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and Nanostructured Materials

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Place: Planet Earth, Solar System, Milky Way, Local Galaxy Group

ABSTRACT BOOK

TITLE

The 19th Conference on Functional and Nanostructured Materials - FNMA 2024

ABSTRACT BOOK

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Intermolecular Interactions in Aqueous Solutions of 2-Aminopyrimidine and Its Tautomers

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2-Aminopyrimidine is an organic compound which is a key building block in medicinal chemistry and pharmaceutical development. This compound can participate in a variety of chemical reactions because it consists of a pyrimidine ring with an amino group attached at the second position. 2-Aminopyrimidine is widely used in the synthesis of pharmaceuticals, agrochemicals and dyes. It is particularly valuable in the development of antiviral, antibacterial and anti-cancer agents due to its ability to interact with biological targets such as enzymes and receptors. In addition, 2-aminopyrimidine derivatives are often found in the structure of several drugs, including some that treat cardiovascular disease, inflammatory conditions and neurological disorders. Its versatility and reactivity make it an important tool in the development of new therapeutic agents [1].

In this work we have studied the 2-aminopyrimidine molecule and its complexes with water by means of Density Functional Theory (DFT) with ωB97XD method. We have checked the stability of the complexes and calculated the Raman and UV-Vis spectra. Additionally, the complexes of tautomers were analysed. Results were confronted with available experimental studies [2].

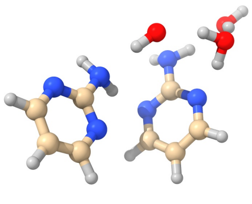

Figure 1: The complex of two 2-Aminopyrimidine and three water molecules

Acknowledgement

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Enhancing Catalytic Activity of the SOECs for the Electroreduction of CO_2-H_2O via the Modification of the Electrodes with Various Promoter Metals

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Recently, Solid Oxide Electrolysis Cells (SOECs) can be considered a solution for the elimination of atmospheric CO_2 and limiting its negative environmental impact. Thanks to high operation temperatures, full-solid construction and high Faradaic efficiency it is a promising method for production of great amounts of relatively cheap and pure hydrogen. Furthermore, the ceramic cells can be set to perform CO_2 electroreduction along with water vapor. Thanks to that, it is possible to simultaneously supply further chemical processes with H_2-CO feedstock using one setup. In that sense the SOECs can provide "green" hydrogen and reduce the CO_2 amount by delivering valuables such as syngas or other chemicals. Recently, high temperature H_2O/CO_2 co-electrolysis in SOECs became a reasonable alternative to other technologies of syngas production such as steam reforming of biogas or coal gasification, which both release huge amount of greenhouse gases.

The main constituent of the water-hydrogen electrode is a bifunctional composite of NiO and $Zr_{0.84}Y_{0.16}O_{2-\delta}$, which upon reduction forms metallic network of Ni within the scaffold of the ionic conductor. This type of electrode is quite well established for working with water vapor in electrolysis mode but struggles under the atmosphere containing CO/CO_2. The Ni grains are an active material for RWGS and electrochemical splitting, but not the most efficient for performing those reactions. Over the years other transition metals - Cu, Fe, or Co - as well as their oxides - MnO, ZnO - were found to be more prominent and used in catalytic reactors. Further increase of the activity and efficiency can be achieved thanks to promoter metals and their oxides *e.g.*, K_2O, Na_2O, Rb_2O, MgO, CaO. The addition of the transition metals can be a promising alternative to the usage of the noble metals considering mostly their much lower price. On the other hand, the addition of alkaline metal oxides can increase the adsorption rate of the CO_2 and prolong the retention time in the proximity of the electrode. As the SOECs are generally non-pressurized systems, the efficiency of the electrode surface catalysts should be pushed to maximum in order to provide valuable outlet gases.

A series of modified SOECs was prepared by the addition of 5 mol. % of the transition metal (Co, Cu, Mn, Fe) or alkaline metal oxide (Na, K, Ca, Mg, Rb, Li, Sr) nanoparticles. The samples have been fabricated by simple wet impregnation method. The SOECs were tested for the coelectrolysis of CO_2/H_2O mixture with addition of H_2 for electrode protection against the reoxidation. The electrical tests were considering the utilization factor of the water vapor and the electrochemical behavior of the cells under various CO_2:H_2:H_2O ratios to better understand the mechanisms of the syngas formation.

It was found out that depending on the reducibility of the metals they were dissolved in Ni grains (*e.g.*, Co, Fe) or formed a secondary phase on the top of the grains (*e.g.* MnO). It was observed as an accumulation of the metal ions inside Ni-rich grains or dissipation of the ions all over the imaging area seen in the STXM imaging. The alkaline metal oxides formed a mixture of the phases on the Ni and the YSZ grains. A series of *in-situ* XAS measurements at ESRF (France) was performed to observe the formation of various mixed compounds and the response of the electrode components to CO_2-rich atmosphere at high temperature. The surficial changes of the oxidation states were determined using in-situ XPS imaging of modified electrode structure using SPEM at Elettra (Italy). The addition of the secondary metal alters the energy levels on the Ni surface and increases the tendency to form carbonates, what prolongs the retention time of CO_2. The addition of guest metal highly increased the CO_2 conversion and selectivity towards CO production as well as the electrical efficiency due to the alterations of basic-acid sites and introduction of active redox couples.

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Methods to Improve the Stability of Biogas-Fed Solid Oxide Fuel Cells – Our Different Material Approaches

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The commercially used Solid Oxide Fuel Cell (SOFC) with Ni-YSZ anode suffer from carbon deposition and sulfur poisoning during the internal reforming of biogas fuel. Therefore some alternative solutions can be applied to improve the stability and the performance of this device.

One of the possibilities is to use the ceria-based catalytic layers deposited on the anode side. They present high mobility of oxygen ions, high oxygen storage capacity (OSC), attractive redox catalytic properties and chemical compatibility with water and carbon dioxide at high temperatures. Moreover, the high oxygen mobility in ceria promotes the mechanism of carbon removal, which in turn should contribute to the stability of the catalysts in hydrocarbon conversion reactions.

