# THE 17th CONFERENCE ON FUNCTIONAL AND NANOSTRUCTURED MATERIALS

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4–11 September, 2021
Paralia Katerinis, Greece

# ABSTRACT BOOK

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*The $17^{th}$ Conference on Functional and Nanostructured Materials – FNMA'21*

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# CONTENTS

# Smoothed particle hydrodynamics simulations applied to nanofluids

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This study is an attempt to show the possibilities of using Smoothed Particle Hydrodynamics (SPH) for simulations of nano-scale materials which is not a very common approach. On the other hand, the popularity of SPH is growing fast and the method grabs new areas, so it is reasonable to give it a closer look.

SPH is a hydrodynamic simulation model used mainly for fluid materials. It is a particle model in the sense that the fluid is divided into small elements treated as particles, which interact using the so-called kernel functions. The kernel function $W(r,h)$ decreases with distance and is most often represented by a Gaussian distribution:

$$W(r,h) = \alpha \cdot \exp\left(-\left(\frac{r}{h}\right)^2\right)$$

where $r$ is a distance between particles, while $h$ is a smoothing length and $\alpha$ is a coefficient depending on the dimensionality of the model (2D or 3D). Any field property of a fluid, $A(\overrightarrow{r})$ in position $\overrightarrow{r}$ can be interpolated by an integral

$$A(\overrightarrow{r}) = \int A\left(\overrightarrow{r}'\right) W\left(\left|\overrightarrow{r} - \overrightarrow{r}'\right|, h\right) dV\left(\overrightarrow{r}'\right),$$

which is then approximated by a sum over particles:

$$A(\overrightarrow{r}) = \sum_j V_j A_j W\left(\left|\overrightarrow{r} - \overrightarrow{r}'\right|, h\right)$$

where $V_j = \frac{m_j}{\rho_j}$ is a volume of a particle j.

The local properties of a fluid, such as velocity, pressure, viscosity, as well as temperature are based on hydrodynamic equations.

As is commonly known, SPH was first designed for large astrophysical models in 1977. In subsequent years it was extended to the simulation of macroscopic fluids and fluid-solid mixtures, especially for free-surface and multiphase flows for both Newtonian and non-Newtonian fluids, as well as for complex geometry systems. The latter simulation aspects show several benefits over grid models due to the meshless nature of SPH.

# ABS01

By nanofluids we understand fluids containing nanometer-sized particles which together form a suspension. In an SPH simulation we do not introduce individual nanoparticles, but rather simulate a two-phase fluid, where one phase is a basic fluid, while the other is a small fraction representing nanoparticles. Nanofluids have many interesting properties, important in technological processes, such as a higher Nusselt number (which is convective to the conductive heat transfer coefficient ratio) compared to the basic fluid.

In our simulations, we investigate changes in the Nusselt number according to different values of Reynolds and Prandtl numbers.

# Investigation of magnetic properties in nanocrystalline iron-ammonia-hydrogen system during nitriding and reduction processes

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Iron catalyst, i.e. nanocrystalline iron, whose surface is covered with oxides of promoters (mainly $Al_2O_3$, CaO, $K_2O$), is also used as a model system to study surface phenomena in reactions between a solid and a gas phase. Reactions in the nanocrystalline iron-ammonia-hydrogen system on the iron surface and the catalyst itself are intensively studied and described in a number of specialized books and articles. The aim of this study was to investigate the kinetics of the nitriding process of iron catalyst and the reduction of the obtained nanocrystalline iron nitrides. Thermogravimetric measurements were performed in a tubular differential reactor (Fig. 1). In addition, a method for in situ measurements of the gas-phase composition, mass, and relative magnetic permeability in a reactor during nitriding and reduction processes has been developed.

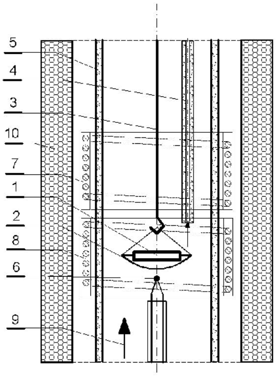

Figure 1: Cross-section of reactor chamber; 1 – sample, 2 – specimen basket, 3 – basket holder, 4 – capillary for gas analysis, 5 – quartz tube, 6 – thermocouple, 7 – measuring coil, 8 – reference coil, 9 – gas flow direction, 10 – furnace

The kinetics studies of the nitriding process and reduction of the obtained iron nitrides were carried out isothermally at 350°C. As a result of the reaction between iron and ammonia, a different form of iron nitrides are formed ($\alpha$-Fe(N), $\gamma'$-$Fe_4N$, $\epsilon$-$Fe_{3-2}N$). During the nitriding process, changes in the relative magnetic permeability values were also measured along with the phase transformation of the forming iron nitride. Moreover, when the transition from one phase to another occurred the directly proportional relation between the relative magnetic permeability and phase

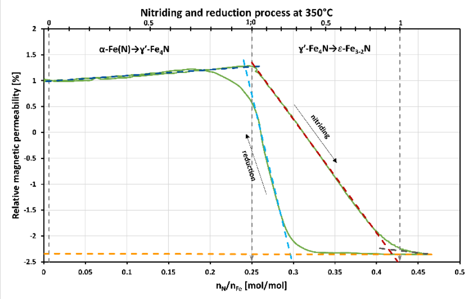

Figure 2: The dependence of the relative magnetic permeability as a function of nitriding degree during nitriding and reduction process at 350°C

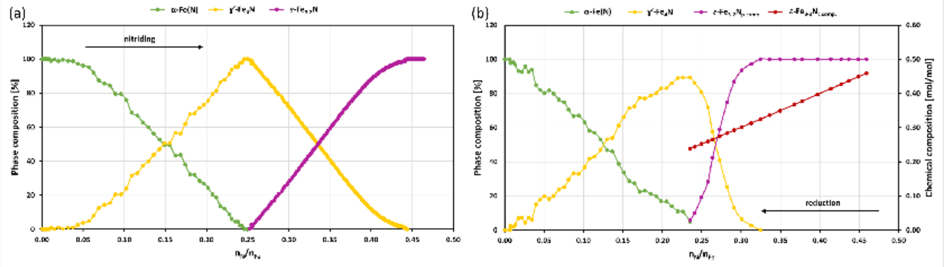

Figure 3: Sample phase composition during (a) nitriding and (b) reduction processes

composition in the sample was observed (Fig. 2). Then the coefficient of change of the relative magnetic permeability to the phase composition was determined, which for the transformation of $\alpha$-Fe(N)$\rightarrow \gamma'$-Fe$_4$N, and $\gamma'$-Fe$_4$N$\rightarrow \epsilon$-Fe$_{3-2}$N was 0.28 and -3.67, respectively. In the final stage of the nitriding process, a paramagnetic phase characterized by a constant value of relative magnetic permeability equal to -2.34 is formed in the material.

Therefore, during the reduction of iron nitrides, a constant value of relative magnetic permeability was observed while the chemical composition of the $\epsilon$-Fe$_{3-2}$N phase was changing. At a value of nitriding degree equal to 0.33 (stoichiometric formation point of Fe$_3$N), a change in magnetic properties was observed. This behavior is caused by a direct transformation to the $\gamma'$ phase. However, another inflection in the curve corresponds to the reduction of $\gamma'$ phase to $\alpha$-Fe(N) phase. Most importantly, the presented dependence of changes in relative magnetic permeability during nitriding and reduction processes allows to determine the phase composition and chemical composition of these phases as a function of nitriding degree (Fig. 3).

## Acknowledgements

This work was supported by the National Science Centre, Poland (grant number 2017/27/B/ST8/02947 and 2017/27/B/ST8/02970)

# Magnetic spin clusters in $Ni_2InVO_6$

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Electron paramagnetic resonance (EPR) and direct current (dc) magnetization were used to investigate the magnetic properties of $Ni_2InVO_6$. A previous study demonstrated the presence of a spin-glass phase in this compound at low temperatures. The EPR spectra showed the existence of four different components, attributed to nickel(II) and additionally to iron(III) as an unintentional admixture. The most intense very broad line was assigned to the nickel spin clusters with strong ferromagnetic short-range interactions. The DC magnetization measurements as a function of temperature and an external magnetic field indicated the presence of spin clusters in the paramagnetic phase and a transition to the cluster spin-glass state below 4.75 K due to the competing ferromagnetic and antiferromagnetic interactions. The EPR and magnetization results were analyzed and compared to draw a comprehensive picture of magnetism in $Ni_2InVO_6$.

# ABS04

# Ionic liquids supplemented with iron III oxides in thermo-electric converters. Redox reactions

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It has recently been demonstrated that ionic liquids supplemented with the so called redox couples can serve as an effective thermo-electric material with the Seebeck coefficient exceeding 2 mV/K. It has been even shown that supplementing the ionic liquid with iron III oxide nanoparticles can further change the material into a ferrofluid, however, there is a surfactant needed to make it possible. The redox couples have been supposed to play the same role when dissolved in ionic liquids as typical redox couples do in typical solvents, i.e. they are considered to be responsible for the flow of current in liquids. In the present work we show the idea of a novel type of a magnetic-thermo-electric device based on an ionic liquid material, and the results of quantum computations of all the possible redox reactions hypothetically occurring in a thermogalvanic cell. We utilized the so-called Born-Haber cycle to determine the redox potentials of all the assumed half-reactions and, as a result, we determined which ions should be responsible for the occurring redox reactions. This electrochemical approach was supported by the chemical one-electron transfer process investigations carried out with the help of quantum chemistry tools.

