behavior of a possible magnetic nanoparticle with the same geometry as the organic molecule Kekulene. Exchange and dipole interactions are considered between the constituting particles in the molecule. Using Monte Carlo simulations we have found that stable magnetic vortices develop and are stable in a wide range of temperature ( $T$ ) and dipole anisotropies ( $\delta = D/J$ ). The importance on synthesizing such molecule grounds in the possibility of building real planar structures. It is worthy to mention that such Kekulene-like molecule is a planar structure with atomic thickness, which is a great advantage compared with other possibilities being of size at least 10 times smaller than earlier proposed permalloy nanodots.

## **Magnetic Nanoparticles in a Thin Elastic Film as a Sensor of Mechanical Deformations - the Theoretical Concept**

K. K. Dudek, M. Marć, W. Wolak, A. Drzewiński, M.R. Dudek

*Institute of Physics,  
University of Zielona Gora,  
Prof. Szafrana 4a, 65-516 Zielona Góra, Poland*

The role of magnetic dipole-dipole interactions during the heating process of single-domain magnetic nanoparticles in an external radio frequency (RF) magnetic field, when magnetic nanoparticles are densely packed in a thin flexible film, is studied. When a thin film is subjected to mechanical deformations, nanoparticles change positions, which affects the interactions of magnetic dipoles. Consequently, during the film deformation, the heating power (namely the specific absorption rates) of the magnetic nanoparticles changes. In order to investigate this effect, a theoretical model was proposed and it was shown that the stretchable magnetic film can act as a mechanical deformation sensor when an RF magnetic field is present. Thus, the proposed concept can be used to design a sensor for medical applications.

## Molecular dynamics simulations of lipid bilayers in the vicinity of chosen synovial fluid components

N. Kruszewska, P. Bełdowski, A. Gadomski

*Institute of Mathematics and Physics,  
Bydgoszcz University of Science and Technology,  
Kaliskiego 7, PL-85796 Bydgoszcz, Poland*

Lipids bilayers are best known for being building materials of biological scaffolds such as cell membranes. They are main players in communication between inter- and outer-cell environments. They are found also in the joints. They cover the articular cartilage surfaces facilitating lubrication. In healthy system, there are few layers of the surface-active phospholipids between which a synovial fluid is present. The synovial fluid is full of different components with which the lipids can react. Diseases change the concentration of the components which causes degradation of lubrication properties. The molecular interactions inside the system have a complex multiscale and synergistic nature [1]. The aim of our studies is to use molecular dynamics simulation method to investigate the interactions between the lipid bilayers and components of the synovial fluid. The main question we try to answer is how the bilayer can help in lowering the friction coefficient between the two juxtaposed cartilage surfaces, and how different components of the synovial fluid can influence the bilayer properties. We will present three problems believed to impact on the mechanism of facilitated lubrication seen within joints: (i) protons (hydrogen ions) transfer through the lipid bilayer [2], (ii) interactions between hyaluronic acid and model phospholipid bilayer (DPPC) [3], (iii) interactions appearing when beta-2-glycoprotein-1 binds to a model phospholipid bilayer (DPPC and POPE) [4]. In addition, another trimer-based model of ion channelling through biomembranes as uncovered by Raik Mikelsaar in the late 1980s [5] will be specially mentioned due to its propensity to supporting the transmission of hydrogen ions through temporarily created lipid layers over the rubbing soft nanosurfaces at a friction-biolubrication event. We will show also viscoelastic properties of two different bilayer system which are crucial for effectiveness of lubrication. Discovery of causes of the destruction of cartilage in the progress of most rheumatic diseases and osteoarthritis are the main goal of our effort.

[1] A. Dedinaite and P. M. Claesson, "Synergies in lubrication", *Physical Chemistry Chemical Physics* 19, 35 (2017).

[2] A. Gadomski et al., *Tribol. Lett.* 30, 83 (2008).

[3] A. Dedinaite et al., *Adv. Colloid Interface Sci.* 274, 102050 (2019).

[4] N. Kruszewska et al., „Inspecting interactions between Beta-2-glycoprotein-1 and phospholipid bilayer”, *Membranes* 10, 396 (2020).

[5] R. Mikelsaar, "A Hypothesis on the Structure of the Biomembrane Lipid Bilayer." *Molecular Crystals and Liquid Crystals* 152 (1987).

## The structural and energetical consequences of chitosan deacetylation degree on its affinity to collagen

Piotr Beldowski<sup>1</sup>, Maciej Przybyłek<sup>2</sup>, Alina Sionkowska<sup>3</sup>, Piotr Cysewski<sup>2</sup>

<sup>1</sup>*Institute of Mathematics & Physics, Bydgoszcz University of Science & Technology, 85-796 Bydgoszcz, Poland*

<sup>2</sup>*Department of Physical Chemistry, Pharmacy Faculty, Collegium Medicum of Bydgoszcz, Nicolaus Copernicus University in Toruń, Kurpińskiego 5, 85-950 Bydgoszcz, Poland*

<sup>3</sup>*Department of Biomaterials and Cosmetics Chemistry, Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarin 7, 87-100 Toruń, Poland*

Chitosan-collagen blends are very promising biomaterials, which have been applied in cosmetics, tissue engineering and wound healing [1]. Chitosan, due to its similarity to hyaluronic acid, has been often applied as its substituent, for instance in joints' diseases treatment. The crucial mechanical properties of chitosan-collagen blends are closely related to the intermolecular interactions. The affinity of chitosan to collagen determines the durability of biopolymeric blends scaffolds and it is an important factor for the functioning of locomotor system components, synovial fluid and articular cartilage. When discussing the properties of collagen-chitosan blends, it should be taken into account, that there are two key factors characterizing these systems namely, chitosan deacetylation degree (DD) and collagen type. In this contribution, the molecular dynamics analysis of type III Collagen collagen-chitosan complexes was presented. It is commonly known that many important physicochemical properties of chitosan are linearly dependent on the DD [2]. As we found, also in the case of chitosan-collagen affinity there is an excellent linear correlation. Importantly, when DD > 40%, the chitosan-collagen complexes were found to be more energetically stable than hyaluronic acid-collagen assembly.

