GDAŃSK UNIVERSITY
OF TECHNOLOGY
FACULTY OF APPLIED PHYSICS AND MATHEMATICS

ABSTRACT BOOK

FNMA 2025
The 20th Conference on Functional and Nanostructured Materials

Video sessions (MSTeams) on December 5 (3.25 P.M.–8.45 P.M.) and December 6 (10.00 A.M.–2.30 P.M.)

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

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CONFERENCE SCHEDULE FOR DECEMBER 5-6, 2025

Day 1, Friday, 5 December 2025

15:25 – 15:30 T. Miruszewski – Opening & Introductory Talk

Session 1. Chair: T. Miruszewski

15:30 – 15:45 Z. Dendzik – Microscopic and macroscopic aspects of prenematic fluctuations in nanoparticles-doped liquid crystals

15:45 – 16:00 M. Dominów – Producing environmental-friendly high-energy gas mixtures for solid oxide fuel cells via unrecyclable plastics pyrolysis

16:00 – 16:15 B. Bochentyn - On the way to understanding the great catalytic activity of ceria-based anode materials for biogas-fed Solid Oxide Fuel Cells

16:15 – 16:30 M. Nowakowska – Structural and transport properties of triple-conducting (Ba,Sr)(Fe,Mo,Zn,Zr)O_3 perovskites for Solid Oxide Fuel Cell technology

16:30 – 16:45 J. Adamczyk – Combining the benefits of conventional and high-entropy materials – mid-entropy perovskites for application in solid oxide fuel cells

16:45 – 17:00 K. Zielińska – Modified multi-component perovskites: the influence of additional 3d dopant in a new group of $SrCo_{0.7-x}Ta_{0.1}Mo_{0.1}Mn_{0.1}X_xO_{3-\delta}$ (X: Cu, Ni, Fe) oxides

17:00 – 17:15 R. Zafar – A-Site Deficiency and B-Site Substitution Synergies in NdBa-Based Double Perovskites for High-Performance IT-SOC Electrodes

17:15 – 17:30 Z. Chen – Laser-Anchored Ruthenium in a Protective TiN-TiO_2 Matrix for Highly Stable Acidic Oxygen Evolution

17:30 – 17:45 I. Shtablavyi – Influence of synthesis conditions on the surface morphology and phase composition of Al-Cu-Ni alloys obtained by selective laser melting

17:45 – 18:00 S. Amatori – The CECOMEC project: CEria-based COmpounds as effective catalyst for electrochemical cells

18:00 – 18:15 Break

Session 2. Chair: B. Bochentyn

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18:30 – 18:45 A. Sikorski – Macromolecules in a solvent of varying quality. Monte Carlo computer simulations

18:45 – 19:00 B. Venhryn – Effect of $FeCl_3$ activation modification on the change in the porous structure of nanoporous biocarbon

19:00 – 19:15 Y. Wang – Identifying the effect of doping and cooling rate on presence of ordered and disordered phases in Mn-based rocksalt-type cathode materials for Li-ion batteries

19:15 – 19:30 J. Winiarski – DFT-based screening of $REBa_{1-x}Sr_xCo_{2-2y}Cu_{2y}O_{5+\delta}$ candidate air electrode materials for solid oxide fuel cells and electrolyzers

19:30 – 19:45 M. Czudec – Determining the influence of Ag and Ni phases on the thermoelectric characteristics of multicomponent oxide composites

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20:00 – 20:15 M. Venhryn - High-Efficiency Terahertz Radiation Modulator Based On Single-Crystalline Germanium

20:15 – 20:30 J. Zdankiewicz – Ceramic–polymer composites for 3D–printed catalytic sieve converting gaseous stream into useful fuels for SOFC

20:30 – 20:45 K. Wojciechowski – A few words on systems exhibiting a negative Poisson's ratio

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10:15 – 10:30 J. Dziedzic – Biochemistry and electrochemistry from first principles using ONETEP

10:30 – 10:45 F. Bagnoli – Synchronization and control of Lorenz systems

10:45 – 11:00 M. Dudek – The effect of the presence of a microwave magnetic field on the magnetic ordering of a ferromagnetic material

11:00 – 11:15 L. Amir – Density Functional Theory Study on the Photovoltaic Properties of End-Capped Acceptor–Modified Phenylsulfonyl Carbazole Materials for Solar Cells

11:15 – 11:30 P. Szatan – Simulations of chemical vapor deposition of a graphene layer on a copper substrate

11:30 – 11:45 A. Rani – Low-Temperature (60°C) Synthesis of Sodium-Doped Triazine/Heptazine g-C_3N_4/Bi_2S_3 Heterostructures for High-Performance Supercapacitors

11:45 – 12:00 K. Hałagan – Quantum Chemical and Biological Insights into Redox Activity of Metallacarborane Complexes in Cancer Cells

12:00 – 12:15 I. Kindrat – Optical Spectroscopy of the Tb-doped and Tb-Ag-co-doped Lithium Tetraborate Glasses

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13:00 – 13:15 I. Shcherba – Valence-Variable Rare-Earth Systems: Candidates for Next-Generation Adaptive Materials

13:15 – 13:30 J. Narojczyk – Systematic study of altering elastic properties of the f.c.c. hard sphere crystal containing different nanolayer–nanochannel inclusions composed of aperiodic phase of hard dumbbells

13:30 – 13:45 K. V. Tretiakov – Magneto-hydrodynamic self-assembly versus a new criterion for forming non-equilibrium self-organization structures

13:45 – 14:00 J. N. Grima - Cornish – Can auxetics be both functional and beautiful?

14:00 – 14:15 E. Bajada – New Auxetic Perforated Sheets Based on the 'Rotating Squares' Model

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Combining the benefits of conventional and high-entropy materials - mid-entropy perovskites for application in solid oxide fuel cells

J. Adamczyk[1], J. Dąbrowa[1], M. Zajusz[1], M. Nowakowska[1], K. Zielińska[2]

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Selected medium-entropy subsystems of Sr-free La(Co,Cu,Fe,Mn,Ni)O_3 perovskite were synthesized and their SOFC-relevant properties were investigated to assess the possibility of their application as cathodes in solid oxide fuel cell technology. Using the Pechini sol-gel method, the following materials were synthesized: La(Co,Fe,Cu,Mn)O_3, La(Co,Fe,Mn,Ni)O_3, La(Co,Fe,Cu,Ni)O_3, La(Co,Fe,Ni)O_3, La(Co,Fe,Cu)O_3, La(Co,Fe,Mn)O_3. The influence of individual dopants (copper, nickel and manganese) on the properties of the obtained compositions is thoroughly examined. XRD measurements show typical perovskite *R*-3*c* and *Pnma* symmetries for Mn-free and Mn-containing materials, respectively, and single-phase structure is retained for five materials (with only a small amount of Ruddlesden-Popper-type phase for La(Co,Fe,Cu)O_3). The oxygen non-stoichiometry remains at relatively low level in the RT-900°C temperature range for four materials, only La(Co,Fe,Cu,Ni)O_3 and La(Co,Fe,Cu)O_3 possess more oxygen vacancies, the amount of which increases at higher *T*. Thermal expansion coefficient values, investigated using dilatometry, are relatively similar for all materials, varying in the range of $15\text{-}17 \cdot 10^{-6}$ 1/K. Most importantly, no sign of deleterious chemical expansion mechanism at higher temperatures is visible. This type of thermomechanical behavior is typical for high-entropy materials and its benefits are still maintained in medium-entropy compositions. The character of conductivity and total conductivity values are profoundly influenced by the presence of Mn, which changes the behavior from metallic-like to typical semiconducting and decreases the maximum total conductivity from > 400 S/cm to 30-120 S/cm. All materials exhibit full chemical compatibility with state-of-the-art GDC and LSGM electrolytes, which enables their application as cathodes in SOFC technology. Electrochemical impedance spectroscopy is used to evaluate the catalytic activity of the investigated materials in symmetrical cell configuration with both GDC and LSGM electrolytes. Cathodic polarization resistance values, in Sr-free compositions, of 0.10 $\Omega \cdot cm^2$ at 750°C for La(Co,Fe,Cu)O_3 and 0.12 $\Omega \cdot cm^2$ at 700°C for La(Co,Fe,Cu,Ni)O_3 are superior to most state-of-the-art cathode materials like LSF or LSCF. The general conclusion is that Cu-based materials are vastly superior in terms of catalytic and transport properties, while maintaining similar thermomechanical and chemical stability in comparison to Cu-free ones. These results indicate that medium-entropy perovskites present a promising approach to combine the benefits of conventional and high-entropy materials.