## Acknowledgements

The investigations were supported by Grant No 731976 from the European Union through the MAGENTA project carried out within the Horizon 2020 Programme

# Open concurrent network communication methods in building distributed web applications

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The attractiveness of real-time multimedia communication as part of an e-learning platform largely depends on the quality of the telecommunications infrastructure and on the services that support the exchange of audiovisual data. The research subject of this work was communication between stationary and mobile devices using distributed services such as Web Real-Time Communication (WebRTC) running in HTML5 compliant web browsers. The test connections were carried out in a peer-to-peer architecture over a local wireless WiFi network and a mobile network supporting the Long Term Evolution (LTE) standard for data interchange. Several audiovisual sessions between two clients were analyzed for different connection scenarios. The parameters responsible for the transmission quality such as delay, jitter, packet loss, or the speed of sending and receiving video frames were measured for each scenario. Open audiovisual communication system performance experiments were conducted under real operating conditions. The obtained results indicated potential applications in the construction of e-learning websites.

# Application of the neural networks for developing new parameterization of the Tersoff potential for carbon

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Penta-graphene (PG) is a 2D carbon allotrope composed of a layer of pentagons having $sp^2$- and $sp^3$- bonded carbon atoms. A study carried out in 2018 has shown that the parameterization of the Tersoff potential proposed in 2005 by Ehrhart and Able (T05 potential) performs better than other potentials available for carbon, being able to reproduce structural and mechanical properties of the PG. In this work, we tried to improve the T05 potential by searching for its parameters giving a better reproduction of the structural and mechanical properties of the PG known from the *ab initio* calculations. We did this using Molecular Statics (MS) simulations and Neural Network (NN). Our test set consisted of the following structural properties: the lattice parameter $a$; the interlayer spacing $h$; two lengths of C-C bonds, $d_1$ and $d_2$ respectively; two valence angles, $\theta_1$ and $\theta_2$, respectively. We also examined the mechanical properties by calculating three elastic constants, $C_{11}$, $C_{12}$ and $C_{66}$, and two elastic moduli, the Young's modulus $E$ and the Poisson's ratio $\nu$. We used MS technique to compute the structural and mechanical properties of PG at $T = 0$ K. The Neural Network used is composed of 2 hidden layers, with 20 and 10 nodes for the first and second layer, respectively. We used an Adams optimizer for the NN optimization and the Mean Squared Error as the loss function. We obtained inputs (about 80 000 different sets of potential parameters) for the Molecular Statics simulation by using randomly generated numbers. The outputs from these simulations became the inputs to our Neural Network. The Molecular Statics simulations were done with LAMMPS while the Neural Network and other computations were done with Python, Pytorch, Numpy, Pandas, GNUPLOT and Bash scripts. We obtained a parameterization which has a slightly better accuracy (lower relative errors of the calculated structural and mechanical properties) than the original parameterization.

# Influence of addition of carbon nanotubes on rheological properties of lubricants — a computer simulation study

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This work is motivated by the improvement of anti-friction properties of lubricants by addition of CNTs proved experimentally in literature. In particular, a methodology is developed to compute the shear viscosity of liquid lubricants (Propylene Glycol) based on Molecular Dynamics simulation. Non-Equilibrium molecular dynamics (NEMD) approach is used with a reactive force field ReaxFF implemented in LAMMPS. The simulations are performed using the canonical (NVT) ensemble with the so-called SLLOD algorithm. Couette flow is imposed on the system by using Lees-Edwards periodic boundary conditions. Suitable parameters such as simulation time and imposed shear velocity are obtained. Using these parameters, the influence of addition of 27 wt% CNTs to Propylene Glycol on its viscosity is analyzed. Results show that 3.2 million time-steps with a 0.1 fs time-step size is not sufficient for the system to reach equilibrium state for such calculations. With the available computational resources, a shear velocity of $5 \times 10^{-5}$ Å/fs was observed to give viscosity value with approximately 43% error as compared to the experimental value. Moreover, the lubricant exhibited a shear thinning behaviour with increasing shear rates. CNTs enhanced the lubricant's viscosity by 100-190% depending upon the averaging method used for calculation.

# An EEG mobile device as a game controller

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In this work the real-time control of computer games was explored by a single electrode mobile electroencephalography (EEG) device with a Bluetooth interface. The amplitude variation in the two frequency bands of 4-12 Hz and 60-200 Hz was selected as the real-time control parameter. The frequency-domain of a raw EEG signal was calculated using the discrete Fourier transform. The time-dependent signal samples equal to 512, 1024, and 2048 time points in size were used in our research. The well-known classic Pong game was used to try out our controller. The developed software handles communication with the device and real-time game rendering. The .NET Framework with the C# programming language was used as a development tool. 50 gameplay trials were made for each controller setup. The obtained results are promising for the possible use of the device in real-time communication with computer devices for people with hand disabilities.

# Tracking the condition of users, based on biometric methods, IoT systems and mobile devices

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The study presents an analysis of the possibilities of using sensory devices and mobile phones available on the market to monitor the condition of users. The article aims to show the possibilities of construction of a general monitoring system that could be used in assessing the possibility of performing work activities by users at the workplace. This type of task is not a diagnostic task in medical terms but is of an auxiliary nature that will increase the reliability of human-dependent technical systems. The study presents methods of assessing the psychophysical condition of users, shows the architectural concept of the monitoring system, and presents a set of sensory devices that may be useful in solving the presented problem.

# Liquid crystalline phases of cyanobiphenyls on different nanostructured substrates - computer simulation study

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Liquid crystalline phases combine the mobility of an isotropic liquid with the long-range orientational order of crystalline solids. Due to these features the are used for applications that rely on their anisotropic electrooptical properties. Since the ordering of molecules is known to be essentially influenced by interfaces and dopants, the anchoring of liquid crystals and other functional organic molecules at a variety of interfaces was studied for fundamental scientific reasons but also due to the fact that the molecular organization of liquid crystals at their interfaces is essential for designing and optimizing a variety of optoelectronic devices and implementing new promising concepts in nano- and biotechnology. We studied the molecular dynamics of cyanobiphenyl family mesogens anchored on different nanostructured substrates of carbon, silicon carbide and boron nitride in order to determine the influence of substrate morphology and polarization of the substrate on the ordering and stability of these phases.

# Destabilization of aqueous suspension of magnetic nanoparticles in AC magnetic field

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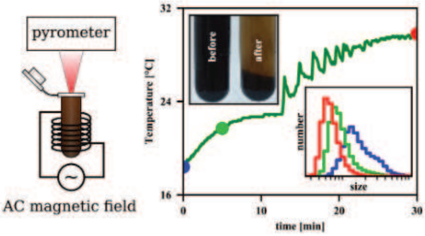
It is known that in the case of single-domain nanoparticles, the energy of the AC magnetic field is converted into heat. The conducted research analyzes the influence of this phenomenon on the stability of the suspension of magnetite nanoparticles in an aqueous solution. We have shown that such local heating makes the nanoparticle suspension unstable, which in turn leads to rapid agglomeration of nanoparticles and, consequently, to rapid sedimentation. Two particular cases of stable colloidal suspensions were considered: a suspension of bare nanoparticles in an alkaline solution and silica-stabilized nanoparticles in a neutral solution. The nature of the phenomenon does not change qualitatively when an alternating magnetic field of a smaller amplitude is used. The obtained results are important primarily for biomedical applications and wastewater treatment.



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# The role of interactions between colloid nanoparticles and substrate for drying pattern formation

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The process of drying a droplet of a colloidal solution and the appearance of a drying pattern of colloid particles deposited on the substrate where such a droplet had dried have been the subject of intensive research in recent years, mainly due to the applications ranging from numerous fields of materials science to inkjet printing technology [1-4]. A brief overview of the current state of research on this issue is presented, both from the point of view of the experiment, analytical results, and modeling with the use of computer simulations. The mechanisms leading to the emergence of the pattern deposit on the surface of the substrate are shown. At the same time, methods of controlling the shape and size of such a deposit of the drying droplet of a colloidal solution using the pH value, temperature, and external fields (electric and magnetic fields, including a variable magnetic field at low radio frequencies) are shown. The experimental results and computer simulations of the drying droplet are presented as an example. The work relates to the recent works concerning deprotonation processes on a silica surface with magnetic nanoparticles and heating magnetic nanoparticles by an external AC magnetic field.

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# Highly-parallel hybrid functionals with plane-wave basis set accuracy

J. Dziedzic[1,2] and C. K. Skylaris[2]

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Local and semilocal functionals widely used in Kohn-Sham density functional theory (KS-DFT) calculations underestimate band gaps and have difficulties describing the energetics of small molecules, among other deficiencies [1]. Hybrid functionals, where Hartree-Fock (or exact) exchange is included in the exchange-correlation functional offers a more accurate description of geometries and improves a number of properties, such as bond energies and band gaps, particularly for metal oxides [2].

We present a higly-parallel resolution-of-identity-based approach [3] for evaluating exact exchange and hybrid exchange-correlation functionals with a computational cost that scales linearly with the number of atoms. We employ a density-matrix formulation with localised, in-situ optimised orbitals. We describe the implementation of this approach in the linear-scaling DFT code ONETEP [4], which can perform such calculations with near-complete basis set accuracy.

We validate our approach against energies, forces and equilibrium bondlengths [2,5] computed with conventional, cubic-scaling DFT codes, demonstrating excellent agreement, even with approaches using an all-electron description and large Gaussian basis sets. We describe a hybrid (MPI+OpenMP) parallelisation strategy for our implementation, which offers excellent scaling up to thousands of CPU cores. Benchmarks for larger systems, demonstrating the linear-scaling of the computational time with the size of the system will also be presented, along with excellent strong parallel scaling, even in regimes where $N_{\text{cores}} > N_{\text{atoms}}$.

We would like to thank the University of Southampton for access to the Iridis [5] supercomputer that was used in this work and to the TASK Academic Computer Centre for access to the Tryton HPC facility.