### References

[1] Sionkowska, A.; Prog. Polym. Sci. 2021, 122, 101452.

[2] Domalik-Pyzik, P. et al.; Chitosan-Based Hydrogels: Preparation, Properties, and Applications. In Cellulose-Based Superabsorbent Hydrogels. Polymers and Polymeric Composites: A Reference Series; Mondal, M., Ed.; Springer: Cham, Switzerland, 2019; pp. 1665–1693.

FRIDAY, 01/21/2022

## Dynamics in complex macromolecular systems

Andrzej Sikorski<sup>1</sup> and Piotr Polanowski<sup>2</sup>

<sup>1</sup>*Faculty of Chemistry, University of Warsaw,  
Pasteura 1, 02-093 Warsaw, Poland*

<sup>2</sup>*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology,  
Zeromskiego 116, 90-924 Lodz, Poland*

The motion of small probe molecules in model disordered systems was studied by means of Monte Carlo simulations. Theoretical studies of dynamics of such systems require special simulation algorithms. We present the applications of the Dynamic Lattice Liquid (DLL) model [1]. Studies of molecules movement in crowded environments by means of extensive Monte Carlo simulations were carried out. Two-dimensional coarse-grained model is supposed to mimic a lateral motion of probe molecules in macromolecular systems. The systems studied contained different types of small particles: fixed, mobile, interacting and having different shape [2-3]. For this purpose a cooperative mechanism of molecular transport based on the DLL model was employed [4]. Our goal was to answer the following question: how do small molecules move in a macromolecular environment that has a complex structure while the motion of small molecules is highly correlated. Short- and long-time dynamic behavior of small molecules were described. The influence of the molecules mobility, their density, the chain length and the polymer concentration on the mobility and the character of motion of small molecules were studied. Conditions of anomalous diffusions appearance and the recovery to Fickian behavior in such systems were discussed. The impact of the mechanism of transport on the dynamics of such systems was suggested.

### Acknowledgement

This work was supported by the Polish National Science Center grant UMO- 2017/25/B/ST5/01970.

### References

- [1] F. Hofling, T. Franosch, Rep. Prog. Phys. 2012 76, 046602.
- [2] P. Polanowski, A. Sikorski, J. Chem. Phys. 2017 147, 014902.
- [3] P. Polanowski, A. Sikorski, Soft Matter 2019, 15, 10045.
- [4] T. Pakula, Simulation on the completely occupied lattices, [in:] Simulation methods for polymers, ed. by M. Kotelyanskii, D. N. Theodorou, Marcel Dekker, New York-Basel 2004, 147-176.

## Dynamic Lattice Liquid model used in the mapping and analysis of shape-memory poly(carbonate-urea-urethane)s synthesis

Karolina Rolińska<sup>1,2</sup>, Andrzej Sikorski<sup>2</sup>, Piotr Polanowski<sup>3</sup>, Paweł Parzuchowski<sup>1</sup>

<sup>1</sup>*Faculty of Chemistry, Warsaw University of Technology,  
Noakowskiego 3, 00-664 Warsaw, Poland;*

<sup>2</sup>*Faculty of Chemistry, University of Warsaw,  
Pasteura 1, 02-093 Warsaw, Poland*

<sup>3</sup>*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology,  
Zeromskiego 116, 90-924 Lodz, Poland*

Polyurethanes gained tremendous popularity due to their excellent physical and mechanical properties such as toughness, durability, elasticity, and abrasive resistance. These materials are used for high-performance coatings, the production of elastic and rigid foams, seals, and adhesives. Conventional polyurethanes are obtained from diisocyanates or polyisocyanates, polyols, and chain extenders. In the presented work, we described the application of Monte Carlo simulations for better understanding the process of poly(carbonate-urethane-urea) elastomers preparation [1–4]. A coarse-grained Dynamic Lattice Liquid model (DLL) was implemented for this purpose. All objects (beads) were put into vertices of a face-centered cubic lattice, corresponding to small molecules or chain fragments. DLL experiments were focused on the simulation of multi-step synthesis. Therefore, we performed a two-step synthesis of oligocarbonate diols, followed by the process in which the prepolymer was obtained and its curing with water vapor. We developed a methodology that allowed us to reflect the essential features of the copolymerization process. The presented methodology allowed us to reflect on crucial components of the multi-step synthesis. The simulation results allowed us to predict the molecular weights of the products obtained during the poly(carbonate-urethane-urea) elastomers synthesis. Moreover, to get acquainted with the progress of the reaction regarding individual components.

Project POWR.03.02.00-00-I007/16-00 implemented under the Operational Program Knowledge Education Development 2014-2020 co-financed by the European Social Fund.

[1] Tomczyk, K.M. et al.: Synthesis of oligocarbonate diols from a “green monomer” — dimethyl carbonate — as soft segments for poly(urethane-urea) elastomers. *Polimery* (5), 2010, p. 366–372.

[2] Kozakiewicz, J. et al.: Studies on the effect of curing conditions on the curing rate and mechanical properties of moisture-cured poly(urethane-urea) elastomers containing oligocarbonate segments. *Polimery* (7), 2011, p. 564–570.