Acknowledgments

This research was supported by the Polish National Science Center (NCN) under project No. UMO-2021/41/B/ST8/04365.

The CECOMEC project: CEria-based COMpounds as effective catalyst for Electrochemical Cells

S. Amatori[1]*, K.Kujawska*[2]*, M. Dominów*[2]*, B. Bochentyn*[2]*, K. Sowa*[3]*, P. Korceki*[3]*, and F. D'acapito*[4]

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Double-doped ceria materials have attracted considerable attention as potential electrolytes for Solid Oxide Fuel Cells (SOFCs) thanks to their high oxygen ion conductivity, thermal stability and flexible redox properties. The aim of the CECOMEC project [1] is to select the best dopants for use in SOFCs. In this study, a series of double doped ceria materials were synthesized using the Pechini method, an approach that enables fine control over cation distribution and homogeneity. The dopants of choice were selected from a number of lanthanides (La, Sm, or Nd), and transition metals (Fe, Co, Ni, Cu, Ru, Ag, Pt, or Au). The investigation focuses on the characterization of the prepared samples to understand their structure and physicochemical properties, and on understanding how those relate to vacancy formation and ionic transport properties.

The samples were subjected to a reduction process in pure H_2 at 900 °C to assess the redox behavior of the dopants and the stability of the resulting oxygen deficient systems. A complete characterization was achieved using complementary techniques such as XAS, XRD, μ-XRF, SEM, TPR/TPO and BET model, revealing distinct behaviors between dopant families. Lanthanide dopants predominantly substitute cerium in the fluorite lattice, generating vacancies without forming segregated secondary phases. In contrast, transition metal dopants exhibited different results: in most cases oxide phases were found in the pristine sample, while in other cases a metallic subphase formed in the pristine sample, indicating and early reduction and segregation during synthesis. The La-Fe co-doped sample displayed an intermediate behavior, with XAS confirming a +3 oxidation state but not showing the presence of a Fe oxide subphase. In all cases the reduction process leads to a metallic phase being formed, which remains homogeneously dispersed.

References

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Density Functional Theory Study on the Photovoltaic Properties of End-Capped Acceptor–Modified Phenylsulfonyl Carbazole Materials for Solar Cells

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Solar energy is a rich, renewable resource that could enhance environmental health that is associated with fossil fuels [1]. Through efficient binding, supported towards a sustainable energy future and efforts to moderate pollution and diminish greenhouse gas emissions [2]. Organic solar cells (OSCs) have emerged as a promising technology owing to their distinct abilities, such as flexibility, low density, and compatibility with roll-to-roll manufacturing [3].

In this study, a series of phenylsulfonyl carbazole-based organic chromophores, labeled PSCD1–PSCD6 (Figure 1), were developed by modifying the terminal group of the parent PSCR chromophore. Quantum chemical analyses were conducted at the M06/6-311G(d,p) level to examine their electronic, structural, chemical, and optical characteristics. All designed derivatives showed decreased band gaps ($\Delta E = 2.742–3.025$ eV) and pronounced bathochromic shifts ($\lambda_{max} = 496.891–545.009$ nm) relative to PSCR. DOS and TDM results highlighted the significant role of the central acceptor unit in facilitating charge transfer. Furthermore, the low exciton binding energy values of PSCD1–PSCD6 indicated improved exciton dissociation and more efficient charge transport compared to PSCR. The calculated open-circuit voltages (V_{oc}) ranged from 1.015 to 1.720 V for the investigated compounds. Among them, PSCD4 exhibited the lowest band gap of 2.742 eV and the most red-shifted absorption maximum at 545.009 nm. Overall, the outcomes suggest that these designed chromophores hold strong potential for application as effective photovoltaic materials.

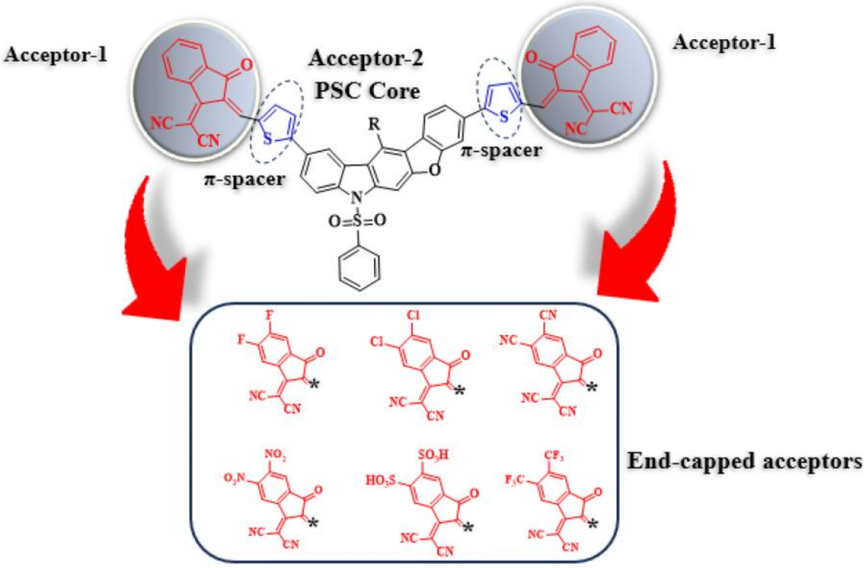

Fig. 1 Modification of the reference compound (PSCR) to design its derivatives using different end-capped acceptor moieties.

Acknowledgments

This work was financially supported by the research project within the program “Excellence Initiative – Research University” for the AGH University of Krakow and National Science Centre Poland (NCN) grant based on decision number UMO-2021/43/D/ST5/00824.

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Synchronization and control of Lorenz systems

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We are interested in developing techniques for meteorological data assimilation and forecasting. We shall use Lorenz systems as toy model, exploiting the replica synchronization scheme for estimating the parameters of a (supposedly unknown) master system, in case of possible access to the dynamical variables and when these are not directly available, and the synchronization can by enacted only through a projection or a data series.

New Auxetic Perforated Sheets Based on the ‘Rotating Squares’ Model

Eucharist Bajada[1], *Pierre-Sandre Farrugia*[1], *Grace Anne Muscat*[1], *James N. Grima Cornish*[1],
Joseph N. Grima[1,2] *and Ruben Gatt*[1]

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We show how the well-known auxetic perforated sheets with diamond-shaped voids reproducing the rotating-square topology can be re-designed via the incorporation of additional triangular voids at the edges of each diamond perforation. We argue that these systems may be better suited for lightweight structural design and applications where specific pore geometries may be required.

Acknowledgments

The funding received from the University of Malta and Xjenza Malta, for and on behalf of the Foundation for Science and Technology, through the Research Networking Scheme (RNS), grant number RNS-2024-062 is most gratefully acknowledged. GAM acknowledges that the work disclosed in this publication is partially funded by the Tertiary Education Scholarships Scheme (Malta). Part of this research has been carried out using computational facilities procured through the European Regional Development Fund, Project ERDF-080 ‘A supercomputing laboratory for the University of Malta’. It has also used equipment and resources provided through the University of Malta Academic Work Resources Fund. Images used courtesy of ANSYS, Inc.

On the way to understanding the great catalytic activity of ceria-based anode materials for biogas-fed Solid Oxide Fuel Cells

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Ceria-based materials present high mobility of oxygen ions [1], high oxygen storage capacity (OSC) [1], attractive redox catalytic properties [2], chemical compatibility with water and carbon dioxide at high temperatures [3], and sufficient resistance to reduction under relatively low oxygen partial pressures [3]. Moreover, the high oxygen mobility in ceria promotes the mechanism of carbon removal, which, in turn, should contribute to the stability of the catalysts on hydrocarbon conversion reactions [1]. Therefore, ceria-based compounds can be applied as catalytic layers deposited on the anode side.

This study focuses on both structural and electrical properties of ceria-based compounds synthesized to improve the stability and catalytic activity of biogas-fed Direct Internal Reforming Solid Oxide Fuel Cells. Compounds from the ceria group were characterized by various methods, i.a. XRD, SEM, TEM, XPS, XAS, 4WDC, and IS. The occurrence of cerium in the mixed valence state of Ce^{3+}/Ce^{4+} was confirmed, which has a significant influence both on catalytic properties and on the resistance to carbon deposition when this material is used as an anode for SOFC.

Progress and obstacles in understanding the anode activity with ceria additives will be discussed.

Acknowledgments

This work was supported by the National Science Center under grant no. 2021/42/E/ST5/00450.

