SOUTHERN FEDERAL UNIVERSITY

SYNCHROTRON RADIATION AND SMART NANOMATERIALS

International workshop
(IWSN 2023)

BOOK OF ABSTRACTS

Rostov-on-Don
2023

Editor: A.V. Soldatov, Scientific Director of The Smart Materials Research Institute at Southern Federal University.

Synchrotron Radiation and Smart Nanomaterials (IWSN 2023) /
Soldatov A.V., 1st edition. - Rostov-on-Don, Bagira, 2023. - 60 p.

The book of abstracts contains the results of the reports presented at the international workshop on Synchrotron Radiation and Smart Nanomaterials. The fields covered nano characterization of advanced materials using the large-scale infrastructure (synchrotron radiation centers), accelerated synthesis of novel functional materials, including microfluidic technologies, the results of supercomputer modeling, including machine learning. A separate block discusses the catalytic processes, their operando characterization and nanocatalysts study.

Time, energy and reagents effective synthesis of advanced nanomaterials

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The technological leadership of the state is largely determined by the possibility of accelerated development of new unique materials with the required characteristics. At present, a long period from the beginning of the development of the material to its practical use in innovative sectors of the economy (on average 10-20 years) is a great global challenge.

We have performed R&D in the field of self-driving systems for accelerated synthesis of functional nanomaterials (at least 5-10 times compared to standard hydrothermal route by human involved batch method) using microfluidics and artificial intelligence technologies (deep machine learning). Another important characteristic of this system is the saving of initial («raw») materials (tens of thousands of times at least).

Significantly smaller volume of the microfluidic channel compared to ordinary chemical flasks results in huge economy of electrical energy as well.

The system was tested for several types of chemical reactions including synthesis of nanoparticles for oncology, nanocatalysts and nanoporous materials (metal-organic frameworks) for ecological applications and long-term storage of fruits and vegetables.

Controllable modular growth of Quantum Dot on metal organic framework Disposition

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Recent advancements in the field of photocatalytic hydrogen generation have emphasized the crucial role of co-catalysts in enhancing the efficiency of solar-to-fuel conversion in various semiconductors. The ability to manipulate the composition, microstructure, crystal phase, and facet of co-catalysts has attended significant attention due to their potential to promote the hydrogen evolution reaction. However, the utilization of a quantum dot-based co-catalyst deposited on a metal-organic framework (MOF) for solar water splitting has not been previously reported widely. In this study, MIL-101, a Fe-based MOF was synthesized using a microwave technique. A stoichiometric mixture of terephthalic acid and $FeCl_3$ in dimethylformamide was subjected to microwave irradiation at 300 W and 150° C for 15 minutes. In the second phase, the obtained MOF was dispersed in DMSO and subjected to a second microwave synthesis technique under similar conditions. The resulting product was then washed multiple times with ethanol and dried in an oven overnight. The synthesized material was characterized using X-ray diffraction (XRD) and X-ray fluorescence (XRF) techniques, which confirmed the successful formation of the MOF with FeS. Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy further supported the presence of the MOF and FeS. Optical absorption properties were investigated using UV-Vis spectroscopy, and the band-gap of the material was calculated. Future studies will focus on examining the microstructure of the material using electron microscopy and conducting photocatalytic hydrogen evolution tests using a solar simulator.

Investigate the key parameters influencing the formation of different morphological $NiCo_2O_4$ nanorods

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Complex oxides with intriguing morphologies have attracted significant attention due to their potential applications. Here, we synthesized $NiCo_2O_4$ nanorods at low temperature annealing followed by a hydrothermal method and explore the crucial parameters affecting their formation.

Initially, the aqueous solutions of cobalt and nickel acetates were prepared with varying concentrations of NH_4F and urea. Then, the clear solution of the precursor was transferred to autoclave for hydrothermal reaction at 180°C for 20h. The resulting composition was washed, dried and then analysed X-ray diffraction (Fig. 1b). We utilized thermogravimetric analysis (Fig. 1a) to identify the optimum annealing temperature, which was found to be approximately 500° C. Subsequently, the samples were annealed at 500° C under both air and N_2 atmospheres for 2 h, resulting in well crystalline spinel structure in the air atmosphere but not in the N_2 atmosphere.

Our study highlights the importance of the annealing atmosphere in obtaining the desired spinel structure and provides valuable insights into the controllable synthesis of $NiCo_2O_4$ nanorods with potential applications.

Loading of D,L-cysteine into biocompatible Zr-MOFs

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MOFs, a new class of three-dimensional hybrid metal-organic porous materials, exhibit highly tunable functional and structural characteristics, enabling them to be used in a wide range of applications [1].

A series of UiO family MOFs, including UiO-66, UiO-66-NH_2, UiO-66-NDC, and one with mixed BDC-NDC linkers, were chosen as drug carriers due to their high biocompatibility. To enhance colloidal stability and to form additional siloxy groups on the surface of MOFs for subsequent loading, all samples also were coated with SiO_2 using the original technique [2]. D, L-Cysteine contains three functional groups: thiol, carboxyl and amino. It was selected as the bioactive compound for loading into the pores to investigate the interaction mechanism. The materials obtained were characterized using various physical and chemical research methods. As a result, we have succeeded in optimizing MOF composition for efficient D,L-cysteine loading.

The research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity, № FENW-2023-0019).

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New routes of synthesis for tungsten-unithiol complex

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Unithiol has many valuable properties such as high sensitivity, selectivity, ability to form strong complex compounds with some metal cations, and exhibits redox properties which allows it to be used for analytical purposes. On the other hand, complex compounds with thiols including unithiol are considered promising antitumor drugs.

To obtain a unithiolate complex of tungsten (V), an excess alcohol extract of prickly spruce Picea pungens Engelm was added to the suspension of sodium dihydrate tungstate. After mixing, a 15-minute synthesis was started under the influence of ultrasound with the following parameters of the VCX-750 ultrasonic homogenizer: frequency 20 kHz, intensity 70 W x cm-2, pulsation with a ratio of operating time and pause 2:1. The reaction time in the CEM Discover SP microwave reactor was 30 min at a set temperature of 110° C with constant stirring. After both synthesis methods, the precipitate was washed, washed once with 96% ethyl alcohol and centrifuged. The XRD patterns and IR spectra of the samples obtained using both synthesis methods prove the structure described in [1].

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Alocasia Indica Assisted Green Synthesis of ZnO Nanoparticles for Improved Anti-Microbial Performance

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The creation of novel materials and applications in a variety of industries, including medicine, has demonstrated the promise of nanotechnology. This paper reports green synthesis of ZnO nanoparticle using Alocasia Indica extract as capping agent. These green synthesized ZnO NPs were characterized using UV Test, Fourier transform Infrared (FTIR), Scanning Electron Microscope (SEM), Energy Dispersive X-Ray Analysis (EDX), X-Ray diffraction (XRD), and Antimicrobial Test to reveal that these synthesized ZnO NPs had the ability to improve the anti-microbial performance. As ZnO has extensive surface area and improved interaction with microbial cells, these nanoparticles exhibit broad-spectrum activity against bacteria, fungi, and viruses. ZnO nanoparticles and Alocasia indica extract work together to improve antimicrobial effectiveness. These results suggest that these green synthesized ZnO NPs using Alocasia Indica extract can be used as effective anti-microbial for controlling pathogenic microbes.