[3] Mazurek-Budzyńska, M. et al.: Poly(carbonate-urea-urethane) networks exhibiting high-strain shape-memory effect. *Polym. Adv. Technol.* (28), 2016, p. 1285-1293.

[4] Mazurek-Budzyńska, M. et al.: Influence of the soft segment length on the properties of water-cured poly(carbonate-urethane-urea)s. *Polym. Adv. Technol.* (26), 2015, p. 57-67.

## From the LCST Transition to Aquamelts: Type-II Phase Transitions in Polymers

Jens-Uwe Sommer

*Leibniz-Institute of Polymer Research Dresden and TU Dresden,  
Hohe Strasse 6, D-01069 Dresden, Germany*

The lower critical solution temperature (LCST) transition is introduced as type-II transition which results in many cases from competing effects of hydrogen bonding and hydrophobic behaviour of water-soluble polymers such as PEO and PNIPAm. As a consequence of the new type of phase separation a switch-like temperature response and phase coexistence is predicted for immobilized polymers such as polymer brushes or gels. I will give an introduction to simple theoretical concepts related with the type-II transition. Furthermore, I will demonstrate that mixed solvents can lead to type-II transitions with the prominent example of so-called co- nonsolvency [1]. Computer simulations and experiments confirm the basic conclusions from the theoretical model for polymer brushes [2,3]. Moreover, this phase transition is most likely driving the formation of protein-RNA-droplets in living cells. Using atomistic simulations it is shown for the example of PEO that stretching of the conformations can induce a phase transition far below the LCST which can be explained by the release of hydrogen bonds in the stretched state of PEO [4]. An aquamelt is introduced in general as a system where stretching/flow induces phase separation and subsequent crystallization, very similar to the process of spider-silk spinning in Nature. Aquamelts break the paradigm that solution properties of polymers are independent of conformation statistics.

[1] J.-U. Sommer, Gluonic and Regulatory Solvents: A Paradigm for Tunable Phase Segregation in Polymers, *Macromolecules* 51, 3066 (2018); Adsorption-Attraction Model for Co- Nonsolvency in Polymer Brushes, *Macromolecules* 50, 2219 (2017)

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## Dynamics and Structure of Opposing Polymer Brushes. A Computer Simulation Study

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A system of two opposing polymer brush systems was virtually synthesized and investigated by molecular modeling. Chains were grafted on two parallel impenetrable walls with the same number of chains on each surface. The polymerization process provided realistic mass dispersity. A very low probability of polymerization allowed to form fully equilibrated brushes. More than 8000 polymer chains were present in the simulation with explicit solvent. The dynamic properties of such systems were studied by Monte Carlo simulations based on the dynamic lattice liquid model with the usage of a highly efficient dedicated machine ARUZ, which enabled the study of large systems and long timescales. Coarse-grained solvent and polymer beads were restricted to face-centered cubic lattice nodes with the excluded volume interactions only. The influence of the surface density and mean polymer length on the dynamic and structure of the system is discussed. The parameters of the polymerization process were found to be crucial for the proper structure of the brush. The self-diffusion coefficient of the solvent strongly depended on the degree of polymerization and the polymer concentration. It was predicted and confirmed that, in a polydisperse sample, the longer chains have unique configurations consisting of a stretched stem and a coiled crown. It was also shown that it is possible to capture changes in solvent mobility that can be attributed to regions of different polymer densities.

Funding: NCN grant UMO-2017/25/B/ST5/01970.



## Binding mechanisms in dendrimer-surfactant complexes

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Molecular dynamics simulations were employed to investigate the impact of interactions between dendritic polyelectrolytes and amphiphilic surfactants on the supramolecular complex formation. We recognize two crucial parameters that govern association of surfactants within dendrimers: surfactant hydrophobicity,  $\epsilon^*$ , and dendrimer generation,  $G$ . We find that depending on the values of  $\epsilon^*$  and  $G$  encapsulation of surfactants by dendrimers is either noncooperative or cooperative. The former binding mechanism is characterized by absorption of surfactants as unimers, whereas in the latter mechanism absorption of unimers is followed by aggregate formation through hydrophobic attractions between surfactant tails. Our results provide guidelines for controlled encapsulation of guest molecules in dendrimer-based guest-host complexes.

## Simulation machines built in TAUR technology: features and examples

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Technology of Real World Analyzers (Technologia Analizatorów Układów Rzeczywistych – TAUR) is a way to produce a scalable, fully parallel data processing system equipped with low-latency communication channels, designed for simulations based on emulation of interactions among huge numbers of molecules. When using TAUR, one can create a electronic structure of cells placed in nodes of the 3D network. All cells contain electronic circuits that perform logical functions. Cells are able to communicate with each other. In these cells it is possible to implement elements of the simulated system, e.g. chemical molecules. The dedicated topology of the electrical circuits of each cell corresponds to the unique property of these molecules. Additionally, all cells in the machine have configured electrical circuits that are responsible for the interaction of molecules inside them with other molecules in neighboring cells. The way in which molecules interact with each other depends on the type of element contained in a given cell, the type of element placed in neighboring cells, and the mechanisms of interactions implemented in the cells. As a result of the interactions, cells can change the state of their molecule and also send and/or receive molecules to/from neighboring cells. After the implementation of molecules in cells and an appropriate model of interactions between them, several million molecules, interconnected in various ways, gradually move over time. As a result, a properly configured machine can be treated as a three-dimensional electronic model of a fragment of real matter with which it is possible to observe and analyze phenomena in any selected simulation step. This can be done by downloading to the memory of external computers information about the spatial structure of the network of connections between molecules and their interactions. The sample results of the simulation of the polymerization process during the formation of a pair of polymer brushes, carried out with the use of the ARUZ (in Polish Analyzer of Real Complex Systems) will also be presented. This machine was built on the basis of TUR assumptions and the mechanism of molecule movements has been implemented in accordance with the principles of the dynamic lattice liquid model.