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Laser-Anchored Ruthenium in a Protective TiN-TiO_2 Matrix for Highly Stable Acidic Oxygen Evolution

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Ruthenium (Ru)-based catalysts are among the most efficient materials for the acidic oxygen evolution reaction (OER), a key process in water electrolysis for sustainable hydrogen production. However, under acidic OER conditions, Ru dissolution leads to the loss of active sites and contamination of the electrolyte, significantly hindering large-scale application. In this study, we introduce an in-situ synthesis of Ru-TiO_2-TiN composite electrode on Ti substrate by the laser method.

The Ru-TiO_2-TiN multiphase doping structure was formed by anchoring Ru within TiO_2-TiN using laser treatment. Ru-TNO/Ti-3 exhibited significant electrocatalytic activity, with an OER overpotential as low as 190 mV at 10 mA cm^{-2}. At the same current density, the lowest voltage required for water decomposition was 1.48 V, with no noticeable degradation observed during long-term acidic oxygen evolution testing. The high activity is attributed to the ability of TiO_2-TiN to enhance electrode charge transport, while Ru-O-Ti promotes the activation of the electronic structure.

The mechanism behind the high stability is linked to the partial oxidation of TiN during the acidic OER process, which further promotes the formation of TiO_2-TiN and Ru-N-Ti. TiO_2-TiN provides external protection, preventing further dissolution of Ru by the acid, while Ru-N-Ti helps maintain the valence state balance of Ru and reduces oxidation. Overall, this work demonstrates that the one-step laser synthesis strategy not only boosts the catalytic activity of Ru-based OER catalysts but also significantly enhances their stability, offering a promising pathway for durable acidic water-splitting electrodes.

Determining the influence of Ag and Ni phases on the thermoelectric characteristics of multicomponent oxide composites

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Strong candidates for thermoelectric applications at high temperatures, multicomponent oxides (MCOs) are distinguished by their exceptional thermal stability, tunable electrical behavior, and compositional diversity. Multiple cations result in disordered and structurally complicated lattices, which offer a variety of ways to customize thermoelectric characteristics through compositional changes and regulated defect chemistry [1–3].

The aim of this research is to create composite thermoelectric materials based on perovskite-type MCOs (ABO_3 structure), in which the B-site is substituted with a mixture of Fe, Zr, Hf, Sn, Ti, Ce, Co, In, Sm, Y, and/or Yb, and the A-site is occupied by barium. The creation and analysis of MCO-based composites including metallic silver (Ag) and nickel (Ni) in various weight % configurations are the main focus of present work. In order to create conductive phases inside the ceramic matrix, these metals are added using solid-state synthesis. The objective is to improve electrical conductivity while maintaining the thermal stability and structural integrity of the oxide host.

X-ray diffraction (XRD) and scanning electron microscopy (SEM) are used to structurally characterize the produced composites in order to assess the phase purity and microstructural distribution of metallic inclusions. Under controlled pO_2 and pH_2O conditions, 4-wire DC is used to study electrical conductivity. The impact of metallic additions on the thermopower response is specifically examined, and the overall Seebeck coefficient is evaluated in a broad temperature range. Additionally, because protonic defects have the potential to improve effective thermoelectric performance, their involvement in transport pathways is taken into consideration. Designing next-generation oxide-based thermoelectrics is made easier by the reported effects of Ag and Ni on microstructure, electrical transport, and thermoelectric performance.

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Microscopic and macroscopic aspects of prenematic fluctuations in nanoparticles-doped liquid crystals

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Liquid-crystal (LC) phases anchored on nanostructures or doped with nanoparticles (NPs) are gaining attention due to their intrinsic properties and their potential for novel technological applications. The incorporation of nanoparticles into a liquid-crystalline matrix is a highly effective strategy to tailor its physical characteristics — including electrical and thermal conductivity, switching voltage and dielectric anisotropy. Furthermore, the use of appropriate polymer substrates, functioning as microcells filled with nanoparticle-doped liquid crystals, facilitates the development of devices such as communication antennas and radiation detectors.

This study integrates broadband dielectric spectroscopy with molecular dynamics (MD) simulations to explore how nanoparticle inclusions influence pretransitional phenomena in liquid-crystal systems. Emphasis is placed on elucidating the relationship between nanoparticles, topological defects and prenematic behavior. Experimental investigations on SiO_2-doped 4-Cyano-4′-pentylbiphenyl composites reveal that, while NP additions do not significantly alter the isotropic-nematic transition temperature (Tc), prenematic effects exhibit universal behavior, confirmed by identical critical exponents across all samples. However, prenematic fluctuations display consistent critical behavior across samples, indicating that the intrinsic nature of these fluctuations is maintained despite the presence of nanoparticles. Importantly, MD simulations elucidate the experimentally observed monotonic reduction in dielectric permittivity as nanoparticle content increases. The simulations identify nanoparticles as nucleation centers for topological defects, inducing a “hedgehog” arrangement in neighboring LC molecules. This defect-driven static structure promotes a local antiparallel orientation of molecular dipoles, resulting in their partial cancellation. Consequently, this provides a mechanistic link between microscopic nanoparticle-induced ordering and the altered macroscopic dielectric response, underscoring the pivotal role of local defect structures in tuning the dielectric properties of nanoparticle-doped LC composites.

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Producing environmental-friendly high-energy gas mixtures for solid oxide fuel cells via unrecyclable plastics pyrolysis

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Waste treatment, particularly of non-recyclable polymers, remains a subject of significant scientific and industrial interest. Various approaches have been proposed to address this challenge, including biotechnological, photocatalytic, and pyrolytic processes aimed at recycling or decomposing such materials. This study addresses catalytic and non-catalytic pyrolysis of polypropylene waste to achieve material decomposition while simultaneously producing valuable gaseous products, notably hydrogen-rich synthesis gas and biogas-type mixtures intended as fuels for solid oxide fuel cells (SOFCs). To ensure process scalability and industrial viability, development of more efficient catalysts is required.

Pyrolysis experiments were performed at a slow to moderate heating rate (10 °C min^{-1}) to investigate the effects of carrier gases (Ar, CO_2, mixture of Ar and H_2O), temperature (600-800 °C) and the presence of a catalyst. Conventional iron oxides and composite materials based on Fe/Fe_xO_y and SrTiO3 were synthesized via various routes and treatments, and compared to identify optimal conditions for producing SOFC-compatible fuels.

A synthetic gas mixture (2:1 CH_4:H_2), formulated from the pyrolysis gas composition, was used to fuel the cell. Potential cell modifications to improve compatibility with different fuel compositions are discussed. Catalysts and fuel cells were characterized by standard techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS).

Acknowledgments

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The effect of the presence of a microwave magnetic field on the magnetic ordering of a ferromagnetic material

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Based on the solutions of the system of stochastic Landau-Lifshitz-Gilbert (LLG) equations [1] for the magnetization of a ferromagnet, an analysis of the dependence of the magnetic ordering in a ferromagnet subjected to a microwave magnetic field $H(\mathrm{t})=H0\cos(\omega \mathrm{t})$ was carried out. It was assumed that the power of absorbed radiation $P(f)=\mu 0\ \pi\ \chi''\ f\ H0$ is converted into heat by changing the temperature of the system [2]. The presented model is related to the atomistic model of a ferromagnet [3].

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Overview of quantum technologies and their availability for science

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The presentation aims to present the most important technological [1] breakthroughs in the field of quantum computers, with particular emphasis on solutions that have gained practical application in recent years.

The focus will also be on technologies available to the scientific community [3]. The evolution of key hardware architectures such as superconducting, photonic and ion trap-based architectures will be discussed (briefly). The development of cloud [4] platforms enabling wide access to real quantum computers for both research and educational purposes will also be addressed.

Slightly more attention was devoted to projects by IBM Quantum, Google Quantum AI, Microsoft Azure Quantum, D-Wave and European initiatives, including Polish EuroQCS systems. The presentation will also cover current limitations [2], challenges and prospects for further [5] development of this dynamic industry.

In addition, participants will learn about the available programming tools and the possibilities of remote use of quantum infrastructure, which enables even centers without their own laboratories to actively join the global technological race.

The presentation is aimed at scientists interested in modern computing technologies and those planning to start research using quantum computers.

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Biochemistry and electrochemistry from first principles using ONETEP

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Accurate studies of crucial biochemical processes, such as protein folding or protein-ligand binding, require taking into account the solvent environment. Similarly, in the study of electrochemical interfaces in devices for energy conversion and storage, solvent and electrolyte need to be accounted for. Explicit inclusion of the solvent and electrolyte with full atomistic detail is usually computationally unfeasible because it necessitates extensive averaging over the solvent and electrolyte degrees of freedom, and increases the system size. The implicit solvent (IS) approach seeks to address this difficulty by introducing an unstructured continuum dielectric to represent the solvent, and point-like Boltzmann ions to represent the electrolyte.