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ABS14

# A generalised model for connected octagonal star-shaped units

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We propose an analytical model for a very general Star-4 system which can be used to predict a wide variety of systems (see Figure 1). We show that by permitting the systems to different ligament lengths, angles and ligament thickness, we can fine-tine the Poisson's ratio properties of the system to practically any reasonable value, both negative and positive.

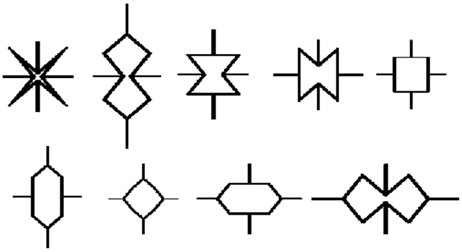

Figure 1: Some examples of the systems which can be modelled through the proposed analytical model

# Modelling of the stress-strain properties of graphene through molecular dynamics

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Ever since the ground-breaking experiments on graphene reported by Geim and Novoselov in 2004, this nanomaterial has received considerable attention from academia and financial circles alike due to its remarkable characteristics. Although high-impact research on graphene is generally directed towards the study of its electronic properties, further positioning it as a promising next-generation material for use in energy storage, spintronics, transistor technology and optoelectronics, among others, its mechanical properties ought not to be ignored. Recent studies on this topic are largely concerned about the mechanical enhancements gained from incorporating graphene into certain types of composites, whereas very few reports exist which detail exactly how the mechanical properties of graphene can be efficiently reproduced through simulation. In this present work, we develop an ad hoc protocol which is executable within the LAMMPS environment for simulating the uniaxial stretching of pristine graphene along its two principal directions, namely the armchair and zigzag direction, until fracture. This is followed by a broad discussion of the design choices that we have made during the creation of the simulation protocol and, in so doing, highlight its key aspects and their respective role in ensuring that the experimentally determined mechanical properties of graphene are replicated satisfactorily.

## Acknowledgements

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# On the structural properties of folded graphene systems: A molecular modelling study

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Graphene is often hailed as the wonder material of the 21st century which is gradually finding its way into a wide variety of applications ranging from biomedical to smart materials. Recent work on graphene by the authors has revealed that, through a random or deterministic placement of 5-8-5 vacancy defects, it is possible to fine-tune the morphology of graphene by forcing it to 'wrinkle' more extensively. Complimentary to this discovery were the identification of energetically stable graphene conformations which resembled crumpled paper or corrugated sheets, and the realisation that folded regions imparts auxetic character, analogously to a 'wrinkled' material that is pulled flat and re-flattened [1,2]. This work investigates further this aspect of graphene through an examination of energetically stable, graphene conformations which exhibit characteristic, folded, pleated-like domains. A comparison is made between folded forms of graphene on the basis of the presence or absence of patterned 5-8-5 vacancy defects within their structure to discern the influence that such topological defects have on fold creation and its unfolding behaviour.

## Acknowledgements

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# Simulation of stretching and unfolding of “folded graphene“

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Graphene, an atomically-thin material, is inherently flexible and therefore highly amenable to both random and controlled corrugation, which is a prerequisite for the formation of folded graphenes. These systems are known to exhibit distinct properties – as exemplified by the manifestation of pseudo-magnetic fields, semiconducting character, and instances of strain-induced negative stiffness – which are absent in standard graphene. However, despite the evident research potential surrounding this intriguing class of graphene-type systems, very few reports exist that examine the mechanism/s involved during the unfolding of folded graphenes under large tensile loads. This study aims to address this shortcoming by simulating in LAMMPS the morphological changes which take place when a set of folded graphene systems are stretched open. From the results, two dominant patterns of unfolding are identified: the first which consists in the re-adjustment of neighbouring folded regions by sliding against each other, and the second which necessitates the opening of a fold to partially release the stress accumulated as a direct result of the stretching action. We expect that a further examination of these mechanisms may be beneficial towards the development of nanodevices where the need for stress relief is desirable.

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# Preliminary results on the anomalous stiffness properties obtained upon uniaxially stretching folded graphene with vacancy-type defects

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Folded graphenes are a loosely defined group of graphene morphologies that contain one or more folding domains, with further differentiation by folding angle and fold spacing. Recent studies have demonstrated that strain-induced, structural modifications to the folds present within these systems have a sizeable influence on their energy band gap, catalytic activity, and compressive strength, among other properties; this naturally implies that such properties can in theory be adjusted simply through straining action. Despite this, the literature pertaining to the nanomechanical unfolding of folded, graphene-type systems remains scarce and even more so on their possible manifestation of anomalous, negative mechanical behaviour in response to large tensile deformation. This work investigates the mechanical behaviour of a folded graphene system as it is being subjected to uniaxial stretching through an MD simulation in LAMMPS using the AIREBO potential. Folds are introduced in the system by inserting 5-8-5 vacancy sites arranged as periodic line defects, which have the effect of constraining the system to a quasi-periodic, highly ordered morphology. The results show instances of pronounced negative tangent modulus which coincide with each fold opening. Moreover, it is observed that initial fold openings are characterised by the stress component in the stretching direction turning slightly negative, an indication of an appreciable reluctance by the system to being further deformed by the applied strain.

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# ABS19

## High entropy materials

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Entropy may be interpreted as the degree of disorder or randomness in the system. It can be used not only to describe theoretical thermodynamic systems or processes but also to describe the disorder in crystalline materials. Metal alloys were considered as the first high entropy materials. However, today the idea of multicomponent materials is not only limited to alloys, but since recently, also to other materials including oxides.

The research on high entropy oxides commenced in 2015 from the pioneering work of Rost et al. [1] who obtained rock-salt HEO in a system of MgO, CoO, NiO, CuO and ZnO mixed in equimolar ratios. Later, oxides of the fluorite-, spinel-, pyrochlore-, perovskite- and other structures were studied in a group of high entropy oxides. Most of the properties of high entropy oxides, especially their electrical properties, have not been sufficiently studied, so far. Only a few published reports have concerned the electrical properties of HEOs. The electrical properties of oxide depend on the mobile charge carriers. The disorder and lattice distortions related to high configurational entropy may influence both the concentration of particular charge carriers and their mobility. For instance, due to the stronger electron scattering on the lattice defects than on phonons, high entropy alloys exhibit high resistivity and a low TCR. The first studies on the proton conduction in high-entropy perovskites have been published recently [2]. In this work, we present selected properties of high-entropy oxides which belong to two groups of proton-conducting oxides. The first group constitutes example perovskites based on barium zirconate, whereas the second one includes modified lanthanum niobates.

Single-phase oxides were prepared using a solid-state reaction method. The electrical properties of the HEOs were characterized by electrochemical impedance spectroscopy and/or by the DC 4-terminal method in different atmospheres. The possible contribution of proton defects, oxygen vacancies and electronic charge carriers to the total conductivity of the oxides was analyzed and discussed.

### Acknowledgements

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# Negative thermo-mechanical properties from rotating rigid units

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Negative Poisson's ratio materials, commonly known as 'auxetics', exhibit the anomalous property of expanding laterally when uniaxially stretched and getting thinner when compressed. This property typically requires the presence of specific geometric features within the nano/macro structure of the material and an amenable deformation mechanism. This work explores the important role and various implementations, both in 2D and 3D, of 'rotating rigid units' which range from 'rotating squares' to much more complex renditions at various scales of structure to generate a negative Poisson's ratio. It also explores the role of rotating rigid units to generate other negative properties, such as negative thermal expansion and negative compressibility.

# Charge transfer in nitrogen-modified titania annealed at 600°C and 650°C

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Four different types of N-$TiO_2$ nanocomposites annealed at 600°C and 650°C were prepared without and with water rinsing and their magnetic response was measured using the EPR technique. An electron transfer between the rutile and anatase phases in N-$TiO_2$ nanocomposites was confirmed with the calcination temperature between 600°C and 650°C. The appropriate calcination temperature causes the electrons to shift from lower to higher energy levels through thermal energy. This results in a 'phase transition' in the photocatalytic process. Undoubtedly, the obtained result may be of significant importance when used in applications in photocatalytic or conductive processes.

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# ABS22

# Dynamic magnetic properties one-pot solvothermal synthesized graphene/25% $ZnFe_2O_4$ composites

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Nanocomposites containing graphene and $ZnFe_2O_4$ were synthesized and characterized. The content of zinc ferrite in the composites was 25 wt.%. The magnetic properties were investigated by the magnetic resonance method. Magnetic agglomerates are present in all composites. The number and the parameters of the resonance spectra depend on the thermal annealing processes with different temperatures and stress values. Some of the magnetic resonance spectra are dominated by an asymmetrical and very intense broad line and others by a symmetrical line. It is characteristic for the magnetic resonance spectra for composites obtained in a $ZnO$-$Fe_2O_3$-$ZnFe_2O_4$ system [1].

The registered magnetic resonance spectra could be very well fitted with the Lorentzian and Gaussian functions for the samples with thermal annealing at 120°C/8h, 160°C/8h, 200°C/8h and with the Lorentzian function only for other samples.