## Description of molecular nanomagnets by the multiorbital Hubbard model with correlated hopping

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We present a microscopic description of molecular magnets by the multiorbital Hubbard model, which includes the correlated hopping term, i.e., the dependence of the electron hopping amplitude between orbitals on the degree of their occupancy [1]. In the limit of large Coulomb on-site interaction, we derive the spin Hamiltonian using the perturbation theory. We determine the magnetic coupling constant between two ions in two different ways: (a) from the expression obtained in the perturbation calculus and (b) from the analysis of distances between the lowest levels of the energy spectrum obtained by diagonalization of the multiorbital Hubbard model. The procedure we use can be applied to various nanomagnets, but we perform the final calculations for the molecular ring Cr<sub>8</sub>. We show that the correlated hopping can reduce the antiferromagnetic exchange between ions, which is essential for a proper description of Cr<sub>8</sub>.

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## Simulations of molecular nanomagnets with various metallic cores and topologies

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We present the results of simulations of a class of molecular nanomagnets with ring, centered ring and dimer topologies. We demonstrate [1,2] that anisotropic Heisenberg model describes quantitatively magnetic properties of a family of the doped Cr<sub>8</sub> molecular rings revealed by the variety of experimental techniques. Interestingly, the nearest neighbor coupling parameters between the localized spins are all transferable across its members. We show that the broken symmetry approach within density functional theory, based on suitable functionals, provides a reliable tool [2,3] to extract magnetic exchange coupling parameters in all rings considered. The molecular complex containing the bimetallic core Ni<sub>6</sub>Cr [3], representing the centered ring geometry as well as its analogue geometrically frustrated are also simulated using the phenomenological and DFT approach. Consequently, the magnetic properties observed are quantitatively explained. In the isotropic limit of the model and the spin frustration switched on, the sequence of the ground states determined by the total spin  $S$  is obtained in agreement with the fundamental Lieb-Mattis theorem. Curiously enough, the temperature dependence of the susceptibility product  $\chi T$  with characteristic minimum and maximum is revealed not only as a signature of competition between the ferro- and antiferro-magnetic interaction but also as a symptom of the spin frustration phenomenon. We have pioneered the application of the Heisenberg-type model to rare-earth dimers [4]. To that end, a new family of 3d–4f coordination polymers has been synthesized in search for new single- molecule magnet materials containing highly anisotropic lanthanides. Their magnetic properties have been explained quantitatively by comprehensive phenomenological modeling.

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## Quench dynamics of magnetization in quantum impurity systems

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We study quench dynamics of magnetization for quantum impurity systems. Considered model precisely describes molecular junctions comprised of molecules or magnetic impurities tunnel coupled to external leads. The real-time evolution is calculated by means of the time-dependent density-matrix numerical renormalization group method implemented within the matrix product states framework. We examine the system's response to a quench in the coupling strength to leads. The magnetization dynamics is analyzed for a single quantum dot system coupled to ferromagnet and/or topological superconducting nanowire. Two time scales are identified, describing the development of the exchange field and the dot's magnetization sign change. We also discuss competition between ferromagnet- and Majorana-induced exchange fields. Finally, we examine time-dependent spintronic anisotropy in magnetic molecule.

## Confirmation of the new Baxter phase in the 3D Ashkin-Teller model

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Although the lattice Ashkin-Teller (AT) model is one of the most important in statistical physics and is being studied for decades [1,2], it still attracts a great interest, raises many applications and intriguing questions that have not found satisfactory answers, as it is a non-trivial generalization of the widely used Ising model. The effective Hamiltonian  $H$  of the AT model is of the form  $-H/(k_B T) = \sum_{\langle ij \rangle} [K_2(s_i s_j + s_i \bar{s}_j) + K_4 s_i s_j \bar{s}_i \bar{s}_j]$ , where Ising spins  $s_i$  and  $\bar{s}_j$  reside on the same cubic lattice site, the summation occurs over the pairs of nearest neighbors interacting with equal energy  $J_2$  for pairs and  $J_4$  for fours, thus  $K_i = -J_i/k_B T$  with  $i = 2$  or  $4$ ,  $k_B$  is the Boltzmann constant, and  $T$  is the temperature of the system. As a result, three order parameters  $\langle s \rangle$ ,  $\langle \sigma \rangle$  and  $\langle s\sigma \rangle$  appear, each of which can order independently. Here, the symbol  $\langle \dots \rangle$  denotes the thermal average. The 3D AT model demonstrates an interesting and complex phase diagram [2] which contains weakly to strong first-order phase transitions, continuous ones, many tricritical and bifurcation points, as well as the wide crossover region. Here we concentrate on the interesting mixed phase region, where  $\langle s\sigma \rangle = 0$  and either  $\langle s \rangle \neq 0$  and  $\langle \sigma \rangle = 0$  or  $\langle s \rangle = 0$  and  $\langle \sigma \rangle \neq 0$  with ferromagnetic order, which is the most complex and least recognized one [1,2]. In particular, the subject of our research is the border region with the Baxter phase, in which all three components are ordered ferromagnetically and  $\langle s \rangle = \langle \sigma \rangle$ . Ditzian et al. [3] observed a narrow region here where  $\langle s \rangle$ ,  $\langle \sigma \rangle$ , and  $\langle s\sigma \rangle$  are nonzero, but  $\langle s \rangle \neq \langle \sigma \rangle$ , despite the symmetry of both order parameters resulting from the Hamiltonian. Recently, Santos et al. [1] presented the MFT results from the Bogoliubov inequality for the 3D AT model on a cubic lattice and they identified this region as the new Baxter(2) phase for the first time. In this paper, we use our extensive Monte Carlo computer experiments [2] to explore this intriguing Baxter(2) phase region in a 3D AT model. Due to the existence of metastable and unstable phases in this region, we based our computer experiments not only on the Metropolis algorithm, but also on our recently discovered cluster one [2]. At the transition of the system from the mixed phase region to the Baxter one, a step energy change is observed for all three order parameters, however, two of them order by reducing their internal energy at the expense of the step change in the internal energy of the already ordered parameter. The sum of the latent heat of the entire system is different from zero, and we demonstrate that it is equal to the sum of the latent heat of individual order parameters computed separately. Moreover, although region indicated as Baxter(2) phase is becoming narrower as the system size increases, it does not disappear in the thermodynamic limit.