Kohn-Sham density functional theory (KS-DFT) is a first principles approach for modelling the behavior of systems at the atomic scale with full details of the electronic structure. The computational cost of conventional KS-DFT calculations scales cubically with the number of electrons in the system. This limits the applicability of this electronic structure method to systems of at most several hundred atoms on today's resources.

The ONETEP approach reformulates KS-DFT in terms of the density matrix, leveraging Kohn's electronic near-sightedness principle. By using strictly localized orbitals and a spatial cutoff in the density kernel, it achieves linear-scaling cost of the calculation. Using a minimal basis of the orbitals keeps the scaling prefactor low, while their *in-situ* optimization to the unique chemical environment of each atom offers near-complete-basis-set accuracy. ONETEP enables alculations with tens of thousands of atoms at the same level of accuracy as plane-wave methods.

In this talk we present a hybrid model combining linear-scaling DFT, a minimal parameter implicit solvent model, and an electrolyte model for grand canonical ensemble calculations under potential control, implemented within the ONETEP framework. Our approach, which automatically achieves the neutralization of the charge on the electrode by a build-up of counter charge in the electrolyte, supports both open and periodic boundary conditions. The model has been parametrized with respect to the reduction potential of standard electrodes and the activity coefficient of electrolytes. We demonstrate the accuracy and feasibility of the solvent model on calculations of free energy of solvation and protein-ligand binding energies in solvent; and of the solvent and electrolyte model by showing results for differential capacitance of graphene based electrodes and lithium nucleation on a graphite anode in Li-ion batteries.

Niobium modification of 9-series Ni-rich NCA cathode materials for lithium-ion batteries: An LSTM model for degradation prediction

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The increasing demand for high-energy lithium-ion batteries, driven largely by the growth of electric vehicles, has intensified interest in the so called 9-series cathode materials (Ni content ≥ 0.9 mol). Although these Ni-rich oxides offer high capacity, they are prone to cycling degradation associated with the H2–H3 phase transition. Niobium incorporation can alleviate these issues by refining particle grains and suppressing detrimental phase transitions, while Nb-based surface coatings further improve interfacial conductivity and stability [1,2].

In this work, the baseline cathode material $Li_{1.02}Ni_{0.905}Co_{0.043}Al_{0.052}O_2$ was modified through Nb doping (0.1-1 mol%) and surface coating using ammonium niobium oxalate (ANO). The resulting material series was thoroughly evaluated with respect to physicochemical characteristics and electrochemical performance. An optimal Nb doping level of 0.5 mol% was identified. Subsequent ANO treatment effectively removed residual lithium and facilitated the in-situ formation of a $LiNbO_3$ coating. To better understand the improved cycling stability, an LSTM model was employed, revealing altered charge-discharge behavior, suppression of the H2–H3 phase transition, and enabling prediction of capacity fade and discharge curve evolution.

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Can auxetics be both functional and beautiful?

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Auxetic materials derive their distinctive behaviour directly from their geometry, making their mechanical performance inseparable from their visual character. Unlike conventional materials, auxetics are inherently expressive: their lattices, whether re-entrant, chiral, or hierarchical, communicate function through dynamic, visible transformations. This work looks into applications where aesthetics are important (e.g. sportswear and sports safety gear) and argues that as auxetics move from research settings into design practice, aesthetic considerations are as critical as mechanical performance. It explores this interplay through classical principles of proportion, symmetry, and rhythm, perceptual frameworks such as Gestalt theory, cultural recognisability, and the evolving role of aesthetics across technological readiness levels. Drawing on examples from nature and design, the study shows that auxetics operate according to a unique visual logic, balancing regularity with inversion, harmony with disruption. This work concludes that for auxetics, form and function are inseparable: aesthetic understanding must guide development from the outset, positioning auxetics as a synthesis of geometry, perception, and cultural form where beauty and functionality coincide.

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Better Sports Safety Gear Through the Use of Auxetics

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We show how auxetics, a unique class of materials and structures that exhibit a negative Poisson's ratio, can be put to good use in the design of next-generation sportswear and personal protective equipment (PPE) for use in sports, with a focus on coastal rowing. We argue that through the use of well-known auxetic motifs, we can produce better PPE with better breathability and an enhanced fit that can adapt more effectively to the contours of the body during movement without sacrificing mobility. These are two of the main characteristics that rowers have been found to look for when making decisions as to whether they should use, or not use, PPE during training and/or competition.

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Quantum Chemical and Biological Insights into Redox Activity of Metallacarborane Complexes in Cancer Cells

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The presented study [1] established a link between the electronic characteristics of metal centers in metallacarboranes and their capacity to influence mitochondrial oxidase function and to promote membrane hyperpolarization in cancer cells. Advanced computational approaches, including density functional theory (DFT) and molecular dynamics, were applied to explore both oxidized and reduced variants of metallacarboranes as well as their internal rotational dynamics. Assuming that the metal ions are low-spin, it was found that the internal movements of the cluster ligands are strongly dependent on the metal type and are consistent with the observed cellular uptake patterns of these complexes during in vitro experiments. Notably, the low-spin iron analogue appears to act as a novel external modulator of redox balance in cancer cells that show resistance to cisplatin, inducing a metabolic breakdown that ultimately leads to cell death.

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Optical Spectroscopy of the Tb-doped and Tb-Ag-co-doped Lithium Tetraborate Glasses

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Lithium tetraborate ($Li_2B_4O_7$) glasses doped with Tb_2O_3 and co-doped with Tb_2O_3 and $AgNO_3$ were obtained by the conventional melt-quenching method and characterised by optical absorption and photoluminescence (emission and excitation spectra, decay kinetics, quantum yield) techniques [1]. The optical absorption spectra of the $Li_2B_4O_7$:Tb and $Li_2B_4O_7$:Tb,Ag glasses reveal narrow and very weak $4f - 4f$ absorption bands related to Tb^{3+} ($4f^8$) ions. The luminescence emission spectra of both investigated glasses in the range of 400–700 nm show numerous narrow emission bands corresponding to the $^5D_4 \rightarrow {}^7F_J$ (J = 6 – 0) and $^5D_3 \rightarrow {}^7F_J$ (J = 5 – 3) transitions of Tb^{3+} ions. The most intense emission band, which accounts for almost 60% of the total integral luminescence intensity, is centered at 541 nm and belongs to the $^5D_4 \rightarrow {}^7F_5$ transition of Tb^{3+} ions. The luminescence emission spectra of the $Li_2B_4O_7$:Tb,Ag glass additionally show two broad weakly-resolved emission bands in the violet-green spectral range attributed to Ag^+ ($4d^{10}$) ions and non-plasmonic Ag nanoclusters (Ag_m^{n+} centres). The decay kinetics of the observed emissions are characterised by ms-scale lifetimes for Tb^{3+} ions and μs-scale lifetimes for Ag^+ ions and Ag nanoclusters.

Enhancement of the Tb^{3+} luminescence intensity and quantum yield was observed in the $Li_2B_4O_7$:Tb,Ag glass, which can be explained by the excitation energy transfer from Ag^+ ions and Ag nanoclusters (donors) to Tb^{3+} ions (acceptors). Overall, silver co-doping is a promising approach to improve the luminescent properties of Tb^{3+} ions in lithium tetraborate glasses and the $Li_2B_4O_7$:Tb,Ag glass is a good light-emitting material for the green spectral range. The main advantages of this borate glass are its simple preparation process and the possibility to produce large luminescent layers, which are difficult to achieve with powders and single crystals.

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Surface modification of Ni-YSZ anodes to improve the stability of biogas-fed SOFC

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Solid oxide fuel cells (SOFCs) have attracted increased attention because they offer high electrical efficiency, fuel versatility, and the ability to reform hydrocarbons internally at elevated temperatures. Their capability to operate on fuels beyond pure hydrogen, such as methane, syngas, or biogas, enables energy production using renewable or waste-derived fuels. However, the conventional Ni–YSZ anode suffers from carbon deposition and sulphur poisoning when exposed to such fuels, which significantly limits its long-term durability.

In this work, the exsolution method was proposed as a strategy to improve the anode's tolerance against these degradation mechanisms. Exsolution is a process in which metal cations migrate from the bulk of the perovskite lattice and nucleate on the surface under reducing conditions, forming finely dispersed and socketed nanoparticles. This strong metal–support interaction provides high structural stability and prevents particle agglomeration during redox cycling. The partially embedded particles act as active catalytic centers, promoting fuel reforming and oxidation reactions while effectively suppressing carbon deposition on the anode surface.