Biomicrofluidics: current trends and prospecs

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The use of microfluidic technologies in chemistry and biology has made it possible to achieve significant progress in scaling «biological» chemical reactions to experiments in laboratory. This review presents the use of microfluidic technologies in medicine (organ-on-chip, human-on-chip), biology and soil science (root-on-chip, soil-on-chip) and others.

An overview of microfluidic devices inspired by the reactions of plants to light, the behavior of jellyfish, and the properties of lizard skin will be presented. An overview of important biological reactions carried out in microfluidic chips will also be given.

Our own research based on the study of reactions occurring in the sprouts of some plants (mung beans, cucumber, squash, hibiscus, soy) allowed us to create a new type of microfluidic chip. This chip reproduces the cross-section of the roots under a microscope and allows substances not only to react under new conditions, but also to mix differently.

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200 MeV Ag^{16+} Swift heavy ion irradiation: Effect on structural and magnetic properties of M-type barium hexaferrite

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Abstract

Sol-gel auto combustion method has been used to synthesize M-type barium hexagonal ferrite ($BaFe_{12}O_{19}$). Utilizing the 15UD Pelletron tandem accelerator, the synthesized M-type barium hexagonal ferrite was exposed to 200 MeV Ag^{16+} ions radiation, and the changes in structural and surface morphology of the material were examined in the present investigation. In order to meet the growing demand for M-type $BaFe_{12}O_{19}$ for different applications such as microwave communication, microwave dark rooms, and anti-electromagnetic wave radiation, it was further investigated. To do this, M-type barium hexagonal ferrite were synthesized and tuned its structural and magnetic characteristics after being quickly bombarded with heavy ions. Different experimental methods, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), and vibrating sample magnetometer (VSM), were used to characterize the pristine (as-synthesised; without radiation exposure) and irradiated (kept under radiation) samples. For both irradiated and pristine samples, the formation of ferrite structure was confirmed by the significant absorption peak between 580 and 440 cm^{-1} in the infrared spectrum and XRD. When compared to samples of pristine ferrite, the XRD peaks for the irradiated barium hexagonal ferrite were slightly widened. It is reliable with TEM images that the crystallite size of the irradiated barium hexagonal ferrite was larger than that of unaltered barium hexagonal ferrite. Due to the reduction in crystallite and grain size brought on by irradiation, coercivity falls in the irradiated sample. Due to ion-induced disorder and a decline in superexchange contacts, the irradiation sample exhibits a lower magnetization value than the clean sample.

Keywords: Barium Hexaferrite; Sol Gel Method; Swift heavy ion irradiation; Structural properties; Hysteresis Properties

3D printed lab-on-a-chip for metal nanoparticles synthesis

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Introduction

Noble metal nanoparticles (NPs) find a wide range of industrial applications, including catalysis, photonics, drug delivery, medical imaging. Their unique optical properties are interesting for surface-enhanced Raman scattering, photovoltaics, molecular detection, and photothermal cancer therapies [1, 2]. In a typical procedure metal nanoparticles grow in the presence of metal ions, reducing agent and stabilizer [3]. The result of the reduction, nucleation and growth depends on many parameters, including temperature and reagent concentrations. Classical synthesis routines are often limited to a few numbers of samples due to high amount of reagent consumption, while also having complex parallelization and reproducibility issues. Flow chemistry and microfluidics, on the contrary, provide unique possibilities for precise control over mixing and heat transfer in tiny reagent volumes. Current methods to produce microfluidic devices involve micromachining, hot embossing, etching and molding [4,5]. However, these processes can be time consuming, imprecise, expensive or challenging to produce complex channel topologies. Moreover, some of them also require clean-rooms and other facilities to ensure error-free devices, which are often expensive to build and maintain. This is where additive manufacturing comes into play with its accessibility and reliability.

Experimental

We have successfully designed microfluidic device (MFD) aka lab-on-a-chip (LOC) for metal nanoparticle synthesis and in situ spectral diagnostic. LOC was were designed in Fusion 360 (Autodesk, USA) and 3D-printed with a FunToDo Nano Clear (Alkmaar, Netherlands) resin on an Asiga MAX UV (Sydney, Australia) DLP-SLA 3D-printer. At 25 μm layer thickness the printing time for an 8 mm thick MFD was typically 40 minutes. After printing, the devices were removed from the build plate and sonicated in IPA for 90 seconds at 50 kHz and 35W power, following with the manual flushing of the channels with IPA. MFDs were then blown dry with compressed air. After drying the channels of MFDs were filled with Vaseline oil and left overnight to improve the surface hydrophobicity.

Synthesis and experimental control

Aqueous solutions of silver nitrate $AgNO_3$, sodium citrate $Na_3C_6H_5O_7$, and L-ascorbic acid $C_6H_8O_6$ prepared from commercial powders (Sigma Aldrich) at concentrations of 2 mM, 6 mM, and 12 mM, respectively, were used as components of the reaction mixture and supplied to the inputs 1-3 of the slug generator. The system of syringe pumps, performing dosing of reaction mixture components, was controlled from PC. The algorithm subdivided the space of reaction parameters into a set of experimental points according to the improved hypercube sampling (IHS, Latin hypercube sampling) method. It then performs automatic transition between these points and collects spectroscopy data according to a preset program.

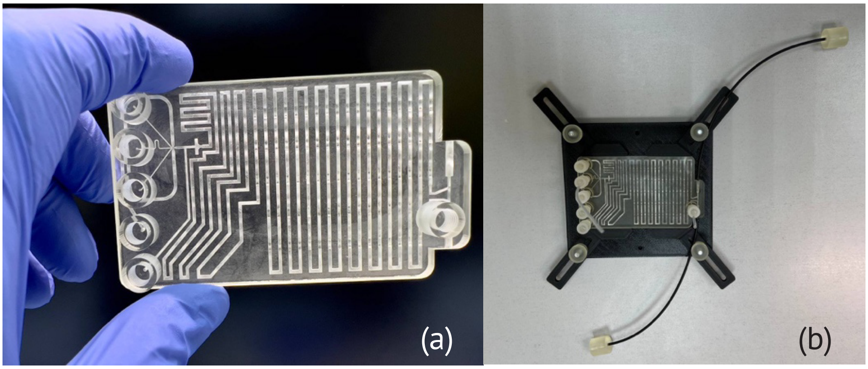

Figure 1: (a) 3D printed lab-on-a-chip. Inlets ports have ¼ 28 thread. Outlet port with integrated optic fiber chamber to measure spectra.

(b) 3D printed lab-on-a-chip and 3D printed devices holder. 4 mounts and optic fiber connected.

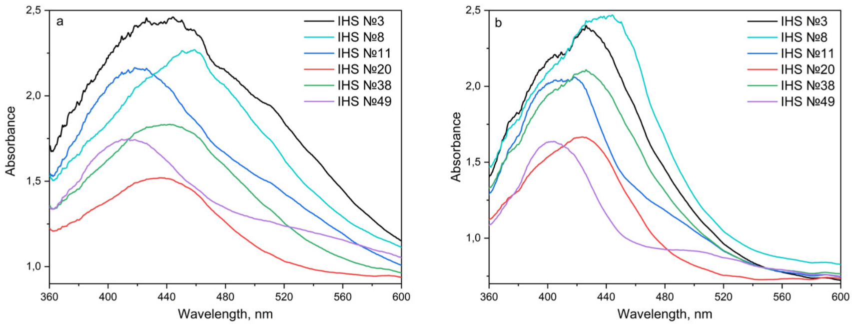

Figure 2. Characteristic UV-Vis absorption spectra obtained for various combinations of reagent in 3D LOC

Conclusion

In our work we demonstrate simple and versatile system based on 3d printed microfluidic device. 3D printing technology allows to easily manufacture microfluidic devices tailored to a specific needs, such as mixing, water-in-oil slug or droplets generation and separation and in situ UV-Vis spectroscopy.