Another method is to exsolve metallic nanoparticles from the perovskite lattice of an anode candidate material. These nanoparticles can act as catalytic centers for the process of electrochemical oxidation of a fuel as well as for the internal reforming reactions. The exsolution process occurs under reducing conditions and offers an even distribution of particles as well as very well attachment to the host material. When bimetallic or even ternary alloys are formed, the properties of the materials can be even further improved. As compared to the monometallic Ni nanoparticles, the Fe-Ni alloy nanoparticles exhibit higher activity, greatly improved durability over long-term testing and increased tolerance towards sulfur-based atmospheres [1]. Simultaneously, these bimetallic alloys demonstrate outstanding microstructural stability and high tolerance towards coking, similar to that presented by monometallic Ni nanoparticles [2].

The aim of this presentation is to show materials synthesized and characterized for SOFC anode application within various scientific projects of our team. Compounds from the ceria group as well strontium titanate-based ones will be presented. Both achievements and obstacles in understanding their anode activity will be discussed.

Acknowledgement

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ABS4

Novel Calixarene-Based Polymers With Potential Auxetic Properties

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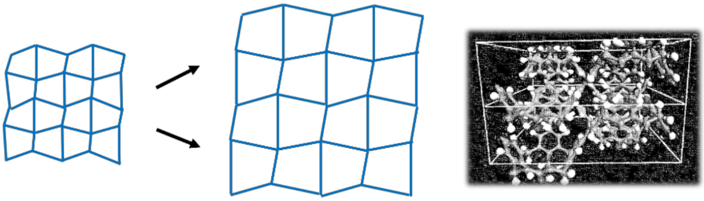
The creation of an intrinsically auxetic synthetic material has long been a challenge in auxetics research, where the goal is to achieve chemical tunability and broaden potential applications. So far, a limited selection of polymers exhibit a negative Poisson's ratio, under specific conditions. Other molecular frameworks, have been proposed as auxetic via simulations but were ultimately deemed too complex to synthesize. This study focuses on designing a feasible, synthesize-able model. This work explores the design principles behind this polymer, along with the steps towards obtaining the synthesized material.



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Thermoelectric Properties of Multicomponent Oxides

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Multicomponent oxides (MCOs) have unique characteristics such as remarkable thermal stability, tunable electrical properties, and a wide range of chemical compositions, making them particularly promising for thermoelectric device applications. To create MCOs with exact compositions and microstructures, several synthesis processes are used, including solid-state reactions and the sol-gel approach. The Seebeck effect is then tested across a wide temperature range to determine MCO thermoelectric performance. The study of the influence of composition, crystal structure, and microstructure on the Seebeck coefficient is a new area of research that will shed information on the underlying thermoelectric mechanisms in multicomponent MCOs. These oxides, distinguished by their complicated and disordered crystal structures caused by the presence of numerous cations, offer new possibilities for modifying thermoelectric performance [1-3].

This research focuses on assessing the thermoelectric and electrochemical properties of chosen multicomponent oxides based on the perovskite ABO_3 structure, with barium in the A-site and several elements – Fe, Zr, Hf, Sn, Ti, Ce, Co, In, Sm, Y, and/or Yb – in the B-site. The structure and microstructure of these materials were investigated using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The temperature dependency of the total Seebeck coefficient was obtained using the 4-wire approach in a variety of water-vapor-containing environments. Electrical tests on total electrical conductivity were performed using 4W-DC and EIS techniques, which varied with pO_2 and pH_2O. A key aspect of this research was studying MCO transport properties in the presence of protonic defects, which could considerably improve thermoelectric effects.

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Structural and Electrical Properties of Ru- and Pt-Doped Strontium Titanate Materials for Catalytic Applications

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Methane reforming, both dry and wet, is discussed as a viable method for producing hydrogen from biogas mixtures, aligning the growing hydrogen industry with environmentally sustainable solutions. Since reforming processes are catalyst-dependent, there is a strong impetus to explore novel catalytic materials. The ex-solution process has garnered significant attention for its potential to yield reliable catalysts for this application [1, 2].

In this study, perovskites with the composition $(\mathrm{La}_{0.3}\mathrm{Sr}_{0.7})_{0.9}\mathrm{Ti}_{1-x}\mathrm{M}_x\mathrm{O}_{3-\delta}$ were synthesized, with platinum and ruthenium as dopants. Doping levels of $x = 0$, 0.01, 0.02, and 0.05 were employed. The synthesis process was based on a modified Pechini method, designed to optimize material porosity and uniformity. Precursors were combined with citric acid and ethylene glycol, and the mixture was heated to 130°C. The resulting organic and powder mixture was then calcined at 1250°C for 12 hours. The properties of these materials were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and temperature-programmed reduction/oxidation (TPx).

The synthesized perovskites were evaluated for their potential as catalysts in dry and wet methane reforming. Electrical properties were measured using the direct current 4-point method.

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ABS7

Optimizing $La_{0.3}Sr_{1.7}Fe_{1.5}Mo_{0.5}O_6$ Double Perovskite in Solid Oxide Fuel Cells: The Role of Transition Metal Doping

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The increase in environmental awareness has led to a significant worldwide trend for the development of alternative energy sources other than the conventional use of fossil fuels. One of the alternatives is the use of Solid Oxide Fuel Cells (SOFCs), which are capable of converting the chemical energy of the fuel (mostly hydrogen) into electricity. In SOFCs, the dense electrolyte is covered with two porous electrodes. So far, the most widely used anode (fuel electrode) material is the Ni-YSZ composite, which degrades significantly under fuels other than hydrogen. Thus, the development of a substation for Ni cermet is desirable. Among many materials, one may find perovskite families, which are known for their high stability and ionic conductivity. Unfortunately, their catalytic performance is rather low and needs to be increased. This can be performed by introducing catalytically active materials as dopants and force them to form nanoparticles in the exsolution phenomenon. The main advantages of exsolving nanoparticles, rather than their deposition, are better connection with the surface and lower tendency for agglomeration.