The $La_{0.27}Sr_{0.54}Ce_{0.09}Co_{0.1}Ti_{0.9}O_{3-\delta}$ (LSCCoT) material was synthesized via the solid-state reaction method and characterized using SEM, XRD, and electrical measurements. The material was then applied as a catalytic layer on the SOFC anode to evaluate its effect on cell performance and direct internal reforming (DIR) of biogas. The cells, with and without the catalytic layer, were tested under a synthetic biogas mixture (60 vol% CH_4 / 40 vol% CO_2) using electrical characterization and electrochemical impedance spectroscopy (EIS) combined with distribution of relaxation times (DRT) analysis. The results demonstrated that the addition of the exsolved catalytic layer delayed cell degradation and significantly extended its operational stability in biogas, highlighting exsolution as a promising route to durable, fuel-flexible SOFC systems.

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Low-Temperature(60°C) Synthesis of Sodium-Doped Triazine/Heptazine g-C_3N_4/Bi_2S_3 Heterostructures for High-Performance Supercapacitors

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Graphitic carbon nitride (g-C_3N_4) has emerged as a promising electrode material for supercapacitors; however, its inherent low capacitance limits practical applications. In the current work, we report the synthesis of a sodium-doped g-C_3N_4/Bi_2S_3 composite featuring a triazine/heptazine heterostructure, synthesized via a low-temperature (60 °C) route using an amine-based precursor. The methodology adopted requires significantly lower energy compared to conventional synthesis (>550 °C) and is scalable. The resulting Na-g-C_3N_4/Bi_2S_3 heterostructure delivers an exceptional specific capacitance of 1680 F g^{-1} at 1 A g^{-1} attributed to enhanced charge transport and interfacial synergy between Na-g-C_3N_4 and Bi_2S_3. This work demonstrates an efficient and green pathway to synthesizing Na-g-C_3N_4/Bi_2S_3 composite-based electrodes, having potential next-generation supercapacitor applications with high performance, durability, and scalability, through structural tuning and mild synthetic conditions.

Performance of Cu-Ag Thin Film Catalysts Deposited by Thermal Evaporation for CO_2 Reduction in Flow cell system

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The persistent challenge of global climate change has accelerated the development of electrochemical technologies for the conversion of CO_2 into valuable chemical products. Among these, the generation of multi-carbon (C_{2+}) hydrocarbons is particularly attractive due to their potential as renewable energy carriers [1]. Copper continues to be the standard catalyst for this transformation, owing to its distinct capability to facilitate C–C coupling reactions [2]. In this work, we investigate thermally evaporated copper-silver alloy thin films as advanced electrocatalysts for CO_2 reduction, focusing on their performance in a gas diffusion electrode (GDE) based flow reactor [3].

By alloying copper with controlled amounts of silver, we systematically tailor the catalyst surface characteristics and electronic properties. The thermal evaporation method enables uniform deposition and precise control of catalyst composition and thickness, optimizing interaction with the gas–liquid interface. Electrochemical tests were conducted at current densities ranging from –150 to –190 mA/cm^2, demonstrate that the incorporation of silver enhances both the selectivity for C_{2+} products and the long-term stability of the catalyst.

Comprehensive characterization using XRD, WD-XRF, SEM, FTIR, and profilometry reveals the structural robustness of the Cu-rich alloys and the stabilizing effect of silver during prolonged electrolysis. Faradaic efficiencies, quantified through GC-MS/TCD confirm the preferential formation of hydrocarbons over a 240-minute operation window. These findings underscore the dominant role of copper in facilitating multi-carbon product formation and highlight silver contribution to improving catalyst durability. Overall, the study offers a tunable, scalable pathway for developing high-performance bimetallic catalysts for CO_2 electroreduction in flow systems.

The Cu–Ag alloy layers fabricated through thermal evaporation exhibited excellent uniformity and well-controlled morphology, as confirmed by SEM imaging and profilometry measurements. XRD analysis verified the formation of bimetallic Cu–Ag phases with varying Ag contents, while WD-XRF provided accurate quantification of elemental composition for all samples.

Electrochemical evaluation showed that decreasing the Ag content enhanced the selectivity toward C_{2+} hydrocarbons, particularly ethylene. The best performance was observed at intermediate Ag concentrations. At current densities between –150 and –190 mA/cm^2, the electrodes delivered high Faradaic efficiencies for the desired products, indicating effective utilization of charge for CO_2 conversion. Furthermore, the electrodes demonstrated strong operational stability with minimal degradation during extended electrolysis.

This work demonstrates that Cu–Ag bimetallic catalysts prepared via a scalable thermal evaporation method are highly effective for the selective electrochemical reduction of CO_2 to valuable multi-carbon products.

The ability to precisely tune the Ag:Cu ratio, film thickness, and surface morphology provides a versatile platform for optimizing catalytic performance. At a fixed current density, the catalytic behavior was strongly dependent on composition:

Higher Cu content → increased CH_4 formation and deeper reduction pathways

Higher Ag content → greater selectivity toward CO or C_{2+} products, with reduced CH_4 formation

These results highlight the importance of compositional and structural control in improving CO_2RR activity and selectivity. Overall, thermally evaporated Cu–Ag alloy catalysts show strong potential as durable and efficient materials for scalable carbon-conversion technologies. Future studies should focus on long-term durability and integration into renewable-energy-powered CO_2 electrolysis systems.

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Systematic study of altering elastic properties of the f.c.c. hard sphere crystal containing different nanolayer–nanochannel inclusions composed of aperiodic phase of hard dumbbells

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The ability to tailor elastic properties of materials to fit a prticular applications is the goal that materials engneering struggles with for quite some time. In recent years, when the technology allows us e.g. to 3D-print structures and systems in sub-micro and even nano scales, such ability seems to be of paramount importance. However, experimenting with structural modification of materials at such scales requires costly equipment. To mitigate this, one might turn to computer simulations as an alterntive approach to gain insight into processes and phenomena at the atomic level that have direct impact on (macroscopic) elastic properties. Despite the fact that the latter are one of the oldest studied physical parameters of matter, our understanding of the microscopic phenomena behind them is still limited. The origin of negative Poisson's ratio [1] (NPR) in materials is one example. The work by Lakes [2] who first obtained a man-made NPR foam by (macroscopic) structural modification of polyurethane, proved that this approach is worth of attention when looking for new materials with extraordinary elastic properties. At the same time Wojciechowski [3,4] showed that negative Poisson's ratio can also result from molecular interactions. Thus, one might expect that modifying material structure at the micro level, the auxeticity [5] would occur in the modified material. The latter term has been coined to negative Poisson's ratio materials. The ones that exhibit NPR only in some directions and zero or positive Poisson's ratio in others are called partial auxetics [6]. The idea of structural modifications at the crystall structure level has been succesfully applied and showed a significant [7] or moderate [8] enhancement of auxeticity in f.c.c. crystals of hard spheres, when using nanochannel or nanolayer inclusions respectively. However, their combination had completely eliminated auxetic properties of the crystal [9]. This showed that our understanding of the microscopic phenomena behind the macroscopic elastic properties of materials is still limited. The study presented during this talk is an in-depth extension of the above mentioned research. With the help of Monte Carlo computer simulations, the otherwise periodic crystal containing a joined nanolayer-nanochannel inclusions, further modified to include a degree of disroder. The latter is introduced in the form of (aperiodic) degenerate crystalline phase [10-14] of hard di-atomic molecules (dumbbells), that constitute the inclusions. Different sizes of inclusions have been studied by varying the size of the nanochannel or by the number of adjecent crystalographic layers. The impact of these modifications on elastic properties has been investigated with the help of the Parrinello-Rahman approach in the isothermal-isobaric ensemble (NpT). Conclusions from the studies [15,16] will be discussed during the talk.

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Structural and transport properties of triple-conducting (BaSr)(FeMoZnZr)O_3 perovskites for Solid Oxide Fuel Cell technology

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Ba and Zn are well known for their ability to improve proton uptake in perovskite-structured oxides, and Zr is helpful in stabilizing the perovskite structure [1]. Therefore, they were used to dope $SrFe_{0.75}Mo_{0.25}O_{3-\delta}$ (SFM), creating series of triple-conducting materials. The base SFM exhibits stability in a wide range of oxygen partial pressures [2], which makes it possible to use it as both cathode and anode in symmetrical Solid Oxide Fuel Cells (SOFCs). However, its cathodic performance still needs further improvement.