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# Proton conduction in high-entropy perovskites

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The first studies of proton conduction in oxides were published in 2020 [1]. In this work, we present the results of the research on high entropy perovskites based on proton conducting barium zirconate in which the zirconium crystallographic site is occupied by between 5 to 10 cations, for example Ba(Zr,Hf,Sn,Ti,Y,In,Sm,Yb)$O_3$. The ceramic materials were prepared by means of a high temperature solid-state route. Dense sinters of the materials were obtained by addition of 1 wt.% of PVB and NiO for the conductivity and diffusion studies. The materials were examined using X-ray diffraction, scanning electron microscopy, thermogravimetric analysis, and electrochemical impedance spectroscopy. The EIS measurements were performed in different atmospheres, namely in dry synthetic air, as well as in H2O- and D2O-containing atmospheres to study proton conductivity. The obtained results allowed calculating the proton and deuterium conductivities reaching $2.61 \cdot 10^{-5}$ $S \cdot cm^{-1}$ and $1.21 \cdot 10^{-5}$ $S \cdot cm^{-1}$ at 500°C, respectively. Additionally, water the diffusion coefficient D and the surface exchange reaction coefficients $k$ were calculated as a function of temperature.

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# Iron III oxides: structures and redox reactions

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The iron III oxide is an interesting material taking the form of various-size structures and nanostructures and frequently displaying magnetic properties.

Moreover, the magnetic nanoparticles of the iron III oxide can be suspended in an ionic liquid and lead to a liquid ferrofluid, however, it is necessary to delicately play with the surfactants and counterions due to the nature of ionic liquids.

The $(Fe_2O_3)_n$ particles, where $n = 1,...,$ can take various forms and spins. Moreover, they can be symmetric or nonsymmetric. They could also exhibit redox properties due to the fact that there are many $Fe^{3+}$ in the structures. In the present work we show the achieved structures of the $(Fe_2O_3)_n$ molecules, where $n$=1,...,10, the spin states examined and their redox properties. We took into account many different quantum methods, basis sets and surrounding solvents. The work is very systematic and comprehensive leading to a direct answer for the question of the possibility of extrapolating the high-level computations and properties found first for small-$n$ iron oxides, to the properties of the nanostructures treated after significant simplifications of the methods used.

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# Investigation of non-magnetic metal welds diagnostics using eddy currents

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This work presents the utilization of the selected NDT (Non-Destructive Testing) method based on measurement of inductive eddy currents involving a differential hybrid probe.

The approach was automated by constructing a 3D positioner and integrated with the authorial LabView program, which enabled high-resolution longitudinal measurements. Both the design and the software of the positioner and the probe were optimized. The calibration of the positioner and the probe was performed and described. The approach was evaluated using superficial and subsurface macro, micro, and nanoscale discontinuities, i.e., laser weld, undersurface material loss, and clamped discontinuity of non-magnetic AISI321 and magnetic Gr.36 steel samples. All measurements were taken in various conditions of the probe-material distance and frequency and intensity of the prime coil current. The characteristics were examined with respect to the prime coil current frequency, hence, the perturbation signal penetration depth. The measurement of eddy currents allowed detecting nanoscale defects. Most importantly, the clamped defects were detected, which is a unique feature of the proposed approach. To conclude, our research reveals the possibility of creating cost-efficient NDT to study the actual propagation of macro and micro defects in metals and alloys. Moreover, eddy currents were proven efficient also for the identification of nanoscale defects.

# Isotope He3 separation from liquid helium - method and results

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The isotope He3 finds application in many areas of science and industry. The most important fields of application are cryogenics, where He3 allows achieving millikelvins in dilution refrigerators, and public security, with He3 detectors of radioactive materials at airports and important buildings. He3 is also used in medicine for lung tomography. One of the most extraordinary future applications assumes the use of He3 in fusion reactors for clean energy.

The low temperature method of the isotope He3 separation from liquid helium which is based on a quantum filtration process with the use of entropy filter is presented. The method used allowed observing an increase in the He3 concentration of more than one order of magnitude. A consistent description of the various stages of the cryostat operation within the cooling process above and below the lambda transition is presented.

# Resistivity switching in activated carbon fibers

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This work presents the effect of switching of the resistivity of activated carbon fibers, observed for a certain combination of specific molecules adsorbed in fiber pores and an external electric field. Clear resistivity jumps were observed, with the amplitude depending on the temperature. Ordering of adsorbed dipolar guest molecules that act as a gating factor for the electrical transport in a granular fiber structure is the most possible cause for the observed phenomenon. The presented research shows that the structure, host-guest interactions, temperature and external fields can be used to gain control over the charge carrier transport in porous carbon systems.

# Second-order nonlinear optical response in chiral ferroelectric liquid crystals

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Noncentrosymmetric (NCS) compounds are of current trend in material science because of their important second-order nonlinear optical properties, with applications such as second harmonic generation (SHG), electro-optical switching, and bioimaging [1–6]. Noncentrosymmetry has a fundamental importance of symmetries in nonlinear optics. Second-order NLO are not observed in centrosymmetric material.

The aim of the present study is to extend the dielectric studies of chiral smectic liquid crystals to nonlinear optical spectroscopy (HRS and SHG) and to check if a HRS (Hyper-Rayleigh Scattering) response exists in these LC. For the study the three classic, known from few decades, chiral liquid crystal have been chosen (MHPOBC, D16 and D17). The small differences in their molecular structures lead to the significant changes in amount and sequences of the phases and subphases, i.e. isotropic-chiral smectic Achiral smectic C. The NLO (TPF and SHG) microscopes were used to obtain the images of studied ferroelectric LC in smectic and isotropic phases. The application of NLO microscopes should be useful because SHG microscopy are usually employed to study the symmetry and local organization of organic microcrystals while two-photon fluorescence (TPF) microscopy to verify the monocrystallinity of the sampled area.

The study of nonlinear optical properties of several ferroelectric LC compounds has allowed the detection of the centrosymmetry or its absence. The HRS measurements of chiral molecules of the compounds MHPOBC and D16 in solution clearly demonstrates the quadratic NLO activity of these chiral ferroelectrics in contrast to D17. The noticeably SHG signal for compounds MHPOBC and D16, in all smectic phases indicates the noncentrosymmetric structure of the molecular order in smectic layers as a result of the loss of the inversion symmetry. The compound D17 does not show a second-order NLO response and the only structural difference is the occurrence of three isolated phenyl rings in the core instead of -conjugated biphenyl core in compounds MHPOBC and D16. It becomes evident that small structural changes in the mesogen molecules lead to the significant differences in the mesogenic and optical properties of the ferroelectric LC material [7].

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# Tuning the physical properties in quasi-low dimensional monophosphate tungsten bronzes

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The family of Monophosphate Tungsten Bronzes (MPTB), represented by the general formula $(PO_2)_4(WO_3)_{2m}$, with $m$ being an integer, constitute a universal platform to explore the physical phenomena associated with the quasi low-dimensional electronic structure [1]. The crystal structure of MPTB is constructed as an alternative stacking of conducting W-O slabs and insulating P-O layers. The parameter $m$, determining the thickness of the conducting slabs, not only plays a crucial role in the tuning of the effective dimensionality, but, due to the fact that the number of free electrons per unit cell is constant, also impacts the electronic carrier density. The latter quantity can be further modified by inserting alkali metal ions into the quasi-pentagonal tunnels located in the P-O environment. A characteristic feature of the phase diagram of this family is the emergence of (multiple) charge density waves [2,3], accompanied by strong, yet incomplete nesting of the Fermi surface (FS). This phenomenon, decomposing the FS into small pockets containing high mobility carriers, gives a rise to the occurrence of quantum effects (such as quantum oscillations) in the low temperature transport [4], together with the enhancement of thermoelectric and galvanothermomagnetic properties [5].

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# The influence of niobium on calcium-phosphate nanoceramics synthesized via low-temperature methods

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As calcium phosphates (CaPs) are major inorganic components of hard tissues, they have been widely studied over the last few decades. Furthermore, owing to their biocompatibility, bioactivity and osteoconductivity, they are widely used in tissue engineering and implantology [1]. In addition, their applications also extend to heavy metal ion sorbents [2].

Naturally, specific properties of a material are needed for different implementations. One of the ways to affect the properties of CaPs is via doping ceramics with metal ions. In this respect, niobium is promising because it influences, inter alia, the crystallinity, morphology and biological parameters of calcium phosphates [3]. Moreover, numerous studies show that calcium phosphates synthesized by different (for example: mechanochemical [4], precipitation [5] and sol-gel [6]) methods exhibit different properties.

In this work, we analyzed the influence of niobium on calcium-phosphate nanoceramics synthesized by three popular methods, namely: mechanochemical, precipitation and sol-gel. The obtained ceramics were examined using: scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The dopant successfully built into the CaPs structure. The grain size of nanoceramics decreased with the addition of Nb. On the other hand, the presence of niobium increased the crystallinity, the size of the crystallites and the number of the absorbed carbonates. Moreover, the results showed that niobium was mainly located on the surface of the ceramics grains.

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# Glasses and glass ceramics enriched with nanostructures as promising materials for optical applications

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In recent years white phosphors and LEDs have been proposed to be the next generation of solid state lighting sources that should replace traditional incandescent and fluorescent lamps owing to their advantages in energy consumption and the related environment benefits. However, materials that could be used in such optical systems must exhibit certain properties such as: good transparency over a wide range of the electromagnetic radiation spectrum, a high refractive index, low phonon energy and chemical and mechanical durability. The group of materials meeting these criteria includes tellurite and borate glasses. On the other hand, materials which not only show the same advantages as glasses, but first of all exhibit improved optical properties are glass-ceramics. And here again tellurite and borate glass-ceramics can be considered, this time enriched with $SrF_2$ nanocrystals or Ag nanoparticles, and doped with rare earth ions. Glass-ceramics can be produced by controlled nucleation and growth of nanocrystals in precursor glasses in a temperature region slightly above the glass transformation temperature Tg. However, when selecting the crystallization conditions, the possibility of growth of undesirable crystalline phases or nanostructures must also taken into account.