Perovskites may be divided into several sub-groups and one of them are double perovskites with general formula $A_2BB'O_6$. Strontium ferrite molybdate (SFM – $Sr_2Fe_{1.5}Mo_{0.5}O_6$) is one of the most prominent compounds in this family. It is well known for its high ionic and electronic conductivity as well as stability in both reducing and oxidizing atmospheres. Those properties make it a promising material for not only the anode, but also a cathode, hence SFM-based compounds can be considered prominent candidates for symmetrical fuel cells. On the other hand, our previous work has shown that, in highly reducing atmospheres, this double perovskite can partially transform into the Ruddlesden-Popper layered perovskite. This transition could increase the amount of exsolved nanoparticles due to internal strain.

Herein, the SFM-based compounds were co-doped with La at Sr-site and one of transition metals (Co or Ni, with doping level 5-20 mol. %) giving the composition $La_{0.3}Sr_{1.7}Fe_{1.5-0.75x}Mo_{0.5-0.25x}O_6$. The fixed Fe:Mo ratio was maintained to prevent formation of either Fe-, or Mo-rich phases. Based on our previous studies, La-doping was found to suppress the phase transition and to simultaneously increase the electrical conductivity. Transition metals were incorporated during the synthesis to boost the catalytic performance of the compound. After the reduction at 800°C in hydrogen, the surface of the grains was almost fully covered with nanoparticles of one metal

(Co or Ni) or bimetallic alloys with co-exsolved iron. Even the small amount (10 mol. %) of introduced transition metal resulted in enormous amount of nanoparticles. The electrical conductivity measurements were performed in both air and hydrogen. It was found that the conduction mechanism is different in both atmospheres: in the air, the conduction occurs by the polaron hopping mechanism through Fe/Mo-O-Fe/Mo bonds. To better understand how the $Fe^{3+/4+}$-$Mo^{5+/6+}$ redox pairs are influenced by transition doping, the XPS technique was used for as-synthesized and reduced compounds. After the reduction, both iron and transition metals were present also in M^0 form, hence the amount of Mo^{6+} cations increased. Lastly, TPR/TPO measurements were performed to understand the reducibility of the compounds and to have a better understanding of the formation of exsolved nanoparticles.

Acknowledgement

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Controllable Dynamic Properties of Magneto-Mechanical Metamaterials

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Over the years, it has been possible to observe numerous studies devoted to the design of mechanical metamaterials capable of exhibiting unusual static mechanical properties such as negative Poisson's ratio (auxetic behavior) or negative stiffness. These studies have been of great practical importance as they were implemented in numerous applications ranging from biomedical to protective devices. However, despite the various advantages that such metamaterials have to offer, they often share one limitation. Namely, once they are fabricated, it is very difficult to significantly change their properties without reconstructing the system. The answer to this problem turned out to be active mechanical metamaterials, *i.e.* composite systems that can be remotely controlled via changes in the external stimuli such as the temperature, light or magnetic field. In recent studies, it has been shown that through changes in the magnetic field, it is possible to observe a significant change in the static mechanical properties of the system. More specifically, in one of such studies [1], it was shown that based on the change in the external magnetic field, a magneto-mechanical system may undergo a transition from the configuration characterized by the positive Poisson's ratio to the highly auxetic configuration and vice versa. However, the same could not be done in terms of the dynamic properties of the system.

In view of the above, in this study [2], a new magneto-mechanical metamaterial was proposed that allows concurrent control over the static and dynamic mechanical properties of the system based solely on the changes in the external magnetic field. Similarly to previous studies, the considered metamaterial can exhibit very different Poisson's ratio depending on the externally induced reconfiguration. However, what makes this work particularly interesting, is that in addition to the control over the Poisson's ratio, the active reconfiguration leads to significant changes in the phononic band structure of the system. This, in turn, makes it possible to fine-tune the wave propagation through the system based solely on the changes in the external magnetic field.

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The Influence of Local Constraints on the Motion of Solvent in Polymer Systems

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The effect of polymer chain obstacles on the diffusion of a low molecular weight solvent was studied by computer experiment. The materials tested were polymer networks with an ideal structure, the so-called constant mesh size. In addition, real networks obtained numerically in the copolymerization process were studied, *i.e.* the mesh size of the polymer network was not constant – the lattice had an irregular structure.

The aim of the study was to understand the effect of the polymer matrix structure, polymer concentration and macromolecular architecture on the mobility and nature of solvent movement.

The research was carried out using computer simulations with Monte Carlo method – the Dynamic Lattice Liquid algorithm [1] – based on the idea of cooperative movements.

The used polymer concentration was well below the percolation threshold [2]. Still, the movement of small solvent molecules was restricted in short and medium time scales, and sub-diffusive behaviour was observed [3]. Dynamic properties of solvent, like MSD, autocorrelation functions and diffusion coefficients were analyzed.

Acknowledgement

This work was supported by the Polish National Science Centre grant UMO-2017/25/B/ST5/01110 and has been completed while the first author was the Doctoral Candidate in the Interdisciplinary Doctoral School at the Lodz University of Technology, Poland. Simulation results were obtained on ARUZ (Analyzer of Real Complex Systems) - a massive FPGA cluster located in Bionanopark, Lodz, Poland.

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Magneto-mechanical metamaterials

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Over the years, researchers have explored active metamaterials due to their controllable geometry and mechanical properties. However, systematic design of these structures in a reproducible and scalable manner has remained a challenge despite their industrial significance. This study addresses this gap by harnessing foldable magneto-mechanical metamaterials controlled via external magnetic fields. Two configurations of the system are presented: one constrained to function like a linear actuator, and another allowing full control of expandability and mechanical properties in all directions. The potential to stack these structures to create large systems with potential auxetic properties in multiple planes is also explored. These metamaterials offer untethered, multi-directional, finely controlled movement, making them promising for applications in actuators, vibration dampers, deployable scaffolds, and impact-resistant materials. Their mechanical properties can be tuned by adjusting the external magnetic field and structural configuration.

