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This 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 section describes computer modeling and automation of the synthesis of biomedical materials.

Development of an intermolecular potential for modeling CO gas absorption on a palladium nanoparticle

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This paper presents the developed interatomic interaction potential based on a sample of data obtained by the density functional (DFT) method. A distinctive feature of the proposed approach is the recording of the potential in the form of a simple analytical formula based on the Pade approximation [1]. This format allows you to efficiently and quickly calculate interatomic interactions without the need to use complex neural networks and resources typical of modern machine learning methods. The developed potential adequately reproduces the energy and structural properties identified in DFT calculations, while providing convenience and high computational performance.

This potential has successfully reproduced the process of CO gas absorption on a palladium nanoparticle. This makes the proposed method a promising tool for multiscale modeling of materials while maintaining accuracy and significantly reducing computational costs.

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References

[1] H. Padé (1892). Sur la répresentation approchée d'une fonction par des fractions rationelles. Ann. École Nor. (3), 9: 3–93 supplement.

In Situ XAS study of Lithiation in Iron Oxide Nanoparticle-Based Anodes During Battery Cycling

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The increasing need for efficient and sustainable lithium-ion batteries fosters the search for alternative anode materials with higher capacity, stability, and cost-effectiveness. Iron oxides, due to their abundance and safety, present a promising option, but their widespread application is limited by structural changes and volume expansion during cycling [1]. Addressing these challenges requires a comprehensive understanding of the chemical and structural evolution of Fe-based anodes under real operating conditions.

In this study, a novel microfluidic method for synthesizing γ-Fe_2O_3 nanoparticles with narrow size distribution and high surface area was developed, enabling superior electrochemical performance. Materials were extensively characterized via XRD, XANES, TEM, and BET, confirming uniform γ-Fe_2O_3 formation. Electrodes based on these nanoparticles exhibited high cycling stability and capacity, with water-soluble CMC binders outperforming PVDF. The discharge capacity of the Fe_2O_3@CMC-based electrodes reached 662 mAh g^{-1} after 50 cycles at 100 mA g^{-1} and 420 mAh g^{-1} at 1000 mA g^{-1}, exceeding the theoretical capacity of graphite. In situ X-ray absorption spectroscopy (XANES/EXAFS) revealed reversible Fe^{3+}/Fe^{2+} transitions and formation of lithium-containing phases (e.g., $LiFeO_2$), with partial irreversible reduction to Fe^0 contributing to low first-cycle Coulomb efficiency and gradual capacity decline.

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References

[1] Huiyu Jiang, Qin Mu, Hideo Kimura, Rui Liu, Wenyue Yang, Liyuan Liu, Wei Du, Chuanxin Hou (2023). Advanced ferroferric oxide-based composites for lithium-ion battery: Recent developments and future perspectives. Progress in Natural Science: Materials International, vol. 6, pp. 743-753.

Investigation and modelling of Mn-doped barium hexaferrite

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During the study of the ways of manganese embedding in the lattice of Barium hexaferrite – $BaFe_{12}O_{19}$, the results of photoelectron spectroscopy and ICP-MC were obtained [1,2]. These results showed an excess on the surface of barium relative to the stoichiometric ratio for this hexaferrite, and therefore its lack inside.

In this regard, a hypothesis was put forward about the replacement of barium with manganese. However, initial theoretical calculations showed that such a replacement was impossible. Therefore, a theoretical calculation was performed for the $MnFe_{12}O_{20}$ system, where MnO replaces Ba. The initial distance between Mn and O was 2 Angstroms.

Quantum-chemical methods, as detailed in article [3], were used to numerically refine the positions of atoms within the crystal lattice, keeping the lattice parameters unchanged. The calculations showed that the potential energy of $MnFe_{12}O_{20}$ is -4970 kcal/mol, while $BaMnFe_{11}O_{19}$ has a potential energy of 5004 kcal/mol. Finally, the distance between Mn and O ions was determined to be 1.7 angstroms.

References

[1] Gudkova S. et al. // Res. Chem. 2025. V 16. P. 102458.

[2] Bairagi K. et al. // Surf. Sci. 2015. V. 641. P. 248. https://doi.org/10.1016/j.susc.2015.05.020

[3] Shramkov E. A. et. al. // Journal of Surface Investigation: X-Ray, Synchrotron and Neutron Techniques. 2025. V 19(2), P. 460–464. https://doi.org/10.1134/S1027451025700685

LED Solar Spectrum Simulator for Photocatalysis

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The spectral composition and irradiation dose are critical for indoor studiesin photocatalytic, photoelectrocatalytic and photovoltaic research. Solar simulator is an instrument that can provide the electromagnetic spectrum in ultraviolet and visible range with intensity similar to the natural sunlight. Such devices are usually constructed using halogen, xenon arc or metal halide lamps for light generation. Solar simulators build using modular arrays of Light Emitting Diodes (LEDs) propose high tunability of the intensity in different spectrum range and could archive Class A AM 1.5 G irradiance (100 mW/cm^2) across the 400 to 1100 nm wavelength range and show spectral match up to 99.5%, a spatial non-uniformity of 2.0%, and a temporal instability of <0.2% [1].