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Advanced silica templated nano spherical particles for photocatalytic hydrogen generation

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The photocatalytic hydrogen generation represents a fascinating way to convert and store solar energy as chemical energy, in the form of hydrogen. However, the current research is aimed to enhance the quantum yield efficiency by the preparation of advanced heterojunction materials which reduce the recombination rate of photogenerated charge carriers. Here, we synthesized silica templated quantum dots deposited titania coating, overnight. The synthesized material was characterized using XRD and XRF techniques, which confirmed the successful formation of the SiO_2 based TiO_2 coating with CdS. FTIR and Raman spectroscopy further supported the results. Optical absorption properties were investigated using UV-Vis spectroscopy, and the band-gap of the material was calculated. The TEM images indicated that obtained material is spherical in shape. Further, photocatalytic test will be performed under solar simulator for the generation of green hydrogen.

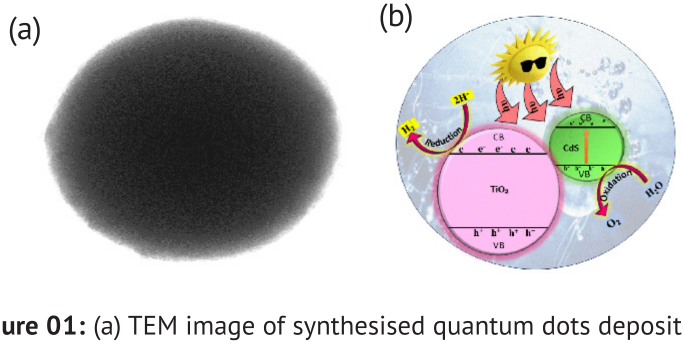

Figure 01: (a) TEM image of synthesised quantum dots deposited titania coating over silica surface (b) Graphical presentation of possible mechanism of hydrogen generation by solar water splitting using studied material.

Acknowledgement: The work is supported by the Strategic Academic Leadership Program of the Southern Federal University («Priority 2030»).

Formation of porous organosilicon matrices using microorganisms as templates

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Sol-gel methods are very attractive for applications in biotechnology, since hybrid silica gels are obtained under mild chemical conditions, at room temperature, at which biomolecules are active. This technology is quite simple to use, does not require expensive equipment, and is more energy and cost-effective. The sol-gel method is characterized by its environmental friendliness and the speed of obtaining a non-toxic and inert matrix capable of maintaining a constant volume, regardless of the composition of the medium. Previously, our research team showed the possibility of encapsulating yeast and bacterial cells in organosilicon sol-gel materials.We suggested that it is possible to use microorganisms as templates for the formation of cavities in sol-gel materials in accordance with the size and shape of microorganisms. To do this, it is necessary to remove microorganisms without damaging the structure of the organosilicon material itself. To do this, it was proposed to use annealing of the material at different temperatures. In the work, yeast cells of Ogataea polymorpha were used as templates and the material was annealed in the range from 200 to 1200° C.

We showed that at temperatures above 200° C, microorganisms are still present in the material, and at 400° C, pyrrolysis of microorganisms occurs, and at temperatures above 600° C, sintering of organosilicon material begins. Thus, it is shown that the use of temperatures above 600° C is not advisable, since the material is sintered and the necessary pores are reduced. In the future, the developed material can be used to adsorb various materials, including antiseptic ones, to develop highly effective antibacterial surfaces with controlled release of the substance.

The reported study was funded by a grant of the President of the Russian Federation for the State Support of Young Russian PhD Scientists, agreement No. MK-4049.2022.1.3

Implementation of microfluidic synthesis technologies to obtain composite based on $BaGdF_5$

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X-ray photodynamic therapy (XPDT) is a relatively new approach to the treatment of deep-located malignant tumors. Nanocomposites for XPDT usually consist of two components: an X-ray-activated nanophosphor and a photosensitizer that converts the energy to the UV-visible range. [1–3]. The selection of optimal luminescent characteristics, biocompatible coatings, and a photosensitizer takes a lot of time and requires expensive components. To obtain nanocomposites quickly and more efficiently, microfluidic synthesis technologies have been introduced. The previously developed new microwave synthesis of nanophosphors made it possible to obtain several series of nanoparticles based on the BaGdF5 structure [4, 5]. In this study, the synthesis technique was modernized by the implementation of microfluidic technologies. Thus, it was possible to obtain a series of BaGdF5:x%Eu, BaGdF5:y%Tb and BaGdF5:x%Eu/y%Tb nanophosphors with different dopant concentrations for a more detailed study of the nanoparticles luminescent properties. Moreover, microfluidic setups have also been used to synthesize the BaGdF5:Tb@RoseBengal nanocomposite.

This research was funded by the Russian Science Foundation (grant no. 19-15-00305-П).

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Phytotoxicity of nanomaterials

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The challenges of regenerative medicine have led to significant advances in cellular and tissue engineering. Advances in molecular biology provide the tools needed to develop gene-based tissue repair strategies. To alleviate the safety problem, a systematic assessment of potential toxic reactions is necessary, in particular, such an assessment can be made by methods of assessing phytotoxicity. Polyvinylpyrrolidone (PVP) is a bio- and hemocompatible polymer. Its toxicity depends on the synthesis conditions and molar mass [1]. To assess phytotoxicity, we conducted an experiment on mung beans [2]. The opened beans were placed in Petri dishes with PVP of various molecular weights: Polydon A, Impiron V200, Impiron V500, Impiron V1000. Every day a photo was taken with each sample and scale. Further, to assess the growth of beans, photos were processed in the ImageJ program. According to the experiment, Polydon sample showed the best growth of roots. On the other hand, the PVP V200 had the worst results. From this we can conclude that \Polydon is the least toxic and can be used as additives of biomaterials.

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Nanocomposite core-shell structures of the UiO-66 family for biomedical applications

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Metal-organic frameworks (MOF) are a class of porous substances consisting of two structural units: a metal cluster (secondary building unit) and an organic molecule (linker) [1]. Coating MOF nanoparticles with silica can improve biocompatibility, drug release, and photocatalytic properties [2].

In this work, several syntheses were carried out to obtain composite materials with a silica shell. The XRF method confirmed the presence of silicon in the obtained materials. According to TEM data, the formation of a shell on the surface of MOF nanoparticles is visible. The results of measuring the specific surface area showed a decrease in the values of the surface area and pore volume. According to the data obtained, materials with mixed linkers UiO-NDC-BDC-NH210BA@PVP@TEOS and UiO-NDC-BDC10BA@PVP@TEOS were selected as the most promising for further research.