To further understand and optimize these materials, the concept of a magnetorheological elastomer (MRE) reinforced with superparamagnetic iron nanoparticles was investigated through a combination of numerical simulations and experimental validation. A W-shaped MRE structure was analyzed under varying magnetic field strengths, examining how geometric parameters influence magnetic forces and contraction dynamics. Experimental results closely matched simulations, with the highest iron nanoparticle concentration (MRE50) achieving over 50% contraction, showcasing the material's potential for dynamic, adaptive applications.

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Protective Gear for Coastal Rowing: Meeting Athletes' Expectations Through the Use of Advanced Materials

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Competitive sports has the overall aim to identify the "winning" participants who need to outperform others in competition. This requires athletes to develop and excel from several aspects including skills, technique, agility, strength and endurance. In addition to this, all athletes and their managers are on the constant search for new equipment, tools and materials which enable athletes perform better, or do so in a safer manner.

As a result, the last decades have seen extensive research being focussed on developing sports equipment, including gear which is used by athletes for added safety and protection. Different sports disciplines may necessitate different types of such protective gear and equipment, and it is essential that that scientists and engineers work together with the sports community to fully understand the needs from a sports perspective, and, match these needs with R&I efforts to provide such gear which permits the athlete to practice the sport safely and without much hindrance.

The last decade has seen the birth of a new sports discipline, Coastal Rowing Beach Sprints, which will become a new Olympic Discipline as for the 2028 Los Angeles Olympic Games. This is generally considered as the "wild cousin" of classic rowing which requires athletes to row on rather challenging and choppy waters. As this is a very young discipline, athletes and the World Rowing governing body are still in the process of learning, sometimes though trial and error, how best to strike a balance between providing the trill and doing so safely.

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This work examines the issue of athlete safety in coastal rowing from the perspective of how equipment and materials used can be optimised for reducing risk to athletes. More specifically, it assesses athletes' perceptions of risks and safety in coastal rowing training and competitions, as well as their perception of the use of protective gear in such sport. With the feedback collected, particularly their perceived negative aspects of using protective gear despite knowing that such a gear would provide them with added safety, we examine whether auxetics could help to provide a new generation of sports protective gear, particularly for use in new sports such as coastal rowing.

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Features and Characterization of Selected Organic Electronics Devices

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Intensive research into new semiconductors has contributed to the development of organic electronics [1]. Electronic circuits can be cheaply fabricated on a large scale by solution techniques using jet printers or by coating devices on the surface of flexible films rolled on drums (roll-to-roll) [2]. The devices produced are lightweight and thin, making it possible to build flexible displays, large area solar cells and other functional devices. Basic electronic circuit components include organic light-emitting diodes (OLEDs), organic thin film transistors (OTFTs), organic photovoltaic cells (OSCs) and organic photodiodes (OPDs).

The construction, operating principle and characterization methods of OLEDs, OTFTs, OSCs and OPDs will be discussed [3]. Selected organic devices will also be presented, such as a nonlinear resistor (electron-only device) [4], a printed flexible logic gate with an OTFT transistor and an organic resistor [5], an OLED subjected to AC tests [6], and a transoptor with an OLED-OPD pair.

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ABS13

High Entropy Cobaltites:
Structure and Electrical Properties

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$BaLnCo_2O_{6-\delta}$ cobaltites (Ln - a lanthanide) are a group of mixed conductors with high total electronic conductivity, partial oxygen ionic conductivity and, in some cases, protonic conductivity. Such mixed ionic-electronic conductors are often applied in the hydrogen technology sector as electrodes for proton ceramic fuel cells and electrolysers [1, 2]. Implementation multiple lanthanides in equimolar proportions into the Ln sublattice can lead these materials to be the so-called high-entropy oxides (HEO), where the presence of profound configurational disorder, originating from multiple elements sharing a single lattice site, can result in new properties [3, 4].

This work is focused on materials with general formula $Ba(Ln_{1/x}Ln'_{1/x}Ln''_{1/x}Ln3'_{1/x} \ldots Lnx'_{1/x})Co_2O_{6-\delta}$ $(8 \leq x \leq 14)$, where Ln, Ln$'$, Ln$''$ and so on are various lanthanides. In such a way were created materials with 8, 10, 12 and up to even 14 different lanthanides occupying the same lattice site. X-ray diffraction (XRD) with Rietveld refinement and Scanning Electron Microscopy (SEM) were used to characterise structural properties. Thermogravimetric analysis (TGA) was used to introduce oxidation and hydration studies. Electrical properties were investigated by the means of DC-4W technique and Seebeck coefficient measurements were performed by the 4W method both in dry and wet air.

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Spectroscopy of the Lithium Tetraborate Glass Co-doped with Cu and Sm

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The lithium tetraborate glass co-doped with CuO (1 mol. %) and Sm_2O_3 (1 mol. %) ($Li_2B_4O_7$:Cu,Sm) was obtained by melt quenching method and characterised by XRD, EPR, optical absorption and photoluminescence (emission, excitation, decay kinetics) techniques [1]. The obtained results have been compared with corresponding data for Sm-doped and Cu-doped $Li_2B_4O_7$ glasses, obtained by us earlier.

The smooth XRD curve was registered and analysed to obtain the local structure details. It was found that the BO_n ($n = 3 - 4$) and LiO_n ($n = 4 - 6$) units dominate in the network of $Li_2B_4O_7$:Cu,Sm glass. The EPR spectrum of the investigated glass reveals an axially-symmetric signal of Cu^{2+} ($3d^9$) ions with a characteristic hyperfine structure caused by the ^{63}Cu and ^{65}Cu isotopes. The optical absorption spectrum shows a broad intense band attributed to Cu^{2+} ions and several weaker narrow bands attributed to Sm^{3+} ($4f^5$) ions.