In this work, we show the method of manufacturing tellurium and borate glasses and glass-ceramics containing $SrF_2$ nanostructures or Ag nanoparticles, and we show the influence of nanostructures on the luminescence of rare earth ions located in the matrix. The structure of the samples was studied by XRD, DSC and FTIR methods, while the optical properties were examined by the UV-Vis spectroscopy. The luminescent properties of the sample were investigated under excitation by UV radiation.

The results show that proposed materials can be considered as matrixes for LEDs.

# Controlling plasmonic band position of AuAg nanoalloy structures by composition

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The unique catalytic and optical properties have attracted the attention of researchers to metallic nanostructures for several years now. Specifically, the key that opens possible application in various fields, such as photovoltaic devices, surface-enhanced Raman scattering or even anti-cancer therapy, is the localised surface plasmon resonance [1,2]. It is bimetallic structures that have been gaining increasing popularity within this group recently. The uniqueness of these nanomaterials is derived from the synergistic effects that can cause fascinating properties, dramatically different from those of the corresponding single component structures. Such properties, and thus the applicability of such nanostructures, are related not only to their size and shape, as is the case with monometallic nanoparticles, but also, and more importantly, to their chemical composition [3].

In the paper, we present the results of the investigation of the parameters of initial fabrication and the influence of experimental conditions on the formation and optical properties of AuAg nanostructures. Nanoislands were fabricated through dewetting Au/Ag thin layers using thermal treatment with temperatures well below their melting temperature. The surface morphology was investigated by means of SEM, HR TEM, EDS and XPS, while the optical parameters were analysed using the UV-vis spectroscopy. The results confirm that the position of the resonance band of alloyed nanostructures can be changed with a linear tendency.

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# Detection of alcohol by nanosensors based on plasmonic structures

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Surface plasmon resonance in metallic nanoparticles has been studied extensively in the past years. Nevertheless, most of the research has been focused on manufacturing plasmonic structures, resonance simulations or applications in the field of luminescence. In this work we focused on the detection of liquids by changing the plasmon resonance frequency. It is well known from the Mie theory that the frequency of plasmon oscillations depends on the three most important factors: the size of nanostructures, the material of nanostructures (its dielectric constant) and the dielectric constant of the material that surrounds the nanostructures. This approach seems to be much more useful than detection of liquids or molecules by recording the variation of the refractive index of plasmon resonance based structures.

Gold, silver and gold-silver nanoalloy nanostructures prepared by thermal treatment of metallic thin films were used as plasmonic structures. The frequency of the plasmon resonance was measured as a position of the absorption peak in the visible light transmission characteristics. We observed that the shift of the resonance position depended on the environment. The shift recorded for water and alcohol was compared to the position of resonance in the air. On the basis of the measurements it is possible to detect not only the presence of water or alcohol, but also the concentration of alcohol in water. Therefore, the proposed platforms can be used in nanosensors.

# The influence of $SrF_2$ concentration on optical properties of $Eu^{3+}$ doped phosphate glasses

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The growing demand for solid light sources forces the search for increasingly sophisticated materials that would combine simplicity of implementation, low production costs, and versatility. Amorphous materials doped with rare earth elements, phosphate glasses in particular, have a high potential in this field. Phosphate glasses stabilized with heavy metal oxides are characterized by a good chemical durability, an exceptional solubility of modifiers and rare earth elements, and a low optical dispersion. The addition of fluorides allows obtaining optical materials with lower phonon energy, high UV transparency, and lower fluorescence linewidth, which makes them promising candidates for phosphors in LEDs.

A series of phosphate glass systems of the nominal composition $P_2O_5$–$Bi_2O_3$–$K_2O$–$Nb_2O_5$–$x$$SrF_2$ ($x = 0$, 5, 10, 15 mol%) doped with 0.5 mol% europium were prepared by the conventional melt-quenching technique. The obtained glasses were structurally characterised by XRD and FT-IR measurements. The glass transition temperature was measured using DSC. The effect of the $SrF_2$ presence on the luminescence of $Eu^{3+}$ ions was analyzed on the basis of the luminescence emission spectra under UV and UV-Vis spectroscopy.

On the basis of the conducted research, an improvement in the luminescence was observed for the amorphous samples containing the $SrF_2$ addition.

# ABS35

# Droplet evaporation method for preparing uniform film of magnetic nanoparticles

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The processes of obtaining thin uniform films of nanoparticles are of great interest for manufacturing fields including protecting layers and functional materials.

Well-known among a wide range of nanoparticle deposition methods is sessile drop evaporation of stabile nanoparticle suspension which is used on a large scale in ink-jet printing.

An outward capillary flow appears during the evaporation of pinned sessile droplets. This phenomenon is induced by a higher rate of evaporation near the edge of the sessile droplet and fast loss of liquid there. The nanoparticles which are present in the suspension are transported towards the edge of the droplet leading to the formation of a ring-like pattern, usually called the coffee-ring effect [1,2].

In the present research, a stabile suspension of magnetic iron oxide nanoparticles was tested for the pattern formation during evaporation as a sessile droplet. The impact of the electric and magnetic fields on suppressing the "coffee ring" effect was investigated.

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# Optical, structural and luminescence properties of borate-bismuth glass and glass-ceramics doped with $Eu^{3+}$ ions

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Owing to their properties such as a high refractive index, good transparency in a wide frequency range, a high thermal and mechanical stability, and the low energy of phonons borate-bismuth glasses seem to be very interesting materials, especially for photonic purposes.

Two types of borate-bismuth glass systems modified by the addition of strontium fluoride ($B_2O_3$-$Bi_2O_3+xSrF_2$ $x$=10,20) and aluminum fluoride ($B_2O_3$-$Bi_2O_3+xAlF_3$ $x$=10,20) were successfully synthesized as host matrices for optically active $Eu^{3+}$ ions. Glasses and glass-ceramics were prepared by the conventional melt quenching technique. Additionally, glass with strontium fluoride was annealed in order to produce $SrF^2$ nanocrystals. $AlF_3$ as well as $SrF_2$ nanocrystals and $Eu^{3+}$ ions leading to the emission enhancement were successfully located in tellurium glasses [1,2].

The structure of the prepared samples was studied by the XRD and DSC methods, while the optical properties were examined by the UV-Vis spectroscopy. The presence of structural units was revealed by the FTIR measurements. The luminescence properties of glasses were investigated by excitation under UV light. A significant influence of fluorides on the luminescent properties was observed.

Based on the obtained results, borate-bismuth glasses appear to be an excellent host for rare-earth ions. Furthermore, they can find application as phosphors in light emitting diodes.

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# ABS37

# FMR study of iron oxides coated with amphoteric sulfohydroxybetaine - type surfactants

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One of the important research methods for magnetic nanoparticles is the magnetic resonance method (EPR/FMR - electron paramagnetic resonance/ferromagnetic resonance) [1]. The dominating particles are nanocrystallites, 7.8 nm in size, insulated by a shell. The FMR study of iron oxides coated with amphoteric sulfohydroxybetaine-type surfactants showed spectra originating from magnetic nanoparticles. The FMR measurements showed a formation of fairly significant internal magnetic fields which can order magnetic moments. Magnetic moments can produce thermal energy as a result of relaxation processes. This plays an important role in heat therapy in combating cancer processes, where the application of an external magnetic field is important [2]. The therapies in the fight against the cancer pathology can be more effective when the formation of internal magnetic fields is taken into account.

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# Molecular Dynamics simulations of thermal conductivity of penta-graphene

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The thermal conductivity of penta-graphene (PG), a new two dimensional carbon allotrope and its dependence on temperature, strain, and direction are studied in this paper. The thermal conductivity of PG is investigated using a non-equilibrium molecular dynamics simulation (NEMD) with the Two Region Method by applying the optimized Tersoff interatomic potential. Our study shows that the thermal conductivity of PG (determined for the [100] direction) at the room temperature of 300 K is about 18.7 W/(m K), which is much lower than the thermal conductivity of graphene. As the temperature increases, the thermal conductivity of PG is decreasing because, unlike graphene, PG has lower phonon group velocities and few collective phonon excitations. The obtained dependence of the thermal conductivity on the temperature can be described as $\kappa \sim T^{-0.32}$. For the [110] direction the thermal conductivity at the room temperature of 300 K is very similar: about 17.8 W/(m K). In this case, the temperature dependence follows the $\kappa \sim T^{-0.3}$ relation. Our investigations reveal that the thermal conductivity of PG is isotropic, meaning that heat transport behavior is independent of the heat flow direction. Our results indicate that the thermal conductivity of PG depends in an interesting way on the applied strain: nonmonotonic up-and-down behavior is observed. The thermal conductivity increases between strains from 0% up to 12.5%, and it decreases above a strain of 12.5%. Our investigation highlights the fascinating thermal transport properties of penta-graphene. The ultra-low thermal conductivity, the decreasing thermal conductivity with the increasing temperature, and the ultra-high mechanical strength of PG show that PG possesses a great potential in thermoelectric and nanomechanics applications. We hope that these findings, made by means of simulations, will become a bridge to inspire and encourage the experimental works, especially in the synthesis of PG.

# Magnetic resonance spectra of hybrid nanocomposites containing nanocrystalline $TiO_2$ and graphene-based materials

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The existence of magnetic agglomerates in nanocomposites based on graphene and $TiO_2$ was shown using the EPR/FMR method. All the parameters of the magnetic resonance spectra strongly depended on the applied modification processes. The reduction in graphene significantly increased the number of magnetic moments which caused important changes in the reorientation and relaxation processes. Some nanocomposites showed a single domain magnetic (ferromagnetic) arrangement, the remainder exhibited magnetic anisotropy. In addition, an EPR spectrum originating from localized magnetic centers was observed. The intensity depended strongly on the method of preparation of the nanocomposites.