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## Universal FMR procedure of probing magnetic properties of ferromagnets

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The phenomenon of ferromagnetic resonance (FMR) is still being widely used for determining the magnetocrystalline anisotropy constants of magnetic materials. We show that one can interpret the resonance condition (the Smit-Beljers equation) as the relationship between resonance frequency and curvature of the spatial distribution of free energy at resonance. Subsequently, taking this relationship into account and using cross-validation of numerical solutions of the Smit-Beljers equation [1,2] we show how to determine accurately all the relevant constants (saturation magnetization, g-factor, magnetocrystalline anisotropy constants) entering this equation and related to the tested sample in FMR experiments. Specifically, three examples are given of calculating such constants from FMR data: we use historical Bickford's measurements from 1950 for bulk magnetite [3], Liu's measurements from 2007 for a 500 nm thin film of a weak ferromagnet (Ga, Mn)As [4], and Wang's measurements from 2014 for an ultrathin film of YIG [5]. In all three cases, the constants we have determined are consistent with the results of other measurements. In the fourth numerical example, we show, using Heinrich et al. FMR measurements from 1991 for ultrathin Co film [6], that the presented method can also be a test for the correctness of the assumed form of the ferromagnet free energy at resonance. Eventually, in the fifth numerical example, basing on Roemer et al. broadband measurements from 2012 for Fe thin films [7], the unambiguity of the determined parameters in the present approach is briefly discussed.

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## About possible unexpected consequences of one unintentional simulation

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The production of neutralizing antibodies and immune memory are outcomes of successful vaccines. Highly effective vaccines were designed against pathogens that had little variability and did not dysregulate the immune system in the way that chronic infections can do. "Chronic viral infections disrupt the ability of the humoral immune response to produce neutralizing antibody or form effective immune memory..." (L. Cooper and K.L. Good- Jacobson: Dysregulation of humoral immunity in chronic infection. *Immunol Cell Biol*, 98 (2020): 456-466; <https://doi.org/10.1111/imcb.12338>). One can expect that the same problem could also occur if the mechanism of action or mode of administration of the vaccine (or both) mimics a chronic infection. In the case of long lasting stimulation of the immune system ("chronic infection"), the results can be completely unexpected owing to "dysregulation of humoral immunity", as is likely the case in many countries now: an increase in infections in highly vaccinated populations. Both, the method of administration (multiple doses) and the mechanism of action of the vaccines result in prolonged stimulation of the immune system, thus mimic a case of chronic infection. This leads to a weakened immune system response resulting in: (1) an increase in the rate of infection in vaccinated population and (2) reduction in the number of severe cases (these are usually caused by an intense response of the immune system, now weakened). This explanation of what we see is well documented in the studies of real chronic infections ([doi:10.1111/imcb.12338](https://doi.org/10.1111/imcb.12338)), and simulation is a widely used, valuable tool, with the results well fitted to reality. Now applied inadvertently.



SATURDAY, 01/22/2022

## Functionalization of fabrics for defense, security, rescue and household

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Fabrics are widely used in defense, security, rescue and household, although their typical properties are often not optimal for such applications. Our improvement program focuses on: 1. Fireproof modification of fabrics to reduce flammability. Fire protection. 2. Fabric modification to reduce near infrared (NIR) reflection for NIR camouflage. 3. Modification of fabrics in order to reduce heat emission, limiting the possibility of thermal imaging detection. 4. Modification of fabrics to reduce wettability in contact with water (hydrophobing). Here we present basic information and examples of successful modification.

## Thermal conductivity of argon nanowire: a molecular dynamics study

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Control of thermal transport at the nanolevel is a significant challenge in the design of various devices at the nanoscale. One of the important issues concerning the research of nanoscale systems is the influence of strong geometrical confinement on thermal conductivity [1]. Studies of simple systems, such as liquid argon in nanochannels or argon nanowires, lead to a deeper understanding of the influence of strong geometrical confinements on the thermal conductivity of confined systems [2,3,4]. The thermal conductivity of liquid argon in nanochannels [3] and of argon nanowires [4] have been calculated using two independent methods of molecular dynamics simulations. The influence of transversal size and shape of a nanochannel and a nanowire on the thermal conductivity of the system has been investigated. The study shows that thermal conductivity increases with an increase of the transversal size of the sample and scales well with the cross-sectional area of the system [3,4]. The phonon confinement effect influences the thermal conductivity of nanowires, but the dominant factor decreasing the thermal conductivity with the thickness of nanowires is boundary scattering [4].

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## CST as a simulation tool for applied physics

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Physicists use many methods to simulate phenomena in the surrounding world. One of the powerful tools is CST Studio, although it is not widely used in the scientific community. The lecture will present the results obtained with the use of various solvers, used in many aspects of physics. The possibility of studying the distribution of electromagnetic waves inside resonating systems and cavities that are made of various materials, distributions of static magnetic and electric fields, and beam trajectories in a magnetic field will be presented.