The photoluminescence emission spectra show a broad band in the blue spectral range assigned to the $3d^9 4s^1 \to 3d^{10}$ transition of Cu^+ ($3d^{10}$) ions and four narrow bands in the yellow-red spectral range assigned to the $^4G_{5/2} \to ^6H_J$ ($J = 5/2 - 11/2$) transitions of Sm^{3+} ions. The photoluminescence excitation spectra show a broad band in the UV spectral range belonging to Cu^+ ions and many narrow bands in the violet-green spectral range belonging to Sm^{3+} ions. The photoluminescence decay kinetics of Sm^{3+} and Cu^+ ions in the $Li_2B_4O_7$:Cu,Sm glass are non-single exponential and characterised by a mean lifetime in the ms and μs time ranges, respectively.

The observed changes in photoluminescence intensity, shortening of the Sm^{3+} lifetime and prolongation of the Cu^+ lifetime are explained by energy transfer and re-absorption processes between Sm^{3+} ions and copper (Cu^+, Cu^{2+}) ions. A wide range of emission colours from blue to yellow is achieved in the $Li_2B_4O_7$:Cu,Sm glass by varying of the excitation wavelength.

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Use of the Exolution Phenomenon to Create Metallic Particles on the Surface of Doped Strontium Titanate Grains as an Anode in Solid Oxide Fuel Cells

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Fuel cells are exceptionally functional devices that convert the chemical energy of fuel and oxidizer directly into electrical energy in an environmentally friendly manner (low, controlled emission of pollutants, silent operation, high durability of construction materials). Among fuel cells one can distinguish Solid Oxide Fuel Cell (SOFC) that operates very efficiently at medium and high temperatures.

The aim of this work is to fabricate metallic particles on the surface of grains of doped strontium titanate ($(\mathrm{La,Ce,Sr})_{0.9}\mathrm{Me}_{0.1}\mathrm{Ti}_{0.9}\mathrm{O}_{3-\delta}$, where Me = Ni, Co. The formation of particles should occur via phenomenon of metal exsolution from the lattice of oxide material when placed in reducing conditions, identical to the operating conditions of the anode in SOFCs. Using the solid-phase synthesis method, a number of compounds were produced, in which the possibility of the exsolution of metal nanoparticles directly from the lattice of oxide material was examined, as well as using the so-called exsolution with topotactic ion exchange after sputtering metallic iron oxide onto material and reduction in H_2 at temperatures of 900°C and 1000°C. Before reduction, the XRD analysis of compounds was performed as well as Rietveld refinement to determine the structure of the synthesized materials. The morphology of nanoparticles formed in the exsolution process as well as chemical composition and stoichiometry was observed with SEM/EDS device. Characterisation of a working cell consisting of an LSCF cathode, YSZ electrolyte, and Ni-YSZ anode with addition of LSCNiT layer sputtered with metal iron was performed. The cells were tested in the Fiaxell Open Flange system while fed with hydrogen fuel on the anode side and synthetic air on the cathode side. First, the cell was heated up to 900°C in an argon atmosphere on the anode side. Then the gas was switched to hydrogen and reduction was carried out for 10 h to force exsolution with topotactic ion exchange. The cell was then cooled at 800, 750, 700, 650, 850°C and the open circuit voltage OCV was measured, the current-voltage characteristics were performed and tests were carried out using impedance spectroscopy.

It was found that the least contaminated compound is LSCNiCoT, in which the composition of strontium titanate was equal to 99.9%, while the amount of additional phases was the greatest for the LSCT reference sample. On this basis, it was concluded that the addition of elements to the LSCT compound improves its structural stability. Examination of the surface morphology of all compounds using SEM showed a significant effect of temperature on the size of particles formed during the exsolution process. The results of EDS analysis allowed to conclude that it is possible to form Ni-Fe, Co-Fe and Ni-Co alloys. The analysis of an oxide cell with an additional LSCNiT+Fe layer while operating at various temperatures showed that the cell operating at a higher temperature, which is 850°C, has the highest power density, the best stability during operation and the lowest losses caused by ohmic and polarization resistance.

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Pyrochlore Thermoelectric Materials, Based on Oxide/Xxide and Oxide/Metal Alloy Composition

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Pyrochlore oxides are widely known for their dielectric properties due to their large band gap. In the thermoelectric aspect they show a low thermal and electrical conductivity and high Seebeck coefficient of mV/K order [1]. However, the figure of merit ZT for standalone pyrochlore oxides is low and not suited for thermoelectric applications.

In recent years, multicomponent compounds have been under intense investigations in a wide range of materials due to massive changes of properties in some cases. One of the important changes is reduction of lattice thermal conductivity in materials mostly thanks to increase of phonon scattering [2].

In this study two pyrochlore oxides were combined with respected compounds to enhance thermoelectric properties. The first composite is based on $SrBi_2Ti_2O_7/La_{0.7}Sr_{0.3}CoO_3$ and second is based on multicomponent pyrochlore (MEP) oxide $(Zr_{0.2}Sn_{0.2}Ti_{0.2}Hf_{0.2}Fe_{0.2})(Sr_{0.25}La_{0.75})O_7$ and metal alloy (FeCu).

The X-ray Diffractometry (XRD) and Scanning Electron Microscopy (SEM) were used to study the structure and microstructure of the materials. The temperature dependence of the total Seebeck coefficient was measured and analyzed. For electrical conductivity measurements, dependent on temperature, a DC four-wire technique was used. Measurements of Seebeck coefficient and electrical conductivity were held in two different atmospheric conditions, with high and low concentration of water vapor during the experiment.

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Numerical Modeling of Ferromagnetic Resonance

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A method of computer simulation of ferromagnetic resonance using the stochastic Landau-Lifshitz-Gilbert equation for magnetic nanoparticle magnetization is presented in the following form [1]:

$$\frac{\mathrm{d}\vec{M}}{\mathrm{dt}} = \frac{-|\gamma|}{1+\alpha}\left[\left(\vec{M}\times\vec{H}^{\mathrm{eff}}\right)+\frac{\gamma}{M_s}\left(\vec{M}\times(\vec{M}\times\vec{H}^{\mathrm{eff}})\right)\right],$$

where $\gamma = 1.76\times10^{11}$ s^{-1} T^{-1} denotes the gyromagnetic ratio, and

$$\vec{H}^{\mathrm{eff}} = \vec{H}_{\mathrm{DC}}+\vec{H}_{\mathrm{AC}}+\vec{H}_{\mathrm{anis}}+\vec{H}_{\mathrm{dipole}}+\vec{H}_{\mathrm{thermal}},$$

$\vec{H}_{\mathrm{DC}}$ is the external static DC magnetic field, $\vec{H}_{\mathrm{AC}}$ is the external AC magnetic field, $\vec{H}_{\mathrm{anis}}$ represents the magnetic anisotropy field, $\vec{H}_{\mathrm{dipole}}$ is the resultant dipolar magnetic field applied to magnetic nanoparticle. The operation of the algorithm will be demonstrated with examples of the ferromagnetic resonance, including new results.