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# Modification of elastic properties of f.c.c. hard sphere crystals using periodically arranged nanoinclusions of hard spheres of another diameter

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Auxetics [1], materials discovered only a little over 30 years ago, distinguish themselves from others by exhibiting a negative value [2,3,4] of the Poisson's ratio [5] . The demand for novel metamaterials and materials with special properties drives the search for auxetic materials and focuses our attention on studying their extraordinary properties and the phenomena behind them. The occurrence of auxetic properties in nature is rare. Thus, one must search for possibilities to modify the elastic properties of the existing materials. One of the ways to find mechanisms to modify the elastic properties of materials in a desired manner is to study simple models with a modified structure, in particular, study models with inclusions to a crystalline structure. In this lecture, the influence of inclusions to an otherwise perfect f.c.c. crystal of hard spheres is reported. The inclusions are filled also by hard spheres, but their diameters differ from the rest of the system. The applied inclusions are organized in the form of layers, channels or a combination of the latter. It is shown that even such simple modifications to the structure are enough to significantly impact the elastic properties (in particular Poisson's ratio) of the model. Layer inclusions are formed by replacing spheres in a selected single crystallographic plane with hard spheres the diameters of which were altered (compared to the original ones – forming a matrix of the system). The inclusion plane was oriented orthogonally with respect to the [001]-direction. The channel inclusions were analogically constructed by replacing the spheres within a specified radius around an axis oriented in the [001]-direction. In order to study the Poisson's ratios of the models, the Monte Carlo simulations using the Parrinello–Rahman [6-8] method in the NpT ensemble were used. It was shown that the elastic properties of a hard sphere system were impacted by the diameters of the inclusion spheres, but even more significantly, by the shape of the inclusions. It was shown that the layer inclusions modified the elastic properties only slightly, merely doubling the negative Poisson's ratio of a cubic system [9], whereas the channel inclusions showed a decrease by an order of magnitude [10]. It was surprising to discover that the combination of the two brought an opposite effect, namely cancelling the auxetic properties from the f.c.c. hard sphere system [11].

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# Nanocrystallization in amorphous metal alloys induced by Joule heating

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Amorphous metal alloys (AMA) have been under research for a long time due to their unique properties caused by their disordered structure and the possibility of forming nanocrystalline materials. Different methods can be applied for amorphous structure crystallization such as annealing, plastic deformation, laser irradiation, etc. [1,2,3].

The present research is focused on the nanocrystallization behavior of amorphous alloys with compositions $Al_{70}Ni_{10}Si_{20}$, $Fe_{73.5}Nb_3Cu_1Si_{15.5}B_7$ and $Co_{70}Fe_3Mo_{1.5}Mn_{3.5}Si_{11}B_{11}$ induced by Joule heating — the effect by which the pass of current through a conductor produces thermal energy. The alloys were manufactured in the form of ribbons by rapid cooling from the melt using the melt-spinning technique. The ribbon thickness was about 25 $\mu$ and the width was about 1-2 cm.

The features of Joule heating-induced nanocrystallization in the the investigated alloys were studied using the back-scattered X-ray diffraction (XRD) method and field emission scanning electron microscopy (FE SEM). The as-obtained ribbons were also investigated by the DTA method using a synchronous thermal analyzer Linseis STA PT 1600 under a dynamic argon atmosphere (~6 liters per hour). The heating was performed at the rate of 10 K/min from 293 K up to 973 K. The temperatures of the onset of the nanocrystallization and further structure transformations were defined.

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# Structural and electrical properties of nanocrystallized vanadium tellurite glasses

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It was recognized a long time ago that properties of some oxide glasses could be improved by temperature treatment [1,2]. The most interesting idea is improvement in conductivity by 6 orders of magnitude. A much better conductivity, high density, and no need to increase the conductivity by adding carbon may found a good use in the field of cathode materials for Li- and Na-ion rechargeable batteries. Being attractive for use, nanocrystallized oxide glasses are of high interest for purely scientific reasons as the conductive mechanism in these materials is not fully understood. Vanadium tellurite glasses can be proposed as a novel material for such use.

In this work the results of the investigation of the crystallization process, structure, and electronic properties of glasses with different vanadium content will be presented. The glasses were prepared by a conventional melt-quenching method. The crystallization was conducted by thermal annealing. Such method of crystallization has been successfully used in the $V_2O_5$-$P_2O_5$ system [3]. The structure of glass and nanocrystallized glass was studied by XRD, FTIR, and SEM methods. The electronic properties were examined by EIS. The crystallization parameters were determined by means of DSC and dynamic DC measurement.

During the research, it was found that vanadium tellurite glasses were an excellent candidate for determining the conductivity mechanisms due to their low complexity. An additional advantage is the low melting point which lowers the production cost.

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# New effective luminescent materials based on borate glasses doped by rare-earth ions and co-doped by silver (Review)

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This presentation is a review of our latest articles devoted to technology and spectroscopic studies of new effective luminescent materials based on borate glasses doped by rare-earth ions [1,2] and co-doped by rare-earth ions and silver [3-5].

Lithium tetraborate ($Li_2B_4O_7$) glasses, co-doped by rare-earth ions ($Er^{3+}$, $Tm^{3+}$, $Nd^{3+}$) and silver (Ag) in amounts 1.0 mol.% and 2.0 mol.%, respectively, were studied in detail by conventional optical spectroscopy and electron paramagnetic resonance (EPR). The optical absorption, luminescence (excitation and emission) spectra and decay kinetics of the $Er^{3+}$ (4f11, 4I15/2), $Tm^{3+}$ (4f12, 3H6), $Nd^{3+}$ (4f3, 4I9/2) as well as $Ag^{+}$ (4d10, 1S0) centers and their aggregates, including Ag metallic nanoparticles, in the rare-earth and silver co-doped $Li_2B_4O_7$ glasses, were analysed in detail according to [1-5]. The presence of the $Ag^0$ (4d105s1, 2S1/2) and $Ag^{2+}$ (4d9, 2D5/2) paramagnetic centers and their aggregates (clusters) in the $Li_2B_4O_7$ glasses, co-doped with rare-earth ions and silver was confirmed by the EPR.

The theoretical and experimental oscillator strengths of the observed absorption transitions as well as the intensity parameters (Ω2, Ω4, Ω6) for the $Er^{3+}$, $Tm^{3+}$ and $Nd^{3+}$ centers were calculated using the Judd–Ofelt theory. The photoluminescence spectra of the $Li_2B_4O_7$:Er and $Li_2B_4O_7$:Er,Ag glasses revealed intense infrared (4I13/2 → 4I15/2 transition, λmax = 1530 nm) and green (4S3/2 → 4I15/2 transition, $\lambda_{\max} = 546$ nm) emission bands. The $Li_2B_4O_7$:Tm and $Li_2B_4O_7$:Tm,Ag glasses showed several intense blue, red, and infrared emission bands characteristic for $Tm^{3+}$. The $Li_2B_4O_7$:Nd and $Li_2B_4O_7$:Nd,Ag glasses revealed three characteristic infrared emission bands corresponding to the 4F3/2 → 4I9/2, 4F3/2 → 4I11/2, and 4F3/2 → 4I13/2 transitions. The characteristic luminescence excitation and emission spectra of the $Ag^{+}$ single centers and their aggregates were also clearly observed in all rare-earth and silver co-doped $Li_2B_4O_7$ glasses.

The radiative properties such as transition probabilities (Arad), luminescence branching ratios ($\beta$), stimulated emission cross-sections ($\sigma$em), and radiative lifetimes ($\tau$rad) were estimated. The obtained experimental and radiative lifetimes were compared and the quantum efficiency ($\eta$) for the main emitting bands of the $Er^{3+}$, $Tm^{3+}$, and $Nd^{3+}$ centers was calculated. A considerable increase in the quantum efficiency (∼10%) of the $Er^{3+}$ green emission (4S3/2 → 4I15/2 transition) in the $Li_2B_4O_7$:Er,Ag glass in comparison with the $Li_2B_4O_7$:Er glass [1,3] was observed. A significant enhancement (by more than 30 %) of the $Tm^{3+}$ visible luminescence for the emission band peaked at 452 nm (1D2 → 3F4 transition) in the $Li_2B_4O_7$:Tm,Ag glass in comparison with the $Li_2B_4O_7$:Er was discovered [4]. The enhancement of the $Nd^{3+}$ luminescence intensity in the $Li_2B_4O_7$:Nd,Ag glass for the emission band with a maximum at 1060 nm (4F3/2 → 4I11/2 transition) in 1.3 and 20 times in comparison with the $Li_2B_4O_7$:Nd glass was achieved under excitation at 585 nm and 350 nm, respectively [2,5].

The observed enhancement of the $Er^{3+}$, $Tm^{3+}$ and $Nd^{3+}$ photoluminescence intensity for their main emission bands is attributed to the energy transfer from $Ag^{+}$ to the rare-earth ions as well as the local field effects induced by the surface plasmon resonance of the silver metallic nanoparticles. Potential applications of the $Li_2B_4O_7$:Er,Ag, $Li_2B_4O_7$:Tm,Ag and $Li_2B_4O_7$:Nd,Ag glasses as promising luminescent materials of the visible and infrared spectral ranges are considered.

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# Tunnelling effects of a two dimensional Gaussian wave packet impinging on a barrier under transverse magnetic field

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The procedure based on momentum-like quantity which provides the reflection and transmission amplitudes for a given barrier sandwiched by reservoirs is extended to include transverse magnetic field within the barrier region. Under the circumstances we consider an initial two dimensional (2D) Gaussian wave packet impinging on the barrier with ignorable barrier overlap. The axis for the second dimension is taken perpendicular to both the impinging and magnetic field directions. Knowledge of the relevant reflection and transmission coefficients leads to the wave function stemming from the initial 2D Gaussian wave packet space and time-wise. This facility leads to obtaining the corresponding probability and current densities. As an application we consider a smooth double barrier. The general picture obtained with regard to the total probability and current densities on account of the extended, in dimension, wave packet due the influence of the magnetic field is relatively small. However, detailed examination of the of the response of the probability and current densities at a given time and location of the impinging direction with respect to the wave extension, along the second dimension, shows significant variations between the cases of zero and applied magnetic field. Apparently, the overall effect of the magnetic field within the additional wave packet extension seems to almost nullify.