## POSTERS

P-1

### **Poly(ethylene oxide)-b-polystyrene block copolymer studied by NMR, DSC, WAXS and AFM**

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The development of lithium-ion batteries in recent years has contributed enormously to the broad field of portable consumer electronics [1]. Their higher efficiency, lower mass and output current density were much higher than older technologies (eg nickel-cadmium cells) [2,3]. The research objective of this project is to use various Nuclear Magnetic Resonance (NMR) methods to characterize the phase behavior and self-assembly in selected block copolymers in the context of further studies of lithium doped systems. Ultimately, this may contribute to the development of innovative, efficient and environmentally friendly (without organic solvents) recycled batteries. In order to investigate the domain structure of self-assembled block copolymers, two complementary techniques were employed, i.e. NMR spin-diffusion and Atomic Force Microscopy (AFM) to determine the size of the domains and the size of the interfacial space. Moreover, Differential Scanning Calorimetry (DSC) and WAXS methods were used to study phase transitions and the degree of crystallinity of the semicrystalline PEO. Conducted research is the basis for further structural analysis of systems based on the admixture of lithium ions.

#### Acknowledgements

The research was supported by project POWER - „Środowiskowe interdyscyplinarne studia doktoranckie w zakresie nanotechnologii” POWR.03.02.00-00-I032/16

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**P-2****Tunable microwave magnetic elements resonator simulated in CST**

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Here we present a tunable resonator consisting of six elliptical elements (petals) made from a magnetic material [1], shield and matching loop. The petals are positioned with their centers at the corners of a regular hexagon. Using numerical simulations (CST Studio) we examine the effect on resonance critical coupling of different: radial petals orientation,  $\mu$  and matching loop position. We study resonance modes with a specific distribution of the electromagnetic field within the resonator as well as the effect of the rotation of petals on the field distribution. The magnetic field distribution inside the resonator volume is crucial to understand the behavior of the EM wave interaction with the potential sample placed inside the maximum of the magnetic field. The system studied is a promising candidate to be an integrated detection sensor, antennas, magnetic spectroscopy and related detection techniques.

This study was partially supported by the Polish agency NAWA under the grant No PPN/BUA/2019/1/00114.

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## P-3

### Electron Transport in Naphthalene Diimide Derivatives

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Two naphthalene diimides derivatives containing two different (alkyl and alkoxyphenyl) N-substituents were studied, namely, N,N'-bis(sec-butyl)-1,4,5,8-naphthalenetetracarboxylic acid diimide (NDI-s-Bu) and N,N'-bis(4-n-hexyloxyphenyl)-1,4,5,8-naphthalenetetracarboxylic acid diimide (NDI-4-n-OHePh). These compounds are known to exhibit electron transport due to their electron-deficient character evidenced by high electron affinity (EA) values, determined by electrochemical methods and a low-lying lowest unoccupied molecular orbital (LUMO) level, predicted by density functional theory (DFT) calculations. These parameters make the studied organic semiconductors stable in operating conditions and resistant to electron trapping, facilitating, in this manner, electron transport in thin solid layers. Current–voltage characteristics, obtained for the manufactured electron-only devices operating in the low voltage range, yielded mobilities of  $4.3 \times 10^{-4} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  and  $4.6 \times 10^{-6} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  for (NDI-s-Bu) and (NDI-4-n-OHePh), respectively. Their electron transport characteristics were described using the drift–diffusion model. The studied organic semiconductors can be considered as excellent candidates for the electron transporting layers in organic photovoltaic cells and light-emitting diodes.

**P-4****Preliminary ESR and VSM studies on magnetic and non-magnetic core silica gels**

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We presented preliminary results of ESR and VSM studies on nanoparticles with the magnetic and non-magnetic core in silica shells modified with functional groups. The materials are potentially intended as drug carriers because of their unique magnetic and biological properties. The measurements were performed by Adani SPINSCAN X benchtop ESR spectrometer intended for spectra registration with continuous wave using the second modulation. Studies of magnetic-core particles with different functional groups using ESR methods are challenging due to the different responses under the influence of the silicone shell and its modification of the sample. Research procedures applied to analyze magnetic-core particles take into account the impact of various functional groups on analyzed samples to achieve comparable results. We also presented results studies by vibrating the sample magnetometer at 100Hz at room temperature for each sample.



P-5

## Structure and molecular dynamics of poly(L-lactic acid)/pine wood bio-based composites

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Bio-based composites made of poly(L-lactic acid) (PLLA) and pine wood were produced by twin-screw extrusion in different compositions, from 10 to 30 wt % of filler content, and characterized for their morphology, physicochemical and mechanical properties. The composites were compatibilized by impregnation of wood with  $\gamma$ -aminopropyltriethoxysilane (APE). The complementary study of structure and molecular dynamics of composites by such experimental techniques as differential scanning calorimetry (DSC), thermogravimetry (TGA), scanning electron microscopy (SEM), wide-angle X-ray diffraction (WAXD) and solid-state <sup>1</sup>H NMR revealed that APE can improve adhesion between the phases, with positive effects on material properties. The composites have a slightly lower thermal stability compared to PLLA, proportional to filler content, due to the lower thermal stability of wood. Molecular dynamics investigated by the solid-state <sup>1</sup>H NMR technique revealed restrictions in the mobility of polymer chains upon the addition of wood, as well as enhanced interfacial adhesion between the filler and matrix in the composites compatibilized with APE. The enhanced interfacial adhesion in silane-treated composites was also proved by scanning electron microscopy and resulted in slightly improved deformability and impact resistance of the composites. Thermogravimetric analysis revealed that wood addition causes a decrease in thermal stability of the material, which occurred to a lower extent in the compatibilized formulations.