Also, commercial xenon solar simulators are expensive and offer limited tunability. LED arrays provide channel-by-channel spectral flexibility, which is advantageous over existing alternatives.When building the device prototype, we used an array of 10 LEDs, each operating at a specific wavelength. All LEDs are placed at angles relative to each other to focus on a defined spot. To collimate the emission from each LED into a narrower beam we used focusing lenses with a 5° divergence. Each LED has dedicated controllers and switches to enable spectral adjustment.

As a result, we formulated the concept of an LED-based solar spectrum simulator, developed a method for focusing the LED array, and assembled a working prototype.

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References

[1] A.Y. Al-Ahmad, J. Holdsworth, B. Vaughan, G.Sharafutdinova, X. Zhou, W.J. Belcher, P.C. Dastoor.Modular LED arrays for large area solar simulation. Prog Photovolt Res Appl. (2019) 27:179–189

Size-controlled synthesis of Ln3+-doped LaF3 nanoparticles

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In this work, we report the size-controlled synthesis of Ln^{3+}-doped LaF_3 nanoparticles with particle sizes tunable from approximately 5 nm to 100 nm, as well as submicron particles. A comprehensive study employing X-ray diffraction (XRD), X-ray fluorescence (XRF), dynamic light scattering (DLS), transmission electron microscopy (TEM), high-resolution TEM (HRTEM), UV-visible spectroscopy (UV-vis), and X-ray excited optical luminescence (XEOL) elucidates the influence of synthesis parameters on nanoparticle size, crystallinity, morphology, and properties. By varying solvent type, solution pH, reaction temperature, time, and precursor concentrations, we achieved precise control over nanoparticle growth kinetics and structural evolution. Ethylene glycol concentration and reaction temperature notably modulate particle size in aqueous media,with pure water promoting the most significant crystallite growth. Solution pH critically affects particle agglomeration and morphology, where acidic conditions accelerate coalescence and alkaline conditions retard growth. Adjustments in fluorine and lanthanide precursor concentrations induce subtle size increases and morphological transitions from nanoprisms to nanorods, particularly at elevated Tb^{3+} doping levels. Core-shell structures were successfully synthesized via a two-step process, maintaining size constraints comparable to single-phase nanoparticles. Precise size and morphology control enable the tuning of optical, magnetic, and catalytic properties, expanding the applicability of Ln^{3+}-doped LaF_3 nanoparticles in photonics, biomedicine, and advanced materials science.

Development and characterization of PVA membranes modified with In(BTC) for pervaporation separation of isopropanol/water

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In this study, pervaporation membranes based on synthetic biodegradable polyvinyl alcohol (PVA) with enhanced properties for isopropanol dehydration were developed by modification with a synthesized metal–organic framework, In(BTC). The improvement of the PVA membrane properties was achieved by varying the In(BTC) concentration (2.5–7 wt.%) in the PVA matrix, which allowed the selection of an optimal membrane composition. This membrane was then chemically cross-linked with maleic acid to increase resistance, and a cross-linked membrane supported on the optimized PVA/5%In(BTC) composite was fabricated for potential industrial applications. The resulting membranes were characterized using spectroscopic, microscopic, X-ray diffraction, and thermogravimetric analysis methods, as well as measurements of swelling degree, contact angle, and Brunauer–Emmett–Teller (BET) adsorption modeling. The cross-linked membrane supported on the PVA/5%In(BTC) composite exhibited optimal transport properties for isopropanol dehydration (20–90 wt.% water), achieving 99.9–89.0 wt.% water in the permeate and a flux of 0.142–0.341 kg/(m^2·h), which was four times higher than that of the pristine PVA membrane during the separation of 20–30 wt.% water/isopropanol mixtures.

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Synthesis and Characterization of a Single-Atom Cobalt Catalyst for Oxygen Reduction Reaction in Hydrogen-Air Fuel Cells

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Proton-exchange membrane hydrogen-air fuel cells represent a promising technology for clean energy conversion. However, their large-scale deployment is hindered by the high cost of platinum-group metal-based electrocatalysts, particularly for the cathodic Oxygen Reduction Reaction (ORR) [1]. Single-Atom Catalysts (SACs) have attracted considerable attention due to their maximum atomic utilization, unique electronic properties, and high catalytic activity.