Research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity, № FENW-2023-0019)

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MOFs as ethylene and 1-MCP absorbents for food preservation technologies

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Metal-organic frameworks (MOFs) have potential application in gas storage/separation. The uptake of ethylene, a plant hormone, from atmosphere or the release of 1-MCP, an ethylene inhibitor, can be used to slow down the ripening process of fruits and vegetables [1]. Here, we investigate the binding sites of ethylene and 1-MCP in $M_3(btc)_2$, CPO-27-M and $M_3(HCOO)_6$ structures by means of X-ray absorption spectroscopy (XAS), IR spectroscopy and DFT simulations. The HKUST-1, CPO-27-Zn and Co-FA samples were activated in Ar at 200° C and then exposed to 10% C_2H_4/Ar at 30° C. The obtained XANES spectra, collected at laboratory source, correspond to Cu^{2+} and were complemented by theoretical spectra to prove the adsorption of guest molecules. Infrared spectra were obtained for HKUST-1, CPO-27-Zn and Co-FA in DRIFTS mode. After activation the samples was exposed to 10% C_2H_4/Ar or in situ produced 1-MCP/Ar flow at 30° C. The peaks at 980 cm^{-1} and 668 cm^{-1} correspond to modes of adsorbed ethylene and 1-MCP in HKUST-1, respectively. Theoretical screening was performed using B3LYP-D4 level of theory to find best candidates for ethylene/1-MCP sorption/release among $M_3(btc)_2$ and CPO-27-M (M=Cr, Mn, Fe, Co, Ni, Cu, Zn) materials and compared with experimental values for $Cu_3(btc)_2$.

The results demonstrated a good correlation between experimental and theoretical data in terms of adsorption geometries, binding energies and vibrational spectra [2] and shed light on ethylene and 1-MCP binding in MOFs for application in food preservation technologies.

The authors acknowledge the Ministry of Science and Higher Education of the Russian Federation for financial support (Agreement № 075-15-2021-1363).

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Size and shape-tunable synthesis of doped rare-earth trifluoride nanoparticles

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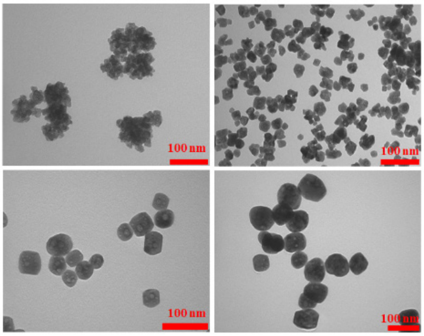
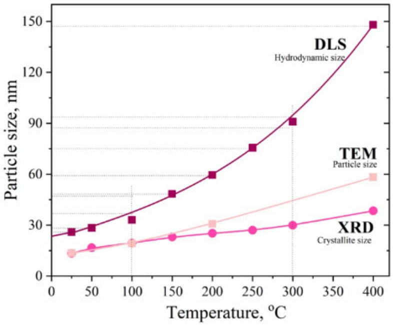
The synthesis of nanoparticles with controlled size, shape, and enhanced functionalities holds significant promise for various technological applications. This work presents a systematic investigation into the fabrication of doped rare-earth trifluoride (REF3, where RE = La, Gd, etc.) nanoparticles with precisely tunable size and shape characteristics. The synthesis process involves a carefully designed sequence of precursor preparation, controlled doping, nucleation, and growth. By manipulating reaction parameters, such as temperature, reaction time, and precursor concentration, a range of nanoparticle sizes and shapes can be achieved.





The resulting nanoparticles are characterized using advanced techniques including electron microscopy, X-ray diffraction, and spectroscopy, confirming their size, shape, composition, and optical properties. The outcomes of this research offer a deeper understanding of the intricate interplay between synthesis parameters and nanoparticle morphology, paving the way for the development of highly customizable materials with tailored functionalities for applications in optoelectronics, catalysis, bioimaging, cancer therapy and drug delivery.

Electronic structure and phase composition of Ni rod arrays formed in silicon dioxide matrix by synchrotron spectromicroscopy studies

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Arrays of Ni particles embedded in a dielectric matrix of silicon dioxide with the enhanced magnetoresistance effect tunable by electric field can be a perspective structure for modern electronic applications (e.g. magnetic tomography) and novel electronic devices. State-of-the-art non-destructive techniques sensitive to the local atomic environment are really demanded for the characterization of such structures.

Swift heavy ion tracks formation with different doses were applied followed by chemical etching of SiO_2 layers aimed at pores formation. Subsequent electrochemical filling of pores by nickel allowed to form rods arrays with different geometry and surface distribution. A complex of techniques was applied to characterize the morphology, atomic and electronic structure of the submicron Ni rods distributed in SiO_2 layer on Si substrate. We used SEM and AFM to study the morphology and surface distribution of Ni rods. Synchrotron XANES in total electron yield and fluorescence modes allowed to study specificity of local atomic surrounding of Ni, Si and O atoms in formed structures. These techniques combination made it possible to perform analysis of electronic structure and phase composition of surface and interfaces (bulk) of the formed structures. Further high energy and spatial resolution PhotoEmission Electron Microscopy (PEEM) technique were applied to investigate simultaneously morphology and electronic structure at microscopic level. Low nickel oxides residuals were found at the surface between metallic Ni rods while no interatomic interactions were detected even if rods concentration led to small surface Ni islands formation. It is shown that further increase of rods amount (island coverage) may lead to low silicide formation. The proposed technological approach allows to effectively form magnetic Ni rods arrays having relatively sharp interphase boundaries with silicon dioxide wide gap matrix.

The study was supported by the Ministry of Science and Higher Education of Russia under Agreement № 075-15-2021-1351.

XANES investigation of the effect of the drying method on the composition and structure of porous silicon nanoparticles

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Silicon nanoparticles (SiNPs) is a prospective material that can be used for therapy and diagnostic issues (theranostics). The properties of nanoparticles depend on the qualities of the initial silicon, the parameters of electrochemical etching of single-crystal silicon wafers, grinding methods used, drying and storage conditions of the obtained powders or suspensions. Aimed at SiNPs biomedicine use it is important to choose the optimal conditions and methods for their obtaining. Application of direct experimental methods for the high-precision composition, atomic and electronic structure diagnostics is necessary for SiNPs production techniques and optimal conditions prospective selection. Ultrasoft X-ray region synchrotron XANES technique is characterized by high surface sensitivity allowing estimation of the local surrounding of the given sort of atoms of nanoparticles.

The suspension of SiNPs obtained by mechanical grinding of porous silicon films in a planetary mill was dried using two approaches. The first is thermal drying in drying box. The second type of SiNPs powder was dried by lyophilic method. XANES (Si $L_{2,3}$ and O K) spectra were registered with the use of the NanoPES beamline of the Kurchatov synchrotron radiation center (NRC «Kurchatov Institute»).

The results obtained allow us to conclude that drying of the lyophilic type prevents the oxidation of SiNPs, at least within the depth of the informative layer of the method used. This result indicates the effect of the drying method on the surface properties and their stability, including during long-term storage, as well as on the further interaction of SiNPs with biological objects e.g. mammalian cells.

This work was supported by the Ministry of Science and Higher Education of Russian Federation under Agreement № 075-15-2021-1351.

TiO_2, MnO_2 and MoO_2 oxides electronic structure: theory and experiment

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The atomic and electronic structure of three commercial powdered samples of transition metal oxides TiO_2, MnO_2, MoO_2 produced by Sigma-Aldrich has been studied. The spatial structure was investigated by powder X-ray diffraction. It is established that the TiO_2 titanium dioxide sample has the spatial structure of classical rutile, the symmetry group P42/mnm (136). The sample of molybdenum dioxide MoO2 has the structure of distorted rutile, the symmetry group P21/c (14). The MnO_2 manganese dioxide sample has a distorted structure characteristic of disordered materials.