**P-6****Manufacturing and structure of poly (vinyl chloride) composites with a hybrid carbon filler carbon fibers/carbon nanotubes**

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The presented research concern the possibility of producing a hybrid carbon filler from carbon fibers (CF) and carbon nanotubes (CNT) and its usage as a modifier of materials based on poly(vinyl chloride) (PVC). The use of CF is a known method of modifying the mechanical properties of plastics. For this purpose, cut and continuous fibers, mats and fabrics are used. However, there are few reports display the properties of composites based on PVC with their participation due to technological problems occurring during the processing of the material (change in viscosity, deterioration of thermal stability). Currently, there is a lot of work on the use of CNT in the modification of polymers, including PVC, in order to obtain nanocomposites with new interesting properties. Works are also carried out to combine the properties of CF and CNT and to attain polymer composites with a carbon hybrid filler micro/nanometric. However, such PVC-based composites have not been reported in the literature so far. Therefore, the research objective of the conducted works was to obtain a hybrid filler suitable for use in PVC composites. During the research work, a carbon hybrid micro with nanometric filler was made. Then, filler was introduced into PVC blends by the extrusion process. The received materials were used to prepare samples for mechanical properties tests (in accordance with EN ISO 527). The cryogenic breakthroughs were used for structural tests using the SEM method. The Congo red method was carried out to determine the time of thermal stability of composites. SEM images of PVC composites indicate a satisfactory homogeneous distribution of the hybrid filler in the matrix, which is confirmed by the obtained values of the mechanical properties of composites containing up to 5% by weight of the filler. With the increase in the hybrid filler content in the matrix, the stiffness of the composites increases, as evidenced by the increase in the value of the tensile modulus of elasticity. The PVC composites are characterized by a slightly longer time of thermal stability compared to unmodified PVC. Based on the research results, it was found that it is possible to obtain PVC composites with a carbon hybrid filler. Further work is required to assess the properties of the new materials developed.

This research was carried out thanks to the support of the National Science Centre in Poland under the program MINIATURA 4 project no. 2020/04/X/ST5/01684.

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## Effect of graphene on physicochemical properties of poly(vinyl chloride) nanocomposite materials

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Poly(vinyl chloride) (PVC) is one of the commonly used thermoplastics due to its good chemical resistance and resistance to atmospheric agents, good mechanical and utility properties, including fire resistance and low production cost. One of the disadvantages of PVC consists in its low thermal resistance. Modification of PVC using nanofillers, including also carbon nanoparticles such as carbon nanotubes (CNT), graphene oxide (GO) and graphene (GN) leads to an improvement in thermal resistance in many cases, but its main goal remains to create new engineering materials having favorable properties, particularly electrostatic and barrier properties, as well as improved chemical resistance. Another effect of the modification of poly(vinyl chloride) with graphene fillers consists in a change of glass transition temperature ( $T_g$ ). The  $T_g$  values depend significantly on the properties of the materials used in production of nanocomposites, concentration of fillers, and interfacial interactions between the fillers and the polymeric matrix. The glass transition is a critical factor limiting the temperature-dependent applications of PVC, accompanied by gradual changes of various polymer properties, such as electrical and heat conductivity, dielectric constant, specific volume, thermal capacity and others. The techniques used for determination of the  $T_g$  are: differential scanning calorimetry (DSC), thermomechanical analysis (TMA), dielectric analysis (DEA) and dynamic mechanical analysis (DMA), where depending on the method used different values of the  $T_g$  for the same material are frequently observed. Another technique used to investigate the glass transition in polymers is nuclear magnetic resonance (NMR), which provides information about the properties of materials on the molecular level. It enables monitoring of complex dynamic behavior of glassy polymers over a wide range of time scales by measuring relaxation times, dramatically changing during the glass transition. The goal of the work was to investigate the influence of multilayer graphene on physicochemical properties of poly(vinyl chloride). PVC/GN nanocomposites were obtained by the solvent evaporation method, and their structure was evaluated using optical microscopy. The NMR technique was used to study molecular dynamics of the obtained materials. The swelling behavior in acetone was also determined.

**P-8****Study of the structure and molecular dynamics of a pharmacologically active substance incorporated into mesoporous silica**

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Untreated properly, acute pain can become chronic and lead to a significant reduction in quality of life. Pain-relieving drugs are among the most purchased drugs in the world. Non-steroidal anti-inflammatory drugs known as NSAIDs, are not only painkillers but also antipyretics, which in higher doses are anti-inflammatory. Lornoxicam (LOX) is an analgesic and anti-inflammatory drug, characterized by high hydrophobicity and relatively low bioavailability in the crystalline form. In this work, the drug was incorporated in Santa Barbara Amorphous no. 15 (SBA-15) onto a silica matrix by two methods - evaporation and adsorption. The aim of the research was to compare the two methods of modified drug and to determine the structure and molecular dynamics of the introduced drug. The research was carried out by means of <sup>1</sup>H nuclear magnetic resonance (<sup>1</sup>H-NMR), wide x-ray diffraction (WXR), Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC). The results of the research indicate that the introduction of the drug into mesoporous silica reduces the proportion of the drug's crystalline phase. We have proved that the absorption equilibrium method is a more advantageous method of loading. It ensures drug absorption in an amorphous state inside the mesopores. However, the solvent evaporation method, despite a greater amount of loaded drug, results in drug adsorption in a crystalline state on the silica surface. The amorphous structure of the drug increases bioavailability as a result of which the dose of the drug introduced into the body may be reduced, which at the same time reduces the occurrence of side effects. In addition our show that silica carriers can be used as potential drug delivery carriers for poorly water-soluble drugs. Due to its crystal structure, LOX is poorly soluble in water, therefore there is a need to develop new drug carriers that improve solubility and increase bioavailability. Therefore, only knowledge of the molecular dynamics of drugs incorporated into a silica matrix and knowledge of the intermolecular interactions is important for a better understanding of drug matrix systems and the future development of drug delivery systems.