The synthesis of a single-atom cobalt catalyst was performedbased on controlled pyrolysis of bimetallic Zn–Co Metal–Organic Frameworks (MOFs) with 2-methylimidazole as an organic ligand. The structural and morphological characteristics of the synthesized materials were investigated using X-Ray Diffraction (XRD) and X-ray Absorption Spectroscopy (XAS).

The electrocatalytic performance of the materials was evaluated using Rotating Disk Electrode (RDE) method. A standardized protocol for catalyst ink preparation and deposition was developed to ensure reproducibility. The optimized catalyst composition is comparable to commercial Pt/C.

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References

[1] Yue M. et al. Hydrogen energy systems: A critical review of technologies, applications, trends and challenges. Renewable and Sustainable Energy Reviews, 146 (2021) 111180.

Atomic and electronic structure of porous silicon nanoparticles by synchrotron study

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The research of atomic and electronic structure of hybrid materials is the key for their properties understanding. Porous silicon nanoparticles (PSI NPS) have a developed surface that determines their properties. In particular, PSi NPs can be a part of biohybrid materials. In this study we used methods that are sensitive to developed surface local atomic surrounding of nanoscale objects – Psi NPs embedded to mammalian cells.

The suspension of PSi NPs 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 PSi NPs powder was dried by lyophilic method. Futher, PSi NPs were integrated into 3T3 NIH cells culture. XANES (Si $L_{2,3}$ and O K) spectra were registered at the NanoPES beamline of the Kurchatov synchrotron radiation centre (NRC "Kurchatov Institute").

The results obtained allow us to conclude that lyophilic type drying 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 nanoparticles surface properties and their stability. The results of the biohybrid structures experimental synchrotron studies by XANES spectroscopy together with scanning electron microscopy data allow us to conclude that nanoparticles combined with biological objects are subject to changes in the composition, structure and physico-chemical state of the surface.

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Studies of biohybrid materials based on Dps molecules of E.coli cells using X-ray and electron spectroscopy and microscopy, including synchrotron investigations

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A complex of X-ray and electron spectroscopy and microscopy techniques, including ones using synchrotron radiation, has been used to study the morphology and physico-chemical state of *E.coli* cells (BL21*(DE3), K12 MG1665), Dps protein molecules obtained from them, and biohybrid structures based on them. The sizes and morphology features of biological containers – molecules of the bacterioferritin protein Dps, inorganic nanoparticles in these molecules containing Fe atoms, as well as *E.coli* cells, the source of the molecules, have been established. The isolating specificity of the Dps by *E.coli* cells in a state of protein superproduction are shown, as well as the peculiarities of combining a molecular culture with a 3D-developed surface of wire-like silicon arrays for the purpose of its targeted functionalization. The applicability of ultrahigh vacuum XPS and XANES spectroscopy and PEEM spectromicroscopy techniques for the study of biohybrid materials based on Dps protein molecules and *E.coli* cells in combination with ion-beam removal of nanolayers has been demonstrated. The presence of iron atoms in the nanoparticles of the biohybrid material in different charge states of Fe^{3+} and Fe^{2+} and different coordination, as well as the possibility of changing the composition of the nanoparticles up to the reduction of iron, is shown.

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Synchrotron and laboratory studies of the physical and chemical state and structure of SnO2 wire-like crystals

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Wire-like SnO_2 crystals are currently important for research due to the gas-sensitive properties of such objects, as well as the possibility of creating high-precision devices based on them. Knowledge about the influence of the formation conditions on the local atomic surrounding, structure, and physical and chemical state will allow for the control of the properties of this functional material, including for practical applications.

In this work, SnO_2 wire-like crystals were formed using gas-transport synthesis at various temperatures in the growth chamber. Surface studies were conducted using XPS and XANES methods, using the KISI-Kurchatov synchrotron radiation source at the Kurchatov Institute in Moscow (the NANOPES station), as well as by the data obtained earlier at the Helmholtz Zentrum Berlin (the BESSY II synchrotron, the RGBL station).

The lack of oxygen atoms in the developed surface layers of the wire-like crystals leads to the formation of a prepeak in the XANES synchrotron spectra, that corresponds to the states in the band gap of tin dioxide. The shape and relative intensity of this prepeak vary depending on the synthesis temperature of the wire-like crystals. The rest shapes of the absorption edges suggest the formation of tetragonal SnO_2 on the surface of the studied objects. The XPS spectra also indicate a lack of oxygen, leading to the formation of SnO_{2-x} in the surface layer of the studied objects.