Based on the above information, $Ba_ySr_{1-y}(Fe_{0.75}Mo_{0.25})_{1-2x}Zn_xZr_xO_{3-\delta}$ was synthesized. Materials with low Ba content showed a cubic structure regardless of the amount of Zn and Zr. The Ba-rich samples show the presence of additional phases, except for a material with a hexagonal structure (Fig. 1a). The highest proton concentration $[OH_O^{\cdot}]$ was measured for almost single-phase cubic $BaFe_{0.45}Mo_{0.15}Zn_{0.2}Zr_{0.2}O_{3-\delta}$ (9 mol% at 250 °C) (Fig. 1b). The standard hydration enthalpy ranges from -23 kJ/mol for SFM to -70 kJ/mol for $BaFe_{0.45}Mo_{0.15}Zn_{0.2}Zr_{0.2}O_{3-\delta}$.

The $y = 0$ series was selected for SOFC testing with a GDC electrolyte (650 µm thickness) [3]. $SrFe_{0.6}Mo_{0.2}Zn_{0.1}Zr_{0.1}O_{3-\delta}$ shows the best combination of properties, resulting in the lowest polarization resistance. Full cell tests have shown that SFM-based materials are a promising Co-free alternative to state-of-the-art SOFC materials (Fig. 1c), and the conducted studies suggest the possibility of using the tested group of materials in PCFCs and symmetrical SOFCs.

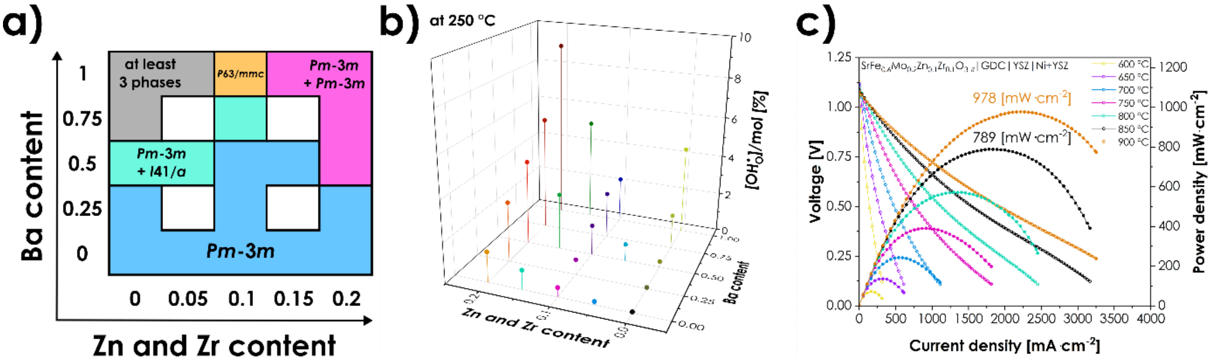

Fig. 1. a) Phase structure for all materials. b) Proton concentration in pH_2O = 16.7 mbar (in N_2) at 250 °C. c) I-V and power density curves for the full SOFC utilizing $SrFe_{0.6}Mo_{0.2}Zn_{0.1}Zr_{0.1}O_{3-\delta}$ as the cathode.

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Spectroscopy and optically stimulated luminescence of the *β*-irradiated $Li_2B_4O_7$:Cu,Eu glass

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In recent decades, the phenomenon of optically stimulated luminescence (OSL) in various materials has been intensively studied with the prospect of its widespread application in radiation protection dosimetry. The basis of OSL dosimeters is a working element in which stable radiation centers are formed under *X*, *γ*, *β* and other types of ionizing irradiation, which can be centers of luminescence upon optical excitation. Borate glassy compounds are promising materials for dosimetry based on both thermoluminescence (TL) and OSL phenomena. Borate crystalline and glassy compounds are also sensitive to neutron irradiation due to the presence of the ^{10}B boron isotope (natural abundance – 19.6 %) with a large interaction cross section that allows the manufacture of OSL dosimeters for a wide range of radiation exposure, including neutrons. The $Li_2B_4O_7$:Cu,Eu glass was first investigated in [1] as a potential active element in OSL dosimetry.

The $Li_2B_4O_7$:Cu,Eu glass containing 1.0 mol.% CuO and Eu_2O_3 impurities was initially studied in [2] by XRD, electron paramagnetic resonance (EPR) and optical spectroscopy techniques. The interatomic distances and coordination numbers were derived from XRD data analysis. The EPR and optical absorption, emission, photoluminescence excitation show that the Cu impurity is incorporated into the $Li_2B_4O_7$ glass network as Cu^{2+} ($3d^9$) and Cu^+ ($3d^{10}$) ions. The Cu^{2+} ions in $Li_2B_4O_7$:Cu,Eu glass show characteristic EPR and optical absorption spectra. Spin Hamiltonian parameters of the Cu^{2+} EPR spectrum were determined. Optical absorption spectrum of the $Li_2B_4O_7$:Cu,Eu glass was analyzed and interpreted. Photoluminescence spectra of the $Li_2B_4O_7$:Cu,Eu glass reveal broad blue emission band of Cu^+ ($3d^94s^1 \rightarrow 3d^{10}$ transition) and narrow emission bands of Eu^{3+} ($4f^6$) ions belonging to the $^5D_0 \rightarrow {}^7F_J$ ($J = 0 – 4$) transitions with characteristic decay kinetics.

The dependence of the integrated total infrared OSL (IR-OSL) signal on the dose of *β*-irradiation (the ^{90}Sr/^{90}Y *β*-source) and the IR-OSL decay curves were obtained and analyzed in [1]. It was established that the IR-OSL intensity becomes sublinear at very high radiation doses, while the OSL decay does not follow either first or second order kinetics, and is instead described by the sum of three exponential components. The mechanism of optical release of charge carriers from deep traps, which are continuously distributed in the glass network is proposed. On the basis of presented results, we posit that the OSL mechanisms in the $Li_2B_4O_7$:Cu,Eu glasses are related to Cu and Eu centers and the energy transfer between them.

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Valence-Variable Rare-Earth Systems: Candidates for Next-Generation Adaptive Materials

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Intelligent materials occupy a special place among the huge number of known materials, and new ones are being created all the time. Despite the impressive number of publications, no attempt has yet been made to classify compounds with a valence unstable rare earth element (R. E.) as smart materials. Our studies demonstrate that the value of the valence of the R. E. in some compounds can be changed by external and internal factors. Examples include the external pressure- or temperature-induced change in the valence value ($YbInAu_2$, $EuCu_2Si_2$), the dependence of the valence on the structural type of a compound ($YbNi_4In$ and $YbNiIn_4$), the dependence of the valence on the second component of ternary intermetallic compounds in YbT_4 (T = Au and Mg) and $Yb_2T_3Sn_5$ (T = Pt and Pd), the effect of d- and f-level occupancy on the valence state of Ce and Yb in compounds with the $ThMn_{12}$ structure (Ce and Yb in RM_4Al_8), the dependence of the valence on the occupation of d-levels. Changing the valence value of the R. E. may significantly alter the electrical and magnetic properties of compounds. Based on our studies, and the review of a considerable number of research papers on the physics of compounds with intermediate valence, we argue that such compounds may be classified in the wide class of materials commonly referred to as intelligent materials. The most difficult part of creating intelligent materials and systems based on them is to provide feedback between the external impact and the object's response. Materials become intelligent when the sensing and actuating elements built on their basis are combined into an intelligent structure to achieve the required advanced functionality.

Influence of synthesis conditions on the surface morphology and phase composition of Al-Cu-Ni alloys obtained by selective laser melting.

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Al-Cu-Ni alloys are widely used as lightweight and high-strength materials in many industries. The excellent mechanical properties of these alloys can be explained by the formation of precipitates based on intermetallic compounds of aluminum with copper and nickel [1, 2]. To create the required phase composition of these alloys, classical methods involve the heat treatment of the finished products [3, 4]. Such post-processing requires additional energy and time, which is impractical from an economic and eco-friendly perspective.

Innovative production technologies enable us to overcome these shortcomings. One of the most promising technologies is the selective laser melting of materials from powder precursors [5]. This method allows obtaining finished products of different shapes and sizes under controlled synthesis conditions. In particular, using the laser melting method, it is possible to control the synthesis temperature and cooling rate, which enables heat treatment of the alloy in a single technological process. As a result, by changing the synthesis conditions, it becomes possible to control the phase composition and microstructure of the metal alloys.

Therefore, in this work, the formation of phases in Al-Cu-Ni alloys was studied in the case of their synthesis by selective laser melting. Special attention was paid to the influence of synthesis conditions on the formation of phases following laser melting. The main task of this work was to obtain phases exhibiting a shape memory effect within an aluminum matrix, aimed at developing high-strength composites.