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Auxetic Potential of Covalent Organic Frameworks: A Molecular Modelling Approach

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Covalent Organic Frameworks (COFs) represent a category of porous organic frameworks, structured through covalent bonding of organic units [1]. Characterised by extensive surface areas, tuneable pore sizes and low densities, COFs offer great versatility for various applications [1]. COFs have been synthesised in 1D, 2D, and 3D forms, with research predominantly concentrating on 2D and 3D structures. 2D COFs such as COF-1 mimic stacked layers, like graphite [2], while 3D COFs like COF-320 exhibit a complex, diamond-like network [3]. The mechanical properties of COFs remain underexplored, with most studies concentrating on 2D COFs [4-6] and revealing the potential for auxetic behaviour in these frameworks, with Poisson's ratios reaching as low as -1.5 [6]. Studies on the mechanical characteristics of 3D COFs, particularly regarding Poisson's ratio and compressibility, are relatively scarce [7, 8]. This study aims to investigate the potential of 3D COFs to act as mechanical metamaterials, by applying force-field-based molecular modelling on different 3D COFs documented in the literature. Modelling these 3D frameworks posed challenges due to the large pore sizes; however, a tailored simulation methodology was developed to address this. Specifically, the impact of nitrogen molecules within COF pores was investigated, demonstrating that their introduction aligns simulations more closely with experimental observations thereby producing more realistic Poisson's ratio values. This research provides insights into the auxetic potential of molecular systems, opening possibilities for designing intrinsically auxetic materials at the molecular level.

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Increase of the Auxetic Properties in the F.C.C. Hard Sphere Crystal Containing Combined Nanolayer-Nanochannel Inclusion Composed of Disordered Crystalline Phase of Hard Dumbbells

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Obtaining materials or metamaterials tailor-made elastic properties is not easy task. To avoid costly and cumbersome design of a new material or composite, one might turn to structural modifications of existing materials in order to change their properties in the desired direction. The latter may also be a tedious process, however, in many cases it can be simplified by computer simulations. Despite the fact that elastic properties are one of the oldest studied physical parameters of matter, our understanding of the microscopic phenomena behind them is still limited. One of many examples can be the origin of negative Poisson's ratio [1], which after few decades of studies still puzzles researchers. The ground breaking work by Lakes [2] who first obtained a man-made auxetic foam by (macroscopic) structural modification of polyurethane, showed the great potential in this approach to thinking about new materials. At the same time Wojciechowski [3, 4] showed that negative Poisson's ratio can result from molecular interactions. Thus, it is meaningful to expect that modifying material structure at the micro level may lead to occurrence of negative Poisson's ratio, coined *auxeticity* [5], in conventional materials or its enhancement in, so called, *partial auxetics* [6]. As appealing as this idea might be, there is a vast set of modifications that can be applied to the crystal structure to change its elastic properties. One of examples are the nanochannels or nanolayers that contribute to significant [7] or moderate [8] enhancement of auxeticity in f.c.c. crystals of hard spheres. However, when combined, these inclusions completely eliminate auxetic properties of the crystal [9]. This demonstrates the limitation in our understanding of the microscopic phenomena behind the macroscopic elastic properties of materials and motivates the further research of simple models of atomic systems. In the present work, with the help of Monte Carlo computer simulations, the above mentioned crystal of hard spheres, containing a combined nanolayer and nanochannel inclusions, is revisited. This periodic model crystal has been extended to include a degree of disorder. The latter is introduced in the form of degenerate crystalline phase constituting the inclusion. The inclusion has been transformed (without changes to its shape, size, or orientation) by randomly connecting the neighbouring spheres into di-atomic molecules (dumbbells). The impact of this modification on elastic properties has been investigated with the help of the Parrinello-Rahman approach in the isothermal-isobaric ensemble (NpT). It has been shown, that the presence of the degenerate crystalline phase [10-14] of hard dumbbells in the system leads to a significant decrease in the Poisson's ratio in [110]-direction ($\nu = -0.235$) and an overall enhancement of the auxetic properties [15].

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Local Structure and EPR Spectroscopy of the $Li_2B_4O_7$:Cu,Eu and $Li_2B_4O_7$:Mn,Sm Glasses

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The $Li_2B_4O_7$:Cu,Eu glass containing 1.0 mol. % CuO and Eu_2O_3 and the $Li_2B_4O_7$:Mn,Sm glass containing 1.0 mol. % MnO_2 and Sm_2O_3 were obtained by high temperature melting technology and studied by XRD, EPR, optical absorption, and photoluminescence methods [1, 2]. The EPR, optical absorption, photoluminescence emission and excitation show that the Cu impurity is incorporated into the $Li_2B_4O_7$ glass as Cu^{2+} ($3d^9$) and Cu^+ ($3d^{10}$) ions. The Cu^{2+} ions (electron spin $S = 1/2$) in the $Li_2B_4O_7$:Cu,Eu glass show an EPR spectrum of axial symmetry with characteristic 4-component hyperfine structure caused by nuclei of ^{63}Cu (natural abundance – 69.17%, nuclear spin, $I = 3/2$) and ^{65}Cu (30.83%, $I = 3/2$) isotopes. Precise spin Hamiltonian parameters ($g_\parallel$, $g_\perp$, $A_\parallel$, $A_\perp$) and peak-to-peak first derivative linewidths of the hyperfine components ($\Delta H_{\mathrm{pp}}^{\parallel}$ and $\Delta H_{\mathrm{pp}}^{\perp}$) for Cu^{2+} ions at $T = 295$ K in the $Li_2B_4O_7$:Cu,Eu glass were obtained by best fitting of the simulated EPR spectrum to the experimental spectrum [1].