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Co-Mn Spinel Coatings for SOFC Interconnect Application

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Solid oxide fuel cells (SOFC) are electrochemical devices designed for direct efficient conversion of organic fuel into electrical energy [1]. One of the most important parts of SOFC are interconnects, which act as an electrical connection of adjacent cells. Ferritic stainless steels (Crofer 22 APU, Crofer 22 H, AISI 430) are favorable for production of interconnects operating in the area of moderate temperatures (750 - 850 °C).

One of the most promising and effective approaches to ensuring a long service life of interconnects is the surface protection coating. The most widespread are coatings based on metal oxides with spinel structure, the application of which keeps area specific resistance (ASR) values low when

interconnects are operated in oxidising atmospheres at high temperatures [2].

In this work coatings based on cobalt-manganese spinel $MnCo_2O_4$ were obtained on the surface of Crofer 22 APU using the method of non-stationary electrolysis. The morphology of the surface of the coatings according to scanning electron microscopy has a crack-line structure. The analysis of the surface layers of the coatings by XPS showed that its main

components are compounds of manganese (4+), cobalt (2+) and oxygen (2-). Area specific resistance is measured at 850 °C for 1000 h in air was equal to 8 mOhm/cm^2.

References

[1] J. Peng, J. Huang, X. L. Wu, Y.W. Xu, H. Chen, X. Li (2021). Solid oxide fuel cell (SOFC) performance evaluation, fault diagnosis and health control: A review, Journal of Power Sources, Vol. 505, P. 230058.

[2] P. Guo, Y. Lai, Y. Shao, Y. Zhang, Y. Wang (2017). Thermal Growth $Cu_{1.2}Mn_{1.8}O_4$ Spinel Coatings on Metal Interconnects for Solid Oxide Fuel Cell Applications, Metals, Vol. 7, P. 522.

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Drying of Methanol as a Critical Step in the Synthesis of Co-N-C Catalysts for ORR

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A reproducible method for drying methanol for the synthesis of Co-N-C catalysts [1] for the oxygen reduction reaction has been developed. Into a 500 ml round-bottom flask, 20 ml of technical methanol (95.5%), 500 mg of magnesium powder, and 20-50 mg of crystalline iodine are added. The mixture is heated to boiling until the iodine color completely disappears. 280 ml of methanol is added and boiled under reflux for 3 hours. The methanol is distilled into a Schlenk flask, achieving a purity of 99.99% by GC.

The formation of the target MOF phase is confirmed by XRD; the metal ratio is determined by XPS. Only the use of methanol activated with magnesium ensures the optimal Zn/Co ratio of ~55/45 in the ZIF precursor. After pyrolysis, such samples contain ~100% cobalt, unlike catalysts obtained with insufficiently dried methanol (9-19% Co).

Electrochemical testing demonstrates outstanding activity: Eonset = 870 mV, E1/2 = 810 mV vs. RHE.

The methanol drying method with Mg/I_2 is a critically important step for the directed synthesis of highly active Co-SAs/N-C catalysts.

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References

[1] Yin, Peiqun, Tao Yao, Yuen Wu, et al. "Single Cobalt Atoms with Precise N-Coordination as Superior Oxygen Reduction Reaction Catalysts". Angewandte Chemie 128, 36 (2016): 10958-63.

Research on the replacement of Fe with Al in BaFe12O19

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Complex oxides, like hexaferrites, are crucial in electrical engineering. Barium hexaferrite ($BaFe_{12}O_{19}$) stands out with its magnetoplumbite structure. It boasts high saturation magnetization, significant coercive force, robust mechanical strength, and chemical stability. Its crystal lattice features five distinct iron positions: 12k, 4f2, 2b, 2a, and 4f1.

To change the properties of $BaFe_{12}O_{19}$, it is alloyed with metals (bismuth, gallium, and zinc) and non-metals (boron and antimony). Alloying affects the coercive forces, lattice parameters, and Curie temperature. In this work, the compound $BaAl_4Fe_8O_{19}$ was studied. Powder neutron diffraction with temperature resolution conducted at the IR-8 reactor [1] revealed the presence of two Curie temperatures.

A theoretical model was created to pinpoint where aluminum can substitute iron in the crystal lattice. The model optimized the positions of atoms with constant parameters using quantum chemical methods. These calculations, based on the techniques detailed in article 2, revealed that systems with iron replaced at positions 2a and 12k are most energetically effective.

References

[1] Gudkova S.A. et.al. // JMMM. , 2023. Vol. 603, 172229
DOI: 10.1016/j.jmmm.2024.172229

[2] Shramkov E. A. et. al. // Journal of Surface Investigation: X-Ray, Synchrotron and Neutron Techniques. 2025. V 19(2), P. 460–464. https://doi.org/10.1134/S1027451025700685