Experimental studies using high-intensity synchrotron radiation were carried out at the «Kurchatov» synchrotron of the National Research Center «Kurchatov Institute». The working pressure was about 10^{-10} Torr, electron energy analyzers Specs Phoibos 250 and 150 were used. Experimental X-ray Absorption Near Edge Structure (XANES) spectra for the K-edge of oxygen absorption in these metal oxides were recorded. The measurements were carried by the sample (drain) current detection mode. The X-ray photoelectronic spectra (XPS) of the valence band and subvalent states were recorded at two values of the excitation energies. For this purpose, radiation with a spectrum excitation energy of 120 eV was used at the synchrotron module of the NANOPES station, and the excitation energy at the ESCA module of the same station was 1486.6 eV (Al Kα laboratory source).

The electronic structure and X-ray spectral characteristics of bulk oxides TiO_2, MnO_2, MoO_2 with the classical spatial structure of rutile were modelled using the linearized augmented plane wave method within the framework of the Density Functional Theory using the Wien2k software package. The results of theoretical calculations are compared with the experimental results of XPS and XANES of the studied materials. There is a good agreement between the results obtained theoretically and experimentally.

Acknowledgement: This work was funded by Russian Science Foundation, project № 22-72-00145.

Copper nanocrystals immobilization in porous SiO2 matrix by electron microscopy and synchrotron XANES studies

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Copper nanostructures (CuNSs) with highly developed surface are potentially perspective functional material for biosensoric application as plasmon-active surfaces for amplification of the Raman scattering signal. Swift heavy ion track technology has been used for the pre-patterning of surfaces for self-organized localized CuNSs growth in porous matrix. Wet-chemical electroless approach for the localized formation of the CuNSs in pores have been applied. According to scanning electron microscopy data, observed tracks in the silica matrix have been partially filled by two types of copper nanocrystals with the grain dimensions of 10 nm and 70 nm as mean sizes. The samples with different pores filling degree have been investigated. First type of surfaces is related to the partly filled pores by Cu and the second type to overfilled pores with spherical copper caps formation on a top. For a careful and detailed analysis of the observed surface atomic and electronic structure as well as physico-chemical state the X-ray Absorption Near Edge Structure (XANES) using large-scale facilities at BESSY II synchrotron storage ring at HZB Berlin have been used. Noticeable changes of electronic structure and phase composition caused by transformation of crystal sizes and filling degree have been detected. The detected local copper and oxygen atomic surrounding reconstruction allowed us to establish a validity for used proposed technique for controlled formation of SERS sensitive surfaces.

The work is supported by the Ministry of Science and Higher Education of Russian Federation under Agreement No. 075-15-2021-1351.

Epitaxial Sn-Si ultrathin nanolayers structure by synchrotron study

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Heat generation can be considered a limiting factor in the creation and production of silicon-based electronic devices. A significant reduction in thermal conductivity can be achieved through the formation of periodic multilayer structures Sn/Si. Thus, disturbances in the movement of phonons are more noticeable due to the higher mass ratio Sn/Si. At the same time, studies of the atomic and electronic structure, the physico-chemical state of such structures are extremely important playing the key-role beyond the formation technology to subsequent application. The aim of this work was to study the atomic and electronic structure of silicon-tin-based epitaxial nanostructures.

The studied samples were obtained by molecular beam epitaxy on a Si(100) substrate with a 50 nm thin epitaxial Si buffer layer. About 5 monolayers of tin were deposited on Si buffer layer. For possible modification of the composition and structure, the obtained samples were annealed in-situ at 800° C for 10 min. Atomic and electronic structure studies were carried out by synchrotron XANES and XPS techniques. First principles calculations of XANES spectra were used.

The characteristic features of the electronic spectrum and the composition of epitaxial nanolayered structure were evaluated. It is shown that the growth of the tin nanolayer on the surface of the silicon buffer layer does not lead to a noticeable interatomic interaction at their interface. As a result, there are no noticeable distortions of the electron-energy spectrum. The formed nanolayer has a complex composition of various tin oxides. However, high-temperature in-situ ultrahigh vacuum annealing leads to a restructuring of the phase composition accompanied by the migration of oxygen atoms from atop tin atoms deep into the structure to silicon. This leads to complete oxidation of the single crystalline silicon buffer layer surface placed under 5 monolayers of the original tin oxide restored to a metallic state.

This work was supported by the Russian Science Foundation, grant 23-22-00465.

Photo-electrochemical cells for in situ and operando X-ray absorption spectroscopy studies

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Hydrogen economy is one of the most promising and encouraging technologies of the near future. Among other alternatives, hydrogen production by electrolysis is an environmentally friendly approach resulting in the green hydrogen. The cost of this process can be optimized by the utilization of solar energy with the help of photo-electrocatalysts. The synthesis of such materials is a complex and somewhat creative task, which requires deep knowledge and good experience. In turn, X-ray absorption spectroscopy (XAS) is a powerful tool providing information about the local atomic and electronic structure as well as its dynamics. Furthermore, in situ and operando studies can help shed some light on the mechanisms of processes occurring during electrochemical reactions.

In this contribution, we present a few designs of photo-electrochemical cells for in situ and operando XAS experiment (Fig. 1). One of them (A) has been successfully utilized at the structural material science beamline of the Kurchatov specialized source of synchrotron radiation «KISI-Kurchatov». All three cells are designed for measurements in fluorescence geometry with light illumination from the back side. The main difference lies in the optical length passing through the electrolyte solution volume, which is dictated by physical limitation of X-ray attenuation length.

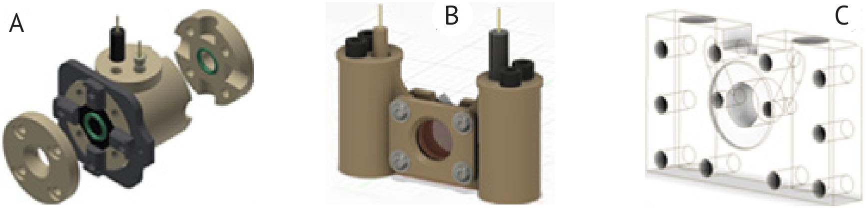

Figure 1. Proposed designs of photo-electrochemical cells.

Acknowledgement: Research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity, № FENW-2023-0019).

Monitoring the hydrosilylation reaction in the flow mode by in situ Raman spectroscopy

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Flow chemistry and, in particular, microfluidics provide a great benefit for the researcher to monitor the product formation on-the-fly easily.

In this work, we in situ monitored the 1-octene and bis(trimethylsiloxy) methylsilane conversion during the heterophasic hydrosilylation reaction. Reactants and the heterophasic catalyst (Pt-precatalyst dissolved in polyol) were injected into the microfluidic chip where the reaction was performed in droplets (Fig. 1a). Spectra of products were recorded by Raman spectrometer EnSpectr R532 each second on the FEP tube in the outlet. As a result, a complete disappearance of bands attributed to **ν**(Si-H) and **ν**(C=C) was observed evidencing a full conversion in less than 7 min (Fig. 1b).