The alloys were synthesized using a fiber laser operated at low laser power. To control the phase composition of the obtained alloys, the amount of absorbed energy was controlled by varying the laser power and scanning strategy. Pure aluminum, copper, and nickel powders were used as raw materials for preparing the alloys. The morphology and phase composition of the obtained alloys were studied by scanning electron microscopy (SEM) and X-ray diffraction (XRD).

Acknowledgments

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Macromolecules in a solvent of varying quality. Monte Carlo computer simulations

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The structure of macromolecular films formed in solvents of varying quality is still not fully understood [1]. Computer simulations of such high-density macromolecular systems require the use of appropriate algorithms, which is why the simulations in this work were carried out using the Cooperative Motion Algorithm (CMA) [2]. For this purpose, a two-dimensional coarse-grained model based on a lattice approximation was used. The behavior of a single homopolymer chain placed in an explicit solvent in a wide range of poor and good solvents was investigated. The theta temperature and the transition temperature from a coil to a disk were determined, and the scaling of the parameters describing the phase transitions of the chain was determined. Differences between the structure of such a disk and the structure of macromolecules in a dense polymer liquid were indicated. It was shown that for systems with polymer-solvent attraction, temporary changes in the size and shape of the chains occur. This is related to the mechanism of chain penetration by the solvent and the formation of structures known as "Bridging-Induced Attraction" [3].

Acknowledgments

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Simulations of chemical vapor deposition of a graphene layer on a copper substrate

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Owing to its superior mechanical, thermal, and electronic characteristics [1–3], graphene is critical for a wide array of applications [4, 5]. Chemical vapor deposition (CVD) on copper substrates stands out as a primary method for the scalable production of high-quality graphene [6]. However, the computational expense of atomistic modeling renders standard simulations of this process impractical.

To overcome this, a hybrid approach combining molecular dynamics (MD) with time-stamped force-bias Monte Carlo (tfMC) is utilized to simultaneously resolve rapid atomic collision dynamics and extended surface relaxation timescales.

This study applies the hybrid MD/tfMC protocol described by Winczewski et al. [7] to simulate graphene growth from atomic carbon on Cu(111) at three different temperatures: 500 K, 900 K, and 1300 K. Incorporating realistic distributions of incident-atom energies and angles further improved the representation of deposition conditions.

Results confirm that the hybrid methodology effectively replicates essential formation stages, including nucleation, grain coalescence, and the propagation of sp^2-hybridized domains. Temperature exerts a governing influence on kinetics and structural integrity: elevated temperatures yield well-ordered monolayers, whereas lower temperatures increase growth rates but induce higher defect densities. These observations align with experimental literature regarding temperature-dependent coverage.

To assess the practical benefits of tfMC for accelerating the exploration of configuration space, additional simulations were performed in which both deposition and relaxation were executed solely with MD. Despite the theoretical potential of tfMC to expedite the sampling of slow relaxation events, practical time gains were negligible, offering important constraints on the method's applicability.

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Magneto-hydrodynamic self-assembly versus a new criterion for forming non-equilibrium self-organization structures

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A decade ago, we showed that outside of thermodynamic equilibrium, the rate at which energy is dissipated to keep an ordered state is connected to how likely it is to observe that state. This was based on a study of a model system where different ("polymorphic") non-equilibrium structures form for the same system parameters [1]. Since the polymorphs differ only in the rates of energy dissipation – and not in their kinetic or potential energies – it is possible to directly link the probabilities of polymorphs occurring to the rates of energy dissipation. A combination of experiments and simulations shows that the likelihood of a polymorph or "state" decreases exponentially as its dissipation rate increases [2]. In other words, far from thermodynamic equilibrium, nature prefers less dissipative states, though more thermodynamically wasteful structures still have small probabilities. Recent research offers new insights and proposes a criterion for the formation of non-equilibrium self-organizing structures [3].

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The computations were partially performed at Poznań Supercomputing and Networking Center (PCSS), Poland.

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Effect of $FeCl_3$ activation modification on the change in the porous structure of nanoporous biocarbon

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Highly porous biocarbon materials, obtained by carbonization of natural wood, attract the attention of researchers due to their unique microstructure and wide potential application for energy storage systems. Natural wood with predominantly channel-type pores (so-called nutrient channels) is carbonized by pyrolysis. As a result, highly porous biochar is formed, which preserves the microstructural features of the original wood.

The study of the electrical transport properties of biocarbon is of great practical interest, since controlling its transport properties by changing the porous structure, fractality, and electronic structure by choosing the appropriate starting tree, degree of graphitization, and activation modification method can significantly affect the properties of the final product.

The porous structure of activated biocarbon materials was studied by the method of small-angle X-ray scattering. The analysis of small-angle scattering spectra reveals the formation of a surface fractal structure, which indicates the formation of a non-smooth boundary between the pores and the carbon matrix. Using the model of polydisperse spherical particles, the calculation of the radial distribution function was carried out. It was established that the main contribution to the formation of the porous structure of the sample is made by microscopic pores with a radius of 0.9-1.0 nm, the volume fraction of which is from 65 to 85 %. It should be noted that an increase in the content of FeCl3 chloride in the initial solution from 0.1 to 0.5 mol % leads to a decrease in the average effective radius of micropores from 2.6 to 2.0 nm, and, accordingly, in the specific surface area of the pores from 490 to 850 m2/kg.

High-Efficiency terahertz radiation modulator based on single-crystalline germanium

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The terahertz frequency range of the electromagnetic spectrum (0.1 – 10 THz) is attractive for various applications often requiring the modulation of THz radiation.

Additionally, terahertz wave is radiation of low photon energy, insufficient to ionize atoms or damage molecules. Therefore, the use of such waves is safe for the study of materials or cells, in particular for medical imaging and non-invasive and label-free identification of living cells [1-4]. In all these applications, terahertz imaging methods based on single-pixel detectors are used. Terahertz modulator is a key component for single-pixel imaging. One of the approaches to creating spatial modulators of terahertz radiation is the optical method of controlling terahertz radiation using semiconductor materials [5].

This study deals with an optically controlled terahertz radiation modulator for a frequency of 130 GHz using single crystal Ge wafer with chemically etched surfaces. Those wafers having resistivity of $\rho = 50\ \Omega$*cm, thickness $d = 0.51$ mm and orientation of (111) have been used. Double-sided etching was performed in a etchant consisting of 4 cm^3 of HF, 2 cm^3 of HNO_3, 4 cm^3 of H_2O, and 200 mg of $AgNO_3$. The etchant was stored for 30 min before use (etching). The choice of such etchant was due to its low surface recombination rate [6]. Etching was carried out for 2 min. The surfaces of the Ge plate after etching appear having a clearly pronounced roughness. The study on the effect of optical illumination on the modulation of terahertz radiation has been carried using a setup depicted in Fig. 1.

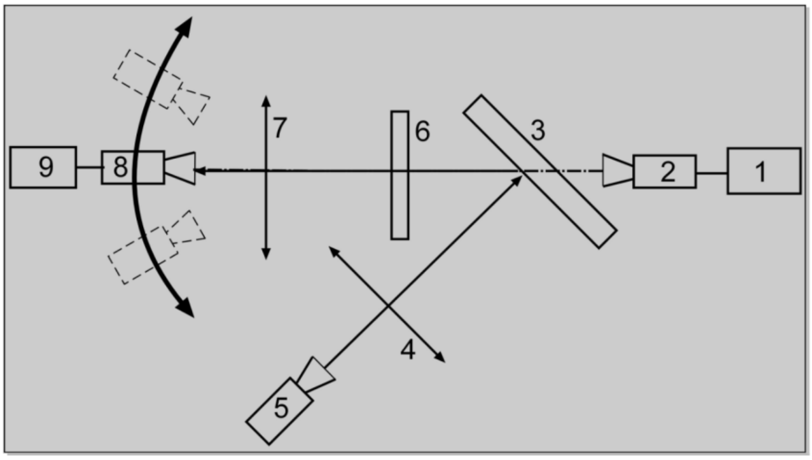

Fig. 1. Layout diagram for measuring optically controlled modulation of terahertz radiation at 130 GHz: 1 – adjustable pulse driver, 2 – Solis-365 D High Power LED lamp (Thorlabs, USA), 3 – ITO film on a glass substrate, 4 – lens, 5 – Si avalanche diode (transmitter), 6 – sample under test, 7 – lens, 8 – GaAs Schottky diode (receiver), 9 – oscilloscope}

The 100 % modulation depth of terahertz radiation has been obtained while illuminating the etched Ge wafer with a power of 0.33 W/cm^2 at λ=585 nm. The modulation time response obtained was 450 Hz. Thus, the performance better than that for single crystal Si based THz modulators has been achieved.