The EPR and optical spectroscopy (absorption, luminescence excitation, emission, decay kinetics) show the presence of Mn^{2+} ($3d^5$) and Mn^{3+} ($3d^4$) impurity ions in the $Li_2B_4O_7$:Mn,Sm glass. The Mn^{2+} ions (electron spin $S = 5/2$) in the $Li_2B_4O_7$:Mn,Sm glass show an isotropic EPR spectrum with a characteristic 6-component hyperfine structure caused by nuclei of the ^{55}Mn isotope (natural abundance – 100%, $I = 5/2$). Parameters of all observed EPR spectra of the Mn^{2+} centres in $Li_2B_4O_7$:Mn,Sm glass were determined at $T = 295$ K. By EPR spectroscopy in the studied glass were identified three types of the Mn^{2+} centres: single Mn^{2+} (1) centres in the strongly distorted sites (ratio of rhombic and axial constants, $|E/D| \leq 1/3$), single Mn^{2+} (2) centres in the sites with almost cubic symmetry ($D \cong 0$, $E \cong 0$) as well as Mn^{2+} pairs and small clusters, coupled by magnetic dipolar and exchange interactions [2].

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Photocatalytic Performance of Nanodiamond-Decorated Potassium Vanadates for Organic Dye Degradation

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Water quality remains a critical challenge for societies in the 21st century, as emphasized by the UNESCO-IHP International Initiative on Water Quality. The growing scarcity of freshwater resources, exacerbated by increasing pollution, demands urgent solutions. Among the various wastewater treatment technologies, photocatalysis stands out as a promising strategy to mitigate environmental pollution. However, the success of this approach relies on the development of new, efficient photocatalysts that can be activated by visible or near-ultraviolet light, while also demonstrating biocompatibility, photostability, and resistance to environmental degradation. Recent studies have identified vanadium-based compounds incorporating d-block or p-block metals as promising candidates for visible-light-driven photocatalysis. Current research has particularly focused on nanostructured vanadates, where properties such as morphology, size, and surface area play a crucial role in determining photocatalytic efficiency. Moreover, the material's microstructure significantly influences its catalytic performance. While vanadates typically exhibit a +5 vanadium oxidation state, variations in valence states can occur based on the synthesis method used.

Among the vanadate family, vanadate bronzes have been relatively underexplored as photocatalysts, and our current research aims to address this gap. We have developed a novel synthesis method called Liquid-Phase Exfoliation with Ion Exchange (LPE-IonEx), designed to precisely control the microstructure and morphology of these materials. This one-step method, which occurs spontaneously at room temperature, enables the tuning of the sample's surface morphology, V5+/V4+ ratio, and band-gap energy by adjusting reaction conditions [1]. Recent findings from our work [2] show that potassium vanadates synthesized via the LPE-IonEx technique exhibit excellent visible-light absorption properties, attributed to their unique structural features and the high surface concentration of V4+ species.

Nanodiamonds are known to enhance light absorption and promote charge transfer. This study investigates the impact of nanodiamond decoration on the photocatalytic performance of potassium vanadates. The structural, morphological, and optical properties of nanodiamond-decorated potassium vanadates were characterized using XRD, FTIR, XPS, SEM, and UV-Vis DRS techniques. The photocatalytic activity of the modified catalysts was evaluated through their ability to degrade an organic dye under simulated solar light.

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Study of Properties of Liquid Crystalline Layers of Selected Cyanobiphenyls on Surfaces of Carbon and Boron Nitride Nanostructures by Computer Simulations Methods

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Composite materials based on liquid crystals and 2D materials such as graphene or hexagonal nitrogen boride are very interesting due to their practical application in optoelectronics, microelectronics and telecommunications. Their properties are largely determined by the interactions between the mesogen and the substrate, which are still not sufficiently studied at the molecular level. As part of the doctoral thesis, the properties of multilayer composites made of cyano-biphenyl located between graphene layers, hexagonal boron nitride or the surface of a bundle of single-walled carbon nanotubes were examined using computer simulations. Both the influence of the distance between the substrate surfaces and the effects related to the length of molecules from the cyano-biphenyl family were investigated.

The performed simulations showed the formation of clearly distinguishable, molecular mesogen layers, the thickness and order of which depend on the distance from the substrate. In addition, in the studied systems with molecules from a series of cyano-biphenyls, the occurrence of a phenomenon related to the length of molecules, the so-called odd-even phenomena. Molecules with an odd number of carbon atoms in the hydrocarbon tail show higher order than molecules with an even number. Increasing the distance between the substrate layers weakens the odd-even effects, which suggests that they are caused by interactions in the mesogen-substrate interface layer. Additionally, the odd mesogens in the series have a higher activation energy of thermal reorientation relaxation. From a practical point of view, it is also important to conclude that the polarization of the substrate (hexagonal boron nitride) significantly affects the structure of mesogen layers and accelerates the reorientation of molecules.

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Self-Repairing Behavior of Phospholipid Membranes After Interactions With Diverse Nanostructures – an MD Simulation Analysis

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Biological membranes serve as highly effective barriers designed by nature to protect the interior of cells from external environmental influences. While these membranes are meant to prevent the entry of molecules into the cell, researchers have been exploring ways to deliver various substances through the phospholipid bilayer [1], aiming to develop efficient and minimally invasive techniques for transporting cargo (such as medicines and markers) into cells. Significant efforts are being made to identify nanomaterials that can serve as containers for targeted drug delivery [2]. However, this process must ensure that the phospholipid bilayer is not permanently damaged, as such damage would lead to cell death.

To gain deeper insights into the self-repair mechanisms of the bilayer, we conducted non-equilibrium steered molecular dynamics (SMD) simulations [3, 4], indenting biological membranes with carbon and silicon-carbide nanotubes, graphene bilayers, and silicon nanocones. After the indentation process, the indenters were withdrawn from the membrane, and the self-sealing mechanisms of the phospholipid bilayer were analyzed.