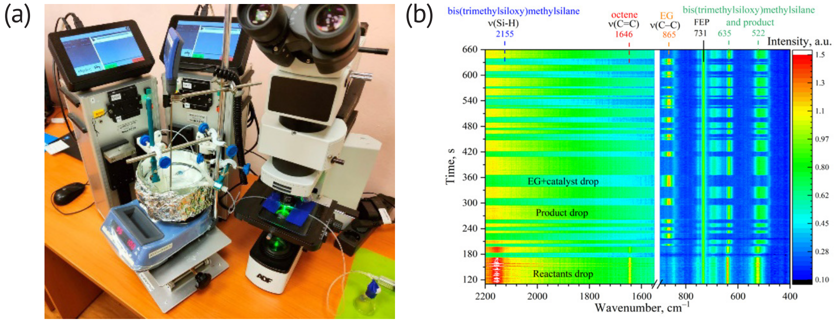

Figure 1. (a) Experimental setup; (b) Series of Raman spectra

XANES Investigation of Oxaliplatin Loaded Zr-MOFs

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Application of metal-organic frameworks (MOFs) as drug delivery systems have received great attention in recent years. MOFs are promising candidates due to the list of their advantages such as high porosity, biodegradability, large BET surface, controlled release of loaded drugs. In this study we estimated the efficiency of different loading methods, including novel freezing-induced loading (FIL) [1]. The experiment was caried out for anticancer drug oxaliplatin loaded into nanoparticles of Zr-based MOFs UiO-66. It was noted that the staged loading of the drug allows to attain increasing loading with each subsequent cycle. Thus, the final loading for the modified zirconium MOF UiO-66-NH_2 with mixed linkers (BDC-NH_2/NDC 50/50) achieved 5.3 wt% after the 7th cycle.

X-ray absorption spectroscopy (XAS) was implemented for clear understanding of loading mechanism. Obtained XANES spectra of pure and loaded oxaliplatin show no pre-edge features and a clear ‘white line’ peak at approximately 11.567 keV. Some significant changes occur after the edge position. In particular, spectral feature at 11591 eV decreases intensity, indicating significant changes in the local environment of the absorbing atom. In this research, we performed XANES modeling of possible resulted structures assuming the binding of the oxaliplatin molecule to the functional groups of MOF.

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Current progress of the SRF «SKIF» project

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The SRF SKIF is a 4th generation synchrotron light source which is being created in the Science town Koltsovo near Novosibirsk. The accelerator complex of the SRF SKIF consists of an electron linear accelerator of 200 MeV, a full-energy synchrotron booster, and a storage ring. The 3-GeV storage ring with a circumference of 476 m and an ultralow theoretical horizontal emittance of 73.2 pm rad will produce synchrotron radiation (SR) beams with the maximum brightness in the photon energy range from 100 eV to 100 keV for 30 experimental beamlines. For a photon energy of ~1.5 keV, the source emittance approaches the diffraction limit, providing a high degree of spatial coherence thus expanding the research capabilities of the facility.

Currently there are six beamlines with different scientific scopes and aims being built in the first phase. The first-phase beamlines of SKIF are as follows: (1-1) «Microfocus,» (1-2) «Structural Diagnostics,» (1-3) «Fast Processes,» (1-4) «XAFS Spectroscopy and Magnetic Dichroism,» (1-5) «Hard X-ray Diagnostics and Imaging,» and (1-6) «Electronic Structure». In total, the SRF SKIF may accommodate up to 30 beamlines; 14 of them will use the radiation of special insertion devices (wigglers and undulators) in straight sections, and 16 will be located at bending magnets.

The main functional task of the SRF SKIF will be infrastructural support of fundamental and applied research of scientific and educational institutions, as well as industrial companies, acting as users, in order to ensure leadership in the priority lines of scientific and technological development of the Russian Federation.

The SRF SKIF will allow one to perform world-leading studies in different fields of physics, chemistry, materials science, molecular biology, medicine, and other disciplines, with an emphasis placed on the most breakthroughs, economically and socially significant multidisciplinary tasks.

Local atomic and electronic structure of magnetic nanoparticles revealed by synchrotron methods

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Synchrotron methods make it possible to obtain information about the local atomic and electronic structure of both crystalline materials and nanosized objects without long-range order in the atomic structure. The physicochemical properties of a series of magnetic nanoparticles based on iron oxide were studied. A method is proposed for the quantitative characterization of the structural features of nanoparticles based on iron oxide using synchrotron X-ray absorption spectroscopies [1].

A combination of μ-XRF (microfocus X-ray Fluorescence Spectroscopy) and μ-XANES (microfocus X-ray Absorption Near Edge Structure) spectroscopies could extend the methodology to probe the localization and chemical stability of the nanoparticles in biological tissues after NPs admission in mice. μ-XRF was used to find the highest concentration of iron in biological tissue, while μXANES at the Fe K-edge has been used to monitor the iron oxidation state in the nanoparticles and in the native tissues. μXANES technique with submicron spatial resolution is sensitive enough to allow a separation of the contributions from the iron atoms present in SPIONs from the contribution of the atoms representing iron contained in the tissues of the body before the introduction of nanoparticles. The analysis of μXANES showed that SPIONs studied in the present research is found to be quite stable and retains its properties after interaction with tissues in vivo. Thus, such SPIONs are promising for further use in the theranostics for oncology [2].

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Investigation of Rh/NR3 catalytic systems in sequential stages of reductive hydroformylation engaging in situ X-ray absorption spectroscopy

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Although reductive hydroformylation over Rh/NR3 catalysts is of great interest to both industry and academia, to the moment, some of its aspects remain controversial or unclear, including those which might turn essential for developing new active catalysts and optimization of parameters. Thus, there are little systematic studies of its two stages separately. Systems of this type were previously studied by in situ NMR and IR methods, but their data are not enough for reliable conclusions on the nature of active species and deactivation processes. Here we report the results of our research of tandem reductive hydroformylation reaction catalyzed by Rh/NR3 complexes. For the first time, we investigated Rh/NR3 catalytic system under the reaction conditions by in situ XAS method to gain the additional structural information and observed the correlation of the obtained data with the results of catalytic experiments. Not intending to draw the final conclusion on the transformations and activities of Rh species under the reaction conditions, our study provides new useful insights into this question, in addition to previously reported data.

In situ FTIR spectroscopy as a tool for UiO-66 active sites tracing

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UiO-66 contains $Zr_6O_4(OH)_4$ clusters. During thermovacuum treatment, these clusters transform into Zr_6O_6. This transformation reduces the Zr coordination number from 8 to 7, forming coordinatively unsaturated Lewis acid sites. The coordination modulator approach presents an alternative technique for introducing Zr Lewis acid sites into defect pores. In this study, we conducted a comparative in situ IR spectroscopic analysis to investigate the accessibility of Zr sites in UiO-66 with defects [1]. We traced the formation of coordinatively unsaturated Zr-sites in the regular pores. After the evacuation of modulator molecules, the opening of Zr in defect pores makes them accessible. We used two probe molecules, CO and CD3CN. Acetonitrile (CD_3CN) is a stronger base and can substitute hydrogen-bonded water. The findings demonstrate that FTIR spectroscopy is a highly effective method for examining the presence and accessibility of acid sites in UiO-66, a critical aspect of its utilization in adsorption and catalysis. Moreover, by combining various probe molecules, essential complementary insights can be gathered.

The research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity, № FENW-2023-0019)

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Synthesis and diagnostic analysis of NBF-substituted dihydroberberine derivatives using microfluidic techniques

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Berberine, a natural alkaloid with diverse biological effects, holds promise for various pharmacological uses. One area of interest involves modified forms of berberine that have reduced structural stability, as they show potential for specific medical applications. Nevertheless, producing disubstituted berberines through synthesis poses challenges. Factors such as the sequence and speed of adding reagents, mixing pace, and the presence of trace acids in the environment impact the purity and stability of the final product. In this investigation, we devised a continuous-flow method to synthesize 8,13-disubstituted berberines, a type that is particularly hard to create in traditional batch methods. The microfluidic system's continuous flow design enabled the production of hybrid berberine derivatives featuring an NBF fragment at the C-13 position, yielding enhanced product amounts of up to 30% compared to the standard batch approach. The combination of the 3D-printed synthesis system and in-situ UV-Vis diagnostics can be applied to enhance and screen synthesis conditions for alkaloid derivatives that are conventionally challenging to generate.