# Nanocrystalline iron oxides with various average crystallite size investigated by magnetic resonance method

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A series of nanocrystalline iron oxides samples differing from each other in the average crystallite size (26 to 37 nm) was studied. Magnetic resonance spectra of all samples (M1-M5) were obtained at room temperature. All the resonance lines were asymmetric and intense. These spectra were fitted by the Lorentzian and Gaussian functions. All the spectral parameters depended on the method of preparation of the nanocomposites. We suppose that the Lorentz fit gives a spectrum from larger agglomerated sizes while the Gaussian fit comes from much smaller magnetic centers. The highest value of the total integrated intensity was obtained for the nanocomposite with the largest size of iron oxide nanocrystallites, indicating a reduction in the magnetic size of the agglomerates.

# Numerical methods for free volume calculation in disordered systems

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One of the methods of obtaining nanostructured materials is their formation from liquid or amorphous phases by controlled cooling or annealing. In this case, the main factor determining the final result is the rate of atomic diffusion. According to the hole theory of liquids [1] and the free volume theory [2,3,4], the diffusion of atoms in liquids and amorphous materials is determined by the volume distribution that is not occupied by atoms. In this regard, the determination of a relationship between the free volume distribution and the processes of nanostructuring in liquids and amorphous materials comes to the fore in obtaining nanostructured materials.

Currently, there are several methods for calculating the free volume. Some methods are based on the tessellation of the atomic configuration into Voronoi polyhedra, as a result of which it is possible to determine the volume per atom [5,6]. Another method for determining the free volume in the frame of the hole theory of fluids is presented by other authors [7]. However, in this method selection of boundaries of interatomic cavities is not determined, which leads in some cases to their unreasonable aggregation. The method proposed in this work makes it possible to avoid such agglomeration by selecting the condition for the existence of interatomic cavity boundaries.

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# Nanoindentation of biomembranes with carbon-based nanostructures using computer simulation methods

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The cell membrane was created by nature to protect the interior of the cell from the outside environment. It consists of integral and peripheral proteins which are located in the phospholipid bilayer. The applied model of the bilayer consists of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and cholesterol molecules. The Steered Molecular Dynamics (SMD) technique was used to indent the membrane with graphene planes as well as carbon nanotubes. All simulations were fully-atomistic and were performed in the physiological temperature.

A vital question concerns the ability of the phospholipid membrane to self-regenerate after the indentation process. A series of simulations of removing nanostructures out of the membrane were performed to assess the damages of the bilayer caused during indentation. The average SMD force and work, deflection and the degree of damage of the membrane during the indentation and withdrawal processes are analysed. The results depend on the type and size of the indenter or the angle and speed of indentation, however, the penetration of the bilayer was effective in each system studied.

Both, graphene planes and nanotubes, seem to be good candidates for targeted drug delivery and for further experimental studies. They penetrate the membrane effectively and after the indentation the phospholipid bilayer is able to restore its original structure, even in case of enormous damages. The presentation will start with an overview of a selected group of empirical potentials which are widely used for simulating of Al-Cu alloy systems. These potentials have been chosen due to their widespread and successful use in various MD simulations. After this introduction, requirements for validating these potentials will be presented. These criteria are focused on the ability of these potentials to correctly predict the formation mechanisms of Guiner-Preston zones and intermetallic precipitates in lowcopper Al-Cu alloys during a precipitation hardening process and how these structures influence the structural, mechanical and thermophysical properties of the alloy. In what follows, a set of computational methods will be outlined. These methods are used to compute each group of the said properties. These methods include, for example, a simulation scheme used for calculating the Gibbs free energy of intermetallic phases or an improvement of the two-phase "sandwich" method used in the estimation of the melting point of pure metals. Based on the results from these simulations, each potential will be categorized in terms of properties for which it predicts values comparable with the available data obtained via experimental and *ab initio* methods.

# Multi-step synthesis of shape-memory poly(carbonate-urea-urethane)s studied by Dynamic Lattice Liquid model

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Shape-memory polymers are a group of macromolecular compounds characterized by the ability to change shape under an external impulse. This type of material is usually segmented. The elastic segments that they contain are in an amorphous form, enabling the stretching of polymer bundles and fixation of a temporary shape and the impulse return to the basic shape. Rigid segments are the cross-linking points responsible for the durability of the basic shape.

We presented the application of Monte Carlo simulations for better understanding of the process of preparation of poly(carbonate-urethane-urea) elastomers [1–4]. A two-dimensional coarse-grained Dynamic Lattice Liquid model was adopted for this purpose. All objects were put into vertices of a face-centered cubic lattice, where these objects (beads) corresponded to small molecules or chain fragments. Computational experiments were focused on the simulation of a multi-step synthesis. Therefore, we performed a two-step synthesis of oligocarbonate diols, followed by a process in which the prepolymer was obtained, as well as its curing with water vapor. We developed a methodology that allowed us to reflect the most important features of the copolymerization process. The presented methodology allowed us to reflect the essential features of the copolymerization process. The simulation results obtained within the frame of the DLL model allowed us to predict the molecular weights of the synthesized products, and moreover, to get acquainted with the progress of the reaction regarding individual components.One of the methods of obtaining nanostructured materials is their formation from liquid or amorphous phases by controlled cooling or annealing. In this case, the main factor determining the final result is the rate of atomic diffusion. According to the hole theory of liquids [1] and the free volume theory [2,3,4], the diffusion of atoms in liquids and amorphous materials is determined by the volume distribution that is not occupied by atoms. In this regard, the determination of a relationship between the free volume distribution and the processes of nanostructuring in liquids and amorphous materials comes to the fore in obtaining nanostructured materials.

Currently, there are several methods for calculating the free volume. Some methods are based on the tessellation of the atomic configuration into Voronoi polyhedra, as a result of which it is possible to determine the volume per atom [5,6]. Another method for determining the free volume in the frame of the hole theory of fluids is presented by other authors [7]. However, in this method selection of boundaries of interatomic cavities is not determined, which leads in some cases to their unreasonable aggregation. The method proposed in this work makes it possible to avoid such agglomeration by selecting the condition for the existence of interatomic cavity boundaries.

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# ABS49

# Comparison of selected empirical potentials available for low-copper Al-Cu systems

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The presentation will start with an overview of a selected group of empirical potentials which are widely used for simulating of Al-Cu alloy systems. These potentials have been chosen due to their widespread and successful use in various MD simulations. After this introduction, requirements for validating these potentials will be presented. These criteria are focused on the ability of these potentials to correctly predict the formation mechanisms of Guiner-Preston zones and intermetallic precipitates in lowcopper Al-Cu alloys during a precipitation hardening process and how these structures influence the structural, mechanical and thermophysical properties of the alloy. In what follows, a set of computational methods will be outlined. These methods are used to compute each group of the said properties. These methods include, for example, a simulation scheme used for calculating the Gibbs free energy of intermetallic phases or an improvement of the two-phase "sandwich" method used in the estimation of the melting point of pure metals. Based on the results from these simulations, each potential will be categorized in terms of properties for which it predicts values comparable with the available data obtained via experimental and *ab initio* methods.

# Preparation, atomic structure and structure sensitive properties of AlCuZnSn medium entropy alloys reinforced with multi-walled carbon nanotubes

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It is known that carbon nanotubes (CNT) have been the strongest materials known to humankind to date. For this reason, as well as due to their superior thermal and electrical properties, a lot of attention has been paid to using carbon nanotubes as reinforcement for composite materials. The major challenge in the production of CNT-metal matrix (CNT-MM) composites is to disperse CNTs uniformly in a metal and alloy matrix. Recently, it has been found that traditional techniques such as the powder metallurgy process only cannot be used to prepare high quality metal matrix-CNT composites. Therefore, other methods for obtaining composites have been developed. Electroplating (EP) of CNT-MM composites is one of the most important techniques of preparing the CNT composite as no melting and solidification of the metal matrix are induced.

This work describes a technique for obtaining nanocomposites based on AlCuZnSn light-weight high-entropy alloys with carbon nanotubes by the combined methods of powder metallurgy and electroplating.

The morphology and structure of such composites were studied by the scanning electron microscopy and XRD methods. The electrical conductivity and microhardness of the obtained composites were studied.

It was shown that dispersed CNTs in a light-weight high-entropy alloy matrix can be uniformly obtained by means of the powder metallurgy and electroplating methods.

# ABS51

# Structure of macromolecular functional films

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A systematic theoretical study of the properties of thin polymer films is presented. Two- and three-dimensional homopolymer and copolymer chains were studied. Some chain sequences such as random copolymers, diblock and multiblock copolymers (consisting of solvophilic and solvophobic blocks) were designed. Different macromolecular architectures were studied: linear, star-branched and cyclic. No atomic details were taken into consideration, and thus, polymer chains were modeled as sequences of statistical segments on square, cubic, triangular lattices. The adsorption of macromolecules on a homogenous flat surface was studied at different solvent conditions [1]. The following Monte Carlo simulation techniques were employed in order to determine the properties of these polymer systems: the Random Sequential Adsorption, the Metropolis scheme, the Replica Exchange scheme, the Dynamic Lattice Liquid and the Cooperative Motion Algorithm [2]. The main question was how the chain sequence, the internal architecture, the strength of the adsorption and the solvent quality influenced the structure of the macromolecular film [3]. The size and shape of chains, their ordering, mutual interpenetration were shown and discussed. The self-assembly in these polymer systems was attributed to a competition between the architecture constraints and the minimization of the polymer-solvent interface. The percolation conditions in polymer films were also presented.