Our results demonstrate the remarkable self-sealing capabilities of phospholipid membranes, which were able to self-repair even after significant damage. Furthermore, the repair process was often observed to be relatively rapid. These findings suggest that carbon-based nanotubes could be promising candidates for applications in targeted drug delivery or as biosensors.

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Influence of External Factors on the Formation of Bulk Amorphous Metal Alloys by Selective Laser Melting

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Amorphous metallic alloys are a unique class of materials with physical properties that are drastically different from their crystalline counterparts. The reason for this is the absence of a long-range order of atoms in the solid state and other features caused by this factor. The problem with producing amorphous alloys using classical methods is their limited size and shape. Therefore, over the past ten years, technologies for obtaining bulk amorphous alloys by additive technologies have been developed. Among the numerous additive technologies enabling 3D printing of materials, selective laser melting is the most optimal for amorphous materials. However, even in this case, the main problem with the formation of bulk amorphous alloys is their partial crystallization, depending on the synthesis conditions. The process of phase formation in the case of selective laser melting is also influenced by external factors, such as the composition of the atmosphere and the possible application of electric or magnetic fields.

Therefore, in this work, the formation of phases in iron-based alloys in the case of their formation by selective laser melting was studied. Special attention was paid to the influence of atmospheric oxygen and the presence of external fields on the formation of phases after sintering.

Morphology and structure of obtained alloys have been studied by scanning electron microscopy and XRD methods.

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Molecular Dynamics Simulation of Zr-Cu-Al Nanoparticles Sintering

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Alloys of the Zr-Cu-Al system are characterized by good amorphization ability, which requires a low cooling rate. For this reason, they are promising for the formation of so-called bulk amorphous alloys with dimensions of few or several tens of millimeters. Amorphous alloys of the same system can be produced in larger sizes using methods of additive technologies. Selective laser sintering and selective laser melting are the most common methods used to produce bulk amorphous alloys. These methods require micro- or nanoparticles of alloys, followed by sintering or melting. At present, it is almost impossible to observe this process at the atomic level using experimental methods, so computer modeling methods come to the forefront. The most promising of these methods is the method of molecular dynamics.

In this work, we have simulated the sintering process of amorphous nanoparticles of the Zr-Cu-Al system with different aluminum content by the molecular dynamics simulation method. The LAMMPS package was used for modeling, and OVITO was used to analyze the results. The modeling was performed at temperatures close to and below the melting point with a step of 50 K. The simulation focused on the formation of a neck between two nanoparticles and atomic diffusion within this neck. In addition, the atomic structure of the particles formed as a result of sintering was studied.

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Structure of Functional Polymer Films: A Computer Simulation Study

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The structure of polymer chains at interfaces is still not fully understood while theoretical prediction of the effective properties for macromolecular materials is very important for the design of new materials [1]. Moreover, the structure of very thin polymer films formed by strongly adsorbed macromolecules was studied by means of computer simulation. A coarse-grained model of strictly two-dimensional polymer systems was built and its properties were determined by an efficient Monte Carlo simulation algorithm employing a sampling algorithm that combines Verdier-Stockmayer, pivot and reputation moves [2-3]. The effects of temperature, chain length, polymer concentration and polydisperity on the macromolecular structure were investigated. It was shown that at low temperatures the chain size increases with the concentration, that is, inversely with high temperatures. This behavior should be explained by the influence of inter-chain interactions. It was also shown that the introduction of polydispersity increases the values of the percolation threshold especially for longer chains. The influence of the type of polydispersity on the percolation threshold in two-dimensional polymer films was found to be significant.

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Thermal Conductivity of Polydisperse Yukawa Crystals: a Molecular Dynamics Study

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Control of thermal transport in colloidal crystals is important in modern technologies and a significant challenge in designing various devices [1]. One of the important issues concerning heat transport processes in such systems is the influence of the particle size polydispersity on the thermal conductivity of polydisperse colloidal crystals. In this study, molecular dynamics simulations have been employed to determine the thermal conductivity of model colloidal crystals using the Green-Kubo method. The model crystals form particles interacting through Yukawa (screened-Coulomb) interaction arranged into a face-centered cubic structure (fcc). The thermal conductivities of monodisperse and polydisperse Yukawa crystals in a wide range of contact potential values and Debye screening lengths have been calculated [2]. This study showed that an increase in the Debye screening length leads to a reduction in the thermal conductivity of monodisperse Yukawa crystals. It was found that the increase in the size polydispersity of particles in fcc Yukawa crystals leads to a strong decrease in their thermal conductivity [2]. Those results qualitatively agreed with a recent report on the effect of disorder on the reduction of the thermal conductivity of colloidal crystals based on binary mixture [3]. However, for the binary mixture, a twofold decrease in the thermal conductivity coefficient associated with the global disorder observed in the glassy state has been found. Whereas in the case of polydisperse Yukawa crystals, a fivefold decrease in the thermal conductivity coefficient was observed caused by a local disorder, with maintaining the regular crystal fcc structure. The origin of those quantitative differences in the results may suggest the presence of different heat transport mechanisms in polydisperse fcc Yukawa crystals and binary colloidal glass. These mechanisms seem to be related to local and global disorders in the system.

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Computer Simulations of Elastic Properties of Model Crystals With Spherical Voids

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One of the most natural ways to understand properties of mechanical (meta)materials to which belong auxetics, *i.e.* systems for which Poisson's ratio [1] is negative [2, 3], is by studying models [4]. The first model exhibiting isotropic auxetic phase was simulated by the Monte Carlo (MC) method in 1987 [5] and then solved analytically in the static limit in 1989 [6]. Recently, certain crystalline systems of high symmetry, to which various (nano)inclusions were introduced, were discussed in the literature [7, 8].

In this lecture, we very briefly review model systems with zero-, one- and two-dimensional nanoinclusions. We also present some very recent results [9], obtained for a class of cubic crystals with spherical (nano)voids which were studied both by the MC method and by the finite element method (FEM).

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