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## Entropy driven phase behavior of grafted block copolymers solutions

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The processes of entropic ordering are taking place, for example, in the formation of crystals or in the separating phases of colloids, may be counterintuitive for the observer [1]. We present the use of the cooperative motion algorithm (CMA) based on Monte Carlo method to study the phenomenon of entropy ordering in various solutions of grafted block copolymers on face-centered cubic lattice. The aim of the research was to investigate the entropic ordering phenomenon in high dense solutions of branched and linear copolymers in various fractional volumes. We treat branched copolymer as a solvent in relation to the linear copolymer, because the arm length of a single star (assumption: all of then arms have the same length),  $NS$ , is much shorter than the chain length of the linear copolymer,  $NL = 12$ . Linear chain systems of length range,  $N = 12-96$ , and grafted stars with volume fraction of a linear chains range,  $\phi = 0.2-0.8$ , were used on lattices of various sizes ( $48 \times 48 \times 48$  and  $96 \times 96 \times 96$ ). The dependance of the influence of the linear chain length  $N$  on the entropy aggregation processes in the system was investigated.

References:

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## P-10

### Monte-Carlo simulations in the design of the new INS spectrometer at FLNP JINR

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Monte-Carlo methods allowed solving problems deterministic in principle, but too complex for analytical approach. Due to their efficiency in optimization and generation of drafts from probability distribution, they have found application in the simulation of neutron scattering. McStas is one of the most popular software packages for modeling neutron scattering instruments and was implemented during the design phase of many modern neutron scattering spectrometers. By using Monte-Carlo algorithms and ray tracing McStas allows to perform a neutron scattering experiment simulation accounting for all variables and contributions, such as broadening, asymmetry, background, distance errors, neutron beam divergence and many other. Due to its effectiveness, McStas was selected as one of the key design tools in the project of a new neutron scattering spectrometer in the Frank Laboratory of Neutron Physics at Joint Institute for Nuclear Research (Dubna, Russia). Presented work describes the use of Monte-Carlo simulation in the evaluation of the new spectrometer's performance, focusing on the prediction of the neutron impulse broadening, neutron beam divergence, beryllium filter efficiency and secondary spectrometer's time and energy resolution. Results obtained from performed simulations allowed to make significant design decisions, such as choices of <sup>3</sup>He detector diameter, HOPG analyzer size and beryllium filter thickness.

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## Double Network of Truncated Octahedrons in Block Copolymers Systems - Monte Carlo Study

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## P-12

**Topological charge scaling a quantum phase transition**

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At quantum phase transition (QPT) ground state properties of the quantum system change drastically due to quantum fluctuations which are most clearly pronounced at zero temperature. Although many approaches have been proposed to examine QPTs, to locate critical points and to calculate values of critical exponents, one still asks an important question: Which observables one should use to explore the critical behavior of a system at QPT? This question is particularly important when there is no possibility to identify a order parameter in a system under consideration nor to establish a pattern related to a symmetry breaking. Therefore there still exists a quest for new approaches, based on scaling and renormalization which enable searching and characterizing QPTs. We propose such a new approach based on Finite Size Scaling (FSS) of a topological charge. We start by defining the topological charge:  $\eta_T = \langle \Psi_0 | W | \Psi_0 \rangle / L$ , with  $W$  being winding number,  $L$  - the system size, and  $|\Psi_0\rangle$  - its ground state. Subsequently, the well-known quantum phase transition in the ground state of an antiferromagnetic spin-1/2 Heisenberg chain with nearest and next-nearest-neighbor interactions is re-investigated from this perspective. FSSS of  $\eta_T$ ,  $\langle \Psi_0 | W | \partial_\lambda \Psi_0 \rangle$  and  $\langle \partial_\lambda \Psi_0 | W | \partial_\lambda \Psi_0 \rangle$  leads to the accurate value of critical coupling  $\lambda_c = 0.2412 \pm 0.0007$  and to the value of subleading critical exponent  $\nu = 2.000 \pm 0.001$ .



**P-13****Fluctuation theorems in non-equilibrium lattice models**

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In this poster we present simulational applications of fluctuation theorems for the calculation of a surface tension in the Ising-doped voter model. Fluctuation theorems of Jarzynski and Crooks give a very useful method for estimating the free-energy differences in various systems. We have examined pure Ising, pure voter and mixed models on a two dimensional lattice with antiperiodic boundary conditions that induce the interface. The Ising model is characterized by curvature-driven dynamics with a power-law coarsening and a finite- temperature phase transition. On the other hand, the voter model is driven by a different spin dynamics, in which the global temperature has no influence on local spin alignment and is inherently nonequilibrium. We obtained non-zero surface tension estimations for pure Ising and mixed models and we numerically demonstrate that the dynamics of voter model does not generate the surface tension. Our work constitute also a numerical attempt to expand the range of applications of fluctuation theorems on nonequilibrium models which do not comply with the principle of detailed balance.



Published on the website of the SFM'22 Conference on June 30, 2022 by  
Functional Materials Physics Division, Faculty of Physics,  
Adam Mickiewicz University, Poznań  
Uniwersytetu Poznańskiego 2,  
61-614 Poznań, Poland