Microfluidic synthesis of magnetic nanoparticles

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Microfluidic syntheses (MFS) are synthesis processes and reactions that occur in microscale devices known as microfluidic chips or Lab-on-a-chip. This technology has several advantages over synthesis in the laboratory, such as saving reagents, high speed and parallelism, and the potential for automation. The use of the MFS method is particularly relevant for magnetic nanoparticles (MNPs) [1]. MNPs are widely used in various fields of ecology, industry, and biomedicine [2]. Due to their properties and the size of nanoparticles, they can be used as agents for improving bio-diagnostics, drug deliverers, sensors, magnetic tags, and used in water purification. Therefore, the development of a technique for microfluidic synthesis of magnetic nanoparticles is very relevant.

In this work, the MFS of MNPs has been worked out and optimized. A MF chip of a special shape has been developed, which uses filtration technology. The syringe filter allowed the reagent to be divided into small droplets-reaction zones, which prevented clogging of the channels. As a result of the synthesis, optimization was carried out in terms of reagent concentration, filter material, and flow rate. The obtained nanoparticles were studied by modern methods using X-ray diffraction, infrared spectroscopy, and X-ray absorption near the edge structure. MNCs have spherical morphology and a size of 7-10 nm, as well as high magnetization.

As a result, a technique for obtaining MNPs using MFS has been developed and optimized.

Research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity, № FENW-2023-0019).

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Synergy of SAXS and Molecular Modeling for DNA Aptamer Bioapplications

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The work presents the results of modeling the atomic structure of aptamers in solution based on small-angle X-ray scattering (SAXS). The methodology of obtaining the atomic structure of small molecules of aptamers from SAXS under the conditions of real solutions is demonstrated. A specific methodology has been developed for this approach. The first step is the modeling of secondary structures based on nucleotide sequences. This step gives a general idea of how the main structural elements of the aptamer will look like, where there will be complementary and non-complementary sites, loops, quadruplexes, single strands of nucleotides, etc. The corresponding full atomic modeling of the 3D structure is then performed based on the secondary structure. This provides a first idea of the atomic structure of the aptamer and the position in space of the major structural elements. Molecular dynamics calculations of the resulting aptamer are then performed under realistic conditions. This provides information on the conformational changes of the aptamer in solution with explicit consideration of solvent, temperature and pressure.

SAXS-based computer modeling provides a basis for subsequent modeling of aptamers and cancer targets. It also provides new ideas for the intelligent design of new aptamers. A methodological approach for the rational design of DNA aptamers based on their structure and interaction with the target is presented. The iterative design procedure with mutual feedback between steps consists of (1) molecular design based on screening in a DNA aptamer library and directed mutagenesis to fit the protein tertiary structure, (2) 3-D molecular modeling of the protein target, (3) molecular docking of an aptamer with the target using the electrostatic potential of the protein, (4) molecular dynamics (MD) simulations of the complexes, (5) accurate quantum mechanical (QM) evaluation of the aptamer-target interaction, and (6) experimental verification with small-angle X-ray scattering, cytometry, and fluorescence polarization.

Acknowledgement: This work was supported by Project FWES-2022-0005 of the Russian Ministry of Science and Education. The authors thank the JCSS Joint Super Computer Centre of the Russian Academy of Sciences for providing supercomputers for computer simulations

Three-dimensional structure determination of DNA oligonucleotides by Small-angle X-ray scattering

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Small-angle X-ray Scattering (SAXS) is a well-established method for structural studies of proteins, peptides, DNA and RNA, and their complexes in solution under quasi-physiological conditions. SAXS has advantages over other methods of structural analysis. These are simplicity of sample preparation, high speed of experimental data acquisition and processing. The method is useful for elucidating the spatial structures of proteins and peptides, short DNA, RNA and other small biological objects in the range of 2 to 1000 nm in their native state. SAXS can also be used to detect binding sites and molecular interactions between different molecules. The SAXS method can be used to obtain information on the maximum particle size, radius of gyration, molecular mass, volume and spatial shape. In this work, initially selected in vitro 80-nucleotide aptamers have two constant 20-nucleotide primer sites on each side for PCR amplification. There is a need to reduce the size of such aptamers to improve their binding properties and make their synthesis cheaper. In this work, a truncated LC-18 (LC-18t) is proposed. A combination of theoretical methods was used to obtain the molecular structure: DNA folding tools, quantum chemical calculations and MD simulations. The modeled structures were compared with the experimental SAXS shape. The efficacy of the new truncated aptamer was tested experimentally on cancer cells. It showed similar binding properties to its predecessor LC-18.

Acknowledgement: This work was supported by the Russian Science Foundation grant no. 21-73-20240.

In situ UV-Vis and SAXS screening of Ag nanoparticles synthesis parameters using 3d-printed microfluidics and machine learning

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Efficient optimization of microfluidic synthesis requires in situ diagnostics and online data processing. In our work we demonstrate simple and versatile system based on 3D-printed microfluidic components. DLP-SLA technology allows to easily manufacture microfluidic devices tailored to specific needs, such as mixing, water-in-oil slug generation and spacing, in situ cells for UV-Vis spectroscopy and SAXS. Use of sufficiently long slugs and optimized optical path in the cuvette allows to obtain high-quality in situ optical spectroscopy data in a single shot from a single slug, enabling the ability to test dozens of combinations of parameters per hour. For synchrotron studies it allows to obtain in situ data from slugs directly through a FEP tube in quasi-stationary regime, without the need for a microfocus beam and synchronization.

The proposed system, combined with automated experiment control software and IHS-based sampling algorithm allows rapid and efficient screening of microfluidic reaction parameters. In this paper we demonstrated application of this approach to study the relationships between Ag nanoparticle optical properties, size distribution and reaction parameters. Using in situ UV-Vis absorption spectroscopy and SAXS we were able to quickly screen the impact of synthesis conditions on the LSPR properties, growth time, size and polydispersity of Ag nanoparticles. ML models were further trained on the in situ data and demonstrated high prediction quality. The trained algorithm can be applied for the inverse problem to predict the experimental parameters required to obtain NPs with given spectral response. We believe that the demonstrated approach will heavily increase the throughput of material diagnostics in laboratories and synchrotrons and accelerate the development of new functional nanomaterials.

X-ray and electron spectroscopy and microscopy studies of the biohybrid material based on E.coli cells

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Bacterial cultures of Escherichia coli and the DPS protein obtained from them are unique nanoscale objects in its properties, including an organic shell and an internal cavity in which an iron-containing core (~ 3-6 nm) consisting of Fe^{3+} ions are formed, which is of wide practical and scientific interest.

In this work, the morphological properties, as well as the atomic and electronic structure, physical and chemical state of E.coli bacterial cells were investigated. Scanning and Transmission (cryo) Electron Microscopy (SEM and TEM) was used as a convenient tool for studying morphological features, as well as a control method of research. Synchrotron methods of X-ray photoelectron spectroscopy (XPS) with high-precision ion profiling, as well as X-ray Absorption Near Edge Structure (XANES) were used to obtain information about the physicochemical state, as well as about the atomic and electronic structure. For the first time the synchrotron method of PhotoEmission Electron Microscopy (PEEM) was used, which combines spectroscopic and microscopic approaches to the study of the cells localized surface parts.