### Acknowledgements

The computational part of this work was done using the computer cluster at the Computing Center of the Faculty of Chemistry, the University of Warsaw. This work was supported by Grant UMO-2017/25/B/ST5/01970 of the Polish National Science Center

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# Strategy locomotion of metastatic cancer cells: Is it a Lévy-like movement?

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Large-scale statistics has been used to describe various types of cells migrating on linear microtracks. The study reveals that metastatic cancer cells follow a different motility strategy than their non-invasive counterparts [1]. In particular, the trajectories of metastatic cells are composed of sequences of many short steps interspersed with longer ”flights”. Such motions are consistent with the so-called Lévy walks which are characterized by heavy-tailed, truncated power-law distributions of persistence times. Regarding non-metastatic cancerous cells, their motion is characterized by a purely diffusive nature [1]. A simple model that could ascribe these walks by the synchronization of the cell's "front" protrusion and "back" retraction has been proposed, although these assumptions need further study and experimental validation.

### Acknowledgements

This work was partially supported by the National Science Centre (Poland) under the grant 2017/27/B/ST3/02955. Part of the computations was performed at the Poznań Supercomputing and Networking Center (PCSS)

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# Structural evolution of Fe local neighborhood in working nitrogen-modified carbon-based fuel cell catalysts: XAFS analysis

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Direct Hydrogen Fuel Cells (DHFCs) represent one of the most promising alternatives for the development of low temperature power devices. However, one of the most severe limitations to a large-scale application of this technology is the high cost of both polymeric membranes and catalytic electrode materials, commonly requiring such noble metals as Pt. In this context, non- precious metal catalysts are actively sought, e.g., to meet the already established operational benchmarks for conventional platinum low temperature FC vehicular requirements, with the additional benefit of a significant cost reduction and increased stability. It is nitrogen-modified carbons containing non-precious transition metals that which are considered interesting and very promising among the various materials [1, 2]. This work is dedicated to nitrogen-modified carbon materials containing Fe centers (about 1-2 wt.%) prepared by high-temperature pyrolysis in an N2 atmosphere of a gel formed by organic precursors of C (fructose or glucose), N (guanidine acetate) and Fe (Fe(II) acetate) [3]. The materials (the so called Fe-FAG and Fe-GAG, respectively) used as electrocatalysts for oxygen reduction in DHFCs were subjected to three types of 50-hour catalysts durability tests: 1) a steady state FC working condition under 0.8V (ss0.8V); 2) a steady state FC working condition under 0.4V (ss0.4V) and 3) accelerated stress testing (AST [4]) by the FC load cycling from 0.4V to 0.6V (square wave potential cycling, sw0.4-0.6V). Then the evolution of the local structure (coordination number, geometry, oxidation

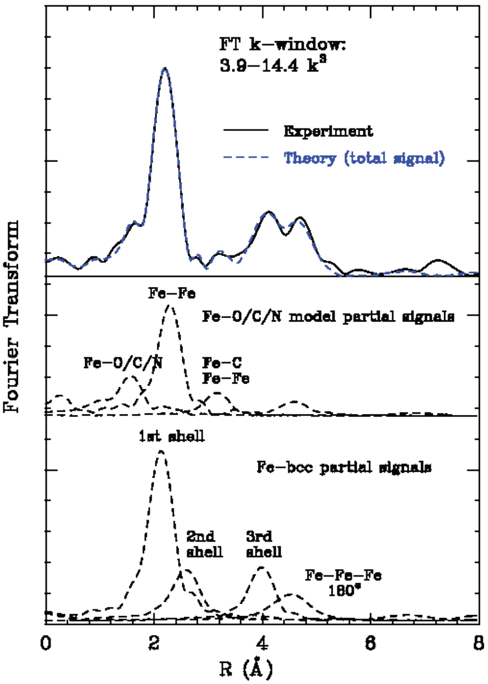

Figure 1: Fourier Transforms of EXAFS experimental signal and theoretical structural model components used in the Fe K-edge spectra analysis of Fe-FAG fresh electrode

state) of Fe ions was studied and the results were combined with the elecrochemical cell performance by means of the advanced X-ray spectroscopy technique (XAFS - X-ray Absorption Fine Structure).

Fe K-edge XAFS spectra in both near-edge (XANES) and extended (EXAFS) ranges were recorded at the ELETTRA 11.1 XAFS station using a double-crystal monochromator equipped with a Si(111) crystal. All the XAFS measurements were taken ex situ at room temperature using transmission geometry. The EXAFS data were analyzed within the framework of the GNXAS method [5,6] using advanced multiple-scattering simulations. The comparison of the XANES spectra with the reference data (Fe-bcc foil, $Fe_3C$, $Fe_2O_3$ and other Fe compounds) showed that the local neighborhood of Fe could consist of atoms forming the Fe metallic phase and of lighter atoms, such as oxygen, nitrogen and possibly even carbon. Thus, proper models were constructed and used to calculate theoretical EXAFS signals. The total signal was composed of the following partial signals: the Fe-bcc model – two-body signals of the three nearest shells and one three-body contribution (configuration with the vertex angle of 180°); the Fe-O/C/N model – two-body signals of the three nearest shells (see Fig. 1).

The results show subtle structural differences at the atomic level between pristine catalysts which depend on the carbon precursor used (e.g. slightly larger metallic Fe nanoclusters and a more ordered Fe-O/N/C phase are formed in in pristine Fe-FAG and then in pristine Fe-GAG, respectively). These differences can be used to explain the different initial electrochemical activity (higher in Fe-GAG) and the different stability of catalysts (higher in Fe-FAG). Regardless of this, both catalysts are more stable and efficient in the steady state FC operation. Moreover, the Fe structure on the atomic level and the electrochemical performance of the FC are closely correlated (this correlation is also independent of the type of the organic precursor of carbon). In both catalysts, Fe-FAG and Fe-GAG, the main changes relate to the Fe metallic phase. The Fe-O/N/C bonds are definitely less influenced by the operating conditions of the fuel cell. The more degraded (a smaller Fe-Fe coordination number and a larger bond length = smaller particle size, probably as an effect of dissolution of Fe particles) the metallic phase is, the largest the loss in the relative current density is observed.

Summarizing, a compromise between the average size of the Fe metallic cluster and the structural ordering in a Fe-O/N/C phase must be found on the catalyst preparation stage to obtain the desired catalyst properties.

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# Extreme Poisson's ratios in some planar systems

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Poisson's ratio (PR) [1] of planar isotropic systems can vary within the range of –1 and +1 [2]. Materials with negative PR values [3-6] are called auxetics [7]. They expand (contract) transversally when stretched (compressed) longitudinally [8-10]. This is an opposite behaviour compared to common materials, like rubber, which expand (contract) transversally when compressed (stretched) longitudinally. It is worth stressing that rubber which exhibits Poisson's ratio very close to the largest positive value possible for isotropic systems, preserves its volume when deformed, at least at small deformations. This is in contrast to perfect auxetics which preserve their shape [11]. In this lecture some simple models, studied recently by analytic methods [11] and computer simulations [12], will be reviewed in the context of extreme values of Poisson's ratio.

## Acknowledgements

This work was partially supported by the National Science Centre (Poland) under the grant 2017/27/B/ST3/02955. Part of the computations was performed at the Poznań Supercomputing and Networking Center (PCSS)

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# ABS55

# The process of drying a droplet of an aqueous suspension of iron oxide magnetic nanoparticles in an alternating magnetic field

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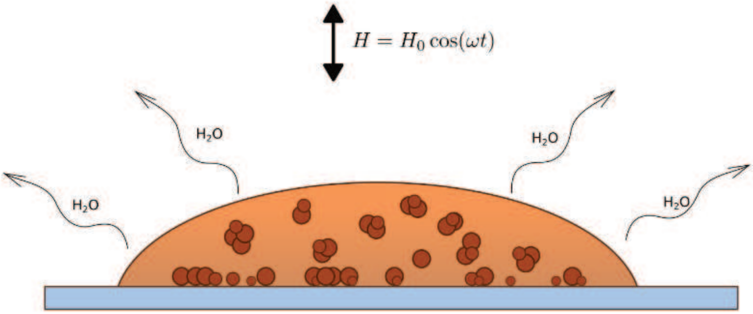
The drying process of a droplet of an aqueous suspension of single-domain iron oxide nanoparticles in an alternating magnetic field was analyzed using the experiment and computer simulation methods.

Single-domain nanoparticles have the unique property of absorbing the energy of an alternating magnetic field which is transferred as heat to their surroundings. The dependence of the temperature increase rate was determined for such a drying droplet. A method of determining the moment of time when the droplet dries up has been developed.



# A hysteresis loop and superferromagnetic state in reduced graphene oxide flakes

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The DC magnetisation of a series of titania nanocomposites modified with a reduced graphene oxide (rGO) was investigated. The hysteresis loops observed at room temperature disappeared at low temperatures. At a temperature of approx. 100 K, a phase transition to the superferromagnetic order state was observed, probably due to the linear expansion and self-reorientation of the magnetic moments. Processes associated with magnetic moment reorientation can cause a hysteresis loop to disappear at low temperatures as well as superferromagnetic ordering. It was suggested that an isolated nanoparticle in the nanopore could be used to create a compass at a nanometer-sized level that would be many times more sensitive than conventional. Measurements of the ZFC and FC modes do not exclude the possibility of the coexistence of a superparamagnetic state.

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