The obtained X-ray spectroscopy and microscopy data show the presence of iron in the studied cells samples, on the surface and in the volume of cells, which correlates well with the data set of «control» methods of SEM and TEM. A slight degradation of the cellular structure was observed as the result of vacuuming and finding the sample under an X-rays or synchrotron beam.

The study was supported by the Ministry of Science and Higher Education of Russia under Agreement N 075-15-2021-1351 and under State Task for Higher Education Organizations in Science for 2023–2025 (Project FZGU-2023-0006).

Local structure in Eu-doped $CaWO_4$

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One of the promising ways to treat cancer cells is photodynamic therapy. It consists in the release of reactive oxygen species (ROS) due to photosensitizers. However, light radiation of the visible spectrum cannot treat cancer cells inside the body because radiation of such a spectrum cannot pass through the skin. For such cases, it is necessary to use X-ray phosphors that create secondary radiation of desired wavelength and intensity.

To obtain our substance, we use the following reagents: the first is a solution of sodium tungstate in water, the second is a solution of calcium chlorides and rare earth metals in water. The method of microfluidic synthesis was used to carry out the reaction. To analyze the composition and structure of the obtained substance, X-ray diffraction and measurements on a synchrotron radiation source at the Kurchatov Institute Research Center were used. The results are shown in Figure 1.

From the XANES region it can be concluded that in the sample Eu-doped there is a significantly higher density of free d-states on the W atom corresponding to the p-d transitions forming the main maximum of the XANES curve beyond the L3 edge of W, which indicates a distortion of the WO4 tetrahedra. This also highlights the inclusion of Eu in the structure of substance.

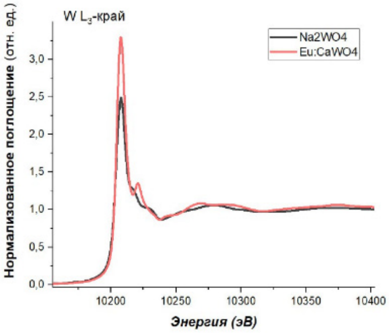

Fig.1 XANES spectra of Eu:$CaWO_4$

Quantitative analysis of the local atomic structure of binuclear molecules based on XANES and EXAFS domain by machine learning methods

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The information obtained from XAS spectra is difficult to process. One of the promising areas is machine learning. To analyze XAS spectra, the pyFitIt software package, developed by The Smart Materials Research Institute at the Southern Federal University, is used, which utilizes machine learning for predicting structures and analyzing XAS spectra. We employed it in our study to investigate binuclear molecules. The aim was to demonstrate which region of the spectrum is more sensitive to the metal-metal bond.

Each chemical element absorbs a photoelectron with a unique wave number k. There is a correlation: the heavier the chemical element, the higher the k value at which the photoelectron is absorbed. Usually, the XAS spectrum has its maximum amplitude immediately after the absorption edge. In addition, energy and wave number have a proportional relationship: the higher the scattering energy, the higher the wave number at which the photoelectron is scattered. Thus, the absorption edge of the XAS spectrum correlates with scattering on lighter chemical elements. In our study, we investigated binuclear copper molecules, with the metal-metal distance playing a key role. However, the information about this bond is primarily embedded in the EXAFS region, where the spectrum amplitude is significantly lower. Therefore, in comparison to the XANES region, where the amplitude is high, the contribution of this region to the machine learning algorithm will be small. To address this, we applied smearing, subtracted the spline, and transformed it into k-space for the entire training dataset. Thanks to this approach, we were able to significantly enhance the intensity of the EXAFS spectrum. Afterwards, we made a prediction of the molecule’s geometry using machine learning (RBF algorithm) and compared it with the prediction based on the regular XAS spectrum. As a result, indeed, the metal-metal distance is better predicted using the chi(k) region, where the contribution of the EXAFS region is significantly higher than in the regular XAS spectrum.

Thus, we were able to correlate theory and experiment and through numerical experimentation, prove that the EXAFS region is more sensitive to the metal-metal bond than XANES.

Application of the neural networks for the task of classification of the 2D colored images

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The problem of classifying WSI patches can be solved by two approaches: multi-class and multi-label. The multi-class approach is aimed at the ML method returning a normalized vector of class probabilities for a given object. The number of elements in the vector coincides with the number of classes and their sum is equal to 1, which in probability theory indicates that an object must belong to exactly one of the classes under consideration. On the contrary, the multi-label approach is applied to tasks where objects may belong to several classes at once or may not belong to any of them.

From the point of view of the neural network structure, the multi-label classification differs from the multi-class one only by the normalization on the last layer. A neural network trained as a multi-label one will assign high probabilities only for classes found in the training sample, the remaining objects will have low probabilities for all classes, so they will not be classified as requiring the attention of a pathologist. The first experiment was the training of a single neural network that classifies patches of a WSI into 6 classes. The quality of the neural network prediction was evaluated using the PR-AUC value for each class. To assess the dynamics of changes in the quality of classification, PR-AUC graphs were plotted during training of a neural network. Neural networks were trained according to the one-cycle policy.

The network weights grow unequally for different classes. That is why, it was decided to use 6 independent neural networks, each of which would solve the One-vs-Rest binary classification problem. The classification quality in this case was evaluated using the accuracy, ROC-AUC and PR-AUC metrics. To find the best solution, neural networks based on ResNet and EfficientNet architectures were compared, and the size of WSI patches (224x224 and 500x500) was also varied.

The Efficient Net architecture generally demonstrated better performance and more consistent results. We expect that having a homogeneous distribution of data across different histological categories may allow more than six classes to be classified.

Good Practice In XAS: Experimental Libraries, Interpretable Machine Learning And User-Friendly Frontend Of The Spectroscopy Ultimate Tool

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Rapidly evolving X-ray absorption spectroscopy (XAS), as well as a family of vibrational spectroscopies, make an important and powerful part of the characterization techniques in the toolbox of modern physical chemistry, condensed matter physics, and many other fields of study. Their unique capabilities to probe local electronic and phonon structure, geometry, and local chemical environment of matter can be enhanced even more in the era of data-oriented science with the use of machine learning (ML) and advanced data handling techniques. However, three main obstacles complicate deciphering of specifically XAS and vibrational spectroscopy by these modern fingerprint approach: (i) XAS community lacks standardized databases of wide range of experimental references; (ii) Whole procedure for reliable and interpretable machine learning analysis is not well established; (iii) There are no user-friendly tools for ML analysis of spectroscopic data, accessible by wide variety of non-programming physicists and chemists. Therefore, in this work we present our steps to address aforementioned problems by building extend dataset of bulk samples with well-defined molecular species and applying novel machine learning approaches for fingerprint analysis of experimental spectra in the form of user-friendly open source set of tools.

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Contents list

Подписано в печать 07.09.2023. Формат 60х84/16
Бумага офсетная. Печать цифровая. Заказ № 5/6
Объем 3.5 печ. л. Уч.-изд. л. 2,4. Тираж 50 экз.

Отпечатано в типографии ООО «Багира»
3440038, г. Ростов-на-Дону, ул. Нансена, 353
тел.: +7(863) 221-88-15, +7-903-401-88-15