Acknowledgments

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Identifying the effect of doping and cooling rate on presence of ordered and disordered phases in Mn-based rocksalt-type cathode materials for Li-ion batteries

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Among the most promising novel cathode materials for Li-ion cells are lithium-excess cation-disordered oxides with a rocksalt structure (DRXs). These materials, for example, $Li_{1.2}Mn_{0.4}Ti_{0.4}O_2$ (LMTO), have the potential to deliver reversible capacities up to 300 mAh g^{-1}, but are hindered by low intrinsic lithium diffusivity. Therefore, to construct a sufficient percolation network for Li^+, the degree of long-range cation-disorder is imperative regarding overall structure. Particularly, there are limited 0-TM pathways available, which hinder Li migration between octahedral and tetrahedral sites [1, 2]. On the other hand, DRXs may contain different transition (and other) metal elements, so they could benefit from flexibility and modified electronic properties according to the high entropy doping strategy.

In this work, we study the significance of the cooling procedure after annealing at a target temperature that effectively inhibits the disorder-to-order conversion during the synthesis of pristine and doped LMTO. The operando XRD method was employed to detect the changes and to select suitable temperature ranges. For the doping strategy, we introduced $Li_{1.2}Mn_{0.4}Ti_{0.25}Al_{0.05}Fe_{0.05}Mo_{0.05}O_2$ composition, aimed at increasing the configurational entropy. This work demonstrates a method for the effective preparation of high-performance DRX cathode materials.

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DFT-based screening of $REBa_{1-x}Sr_xCo_{2-2y}Cu_{2y}O_{5+\delta}$ candidate air electrode materials for solid oxide fuel cells and electrolyzers

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Looking for highly efficient, durable and cheap air electrode materials for solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs) is still a challenging task, which is crucial to achieve stable performance of these devices. In commonly used ABO_3 or $AA'BB'O_6$ perovskite materials, there are many substitution possibilities and doping strategies to tune the structural and electrochemical properties. However, such an approach is time-consuming and not efficient. Therefore, density functional theory (DFT) may be used as a tool to theoretically predict essential parameters and properties which are demanded for a good air electrode.

In our work, we performed DFT calculations for the $REBa_{1-x}Sr_xCo_{2-2y}Cu_{2y}O_{5+\delta}$ (RE = chosen rare earths; $x = 0, 0.5, 1$; $y = 0, 0.5, 1$; $\delta = 0, 0.25, 0.5, 0.75, 1$) group, by computing unit cell parameters, VASP energies, energies of oxygen vacancy formation, electron localization functions and density of states. Based on the computational results, four best-chosen air electrode materials were experimentally synthesized using a typical sol-gel method and investigated. All of the materials were single-phase; however, depending on the RE ion, they crystallize either in Pm-3m cubic or P4/mmm tetragonal structure. For these materials, electrical conductivities are between 10 – 100 $S\cdot cm^{-1}$ in the 200 – 400 °C range. In symmetrical cells, using a typical $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ electrolyte, polarization resistances ranged between 0.072 to 0.035 $\Omega\cdot cm^2$ at 800°C. For an in-depth electrochemical analysis, full anode-supported cells were prepared. All of the experimentally obtained results follow the theoretical predictions, confirming that DFT screening is a reliable method in SOFC/SOEC air electrode trial searching.

A few words on systems exhibiting a negative Poisson's ratio

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Systems exhibiting negative Poisson's ratio [1], studied since almost 40 years [2-5], are often referred to as auxetics [6]. Many auxetic materials belong to the class of mechanical metamaterials [7].

The first International Workshop on auxetics and other unusual systems, organized in Poznań in 2004 [8], was followed by the first special issue in this field in Compurtational Methods in Science and Technology (CMST) in 2004 [9] and by the first thematic issue in Physica Status Solidi B in 2005 [10]. Since that time, almost every year a thematic issue of the Physica Status Solidi B (PSSB) has been published [11,12]. The next international Conference on "Auxetics and Other Unusual Systems" is planned to occur in 2026 [13].

This lecture will provide a very brief overview of the latest simulations of auxetics in Poznań [14-15].

Acknowledgments

The computations were partially performed at Poznań Supercomputing and Networking Center (PCSS), Poland.

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A-Site Deficiency and B-Site Substitution Synergies in NdBa-Based Double Perovskites for High-Performance IT-SOC Electrodes

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Intermediate Temperature Solid Oxide Cells (IT-SOCs) offer a highly promising pathway for green energy generation from diverse fuel sources and for energy storage through hydrogen generation. Their wide implementation and usage could significantly contribute to reducing the effects of climate change associated with fossil fuels. However, because of their relatively lower operating temperature range (600°C~700°C), IT-SOCs exhibit slower electrochemical kinetics compared to conventional high temperature SOCs (800°C~1000°C). Therefore, designing electrode materials that operate efficiently within the intermediate temperature range is crucial. Barium-based cobalites ($LnBaCoO5+\delta$, where Ln represents lanthanides) are strong candidates due to their mixed ionic–electronic conductivity and notable electrochemical activity [1]. However, the presence of Co introduces challenges, such as electrode delamination, stemming from their high thermal expansion coefficient (TEC). To overcome these limitations, approaches including B-site substitution of Co to decrease TEC as well as introducing A-site deficiency to increase oxygen vacancy concentration can be adopted. These modifications enhance electrochemical performance, improve oxygen-ion transport kinetics, and may contribute to improved stability owing to favorable lattice distortions [2, 3, 4].

In this work, A-site-deficient and B-site Co-substituted $(NdBa)2-\alpha CoFe1-xMnxO5+\delta$ ($\alpha = 0.1$, $x = 0$, 0.25, 0.5, 0.75, and 1) double perovskites show highly promising behavior as new electrode materials for intermediate temperature SOCs. Their physicochemical characteristics, including crystal structure, thermomechanical behavior, transport properties, microstructure, and electrochemical properties are systematically investigated using a suite of techniques such as XRD analysis, HT-XRD, dilatometry, SEM+EDS, TGA, TEM, EIS, and full fuel-cell performance tests. Among the tested compositions, $(NdBa)1.9CoFeO5+\delta$ demonstrates excellent electrochemical performance, achieving an electrode polarization resistance of 0.094 $\Omega\cdot cm^2$ at 700°C. Moreover, the material displays minimal degradation, showing only a 0.018 $\Omega\cdot cm^2$ increase over a 100-hour long term test, whereas the stoichiometric $(NdBa)2CoFeO5+\delta$ fails to sustain its performance, highlighting the beneficial effects of A-site deficiency. $(NdBa)1.9CoFeO5+\delta$ also delivers higher activity under elevated oxygen partial pressure, further confirming its strong capability as an oxygen electrode. Overall, $(NdBa)1.9CoFeO5+\delta$ exhibits outstanding performance, combining low impedance with excellent long-term stability. These results demonstrate the effectiveness of A-site deficiency and B-site substitution in developing robust electrode materials for sustainable energy applications.

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Ceramic–polymer composites for 3D–printed catalytic sieve converting gaseous stream into useful fuels for SOFC

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Metal–support catalysts are widely used for gas conversion processes including methane reforming, CO_2 conversion, and hydrogenation [1]. One of the biggest challenges in designing catalysts for gas conversion is preventing catalyst particles from sintering and deactivation caused by carbon deposition. One promising technique to address these issues is the exsolution of metal nanoparticles from a perovskite structure support. Exsolved nanoparticles are partially embedded in the support, which significantly improves their thermal stability and metal-support interactions [2].

Fused filament fabrication (FFF) is the most widely used commercial 3D printing method and can be applied to fabricate ceramic structures. Ceramic FFF is performed using ceramic particles suspended in a thermoplastic polymer as a printing material. The printed element is then thermally debinded, and the remaining ceramic particles are sintered [3]. This method enables the production of porous ceramic structures, which can be advantageous for catalytic applications [4].

The most significant challenges include preparing a sufficiently homogeneous ceramic–polymer composite, which is essential for repeatable FFF processing, and optimizing the debinding heating program, which is crucial for maintaining the stability of the printed structure during sintering. The goal of this work is to optimize the ceramic FFF method to print a porous, transition metal (TM) doped perovskite structure of a general formula $SrTi_{1-x}TM_xO_3$ with a sieve geometry and to exsolve catalytically active metal nanoparticles from it. Such a structure will then act as a catalytic sieve converting gaseous stream into useful fuels for SOFC.

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Modified multi-component perovskites: the influence of additional 3d dopant in a new group of $SrCo_{0.7-x}Ta_{0.1}Mo_{0.1}Mn_{0.1}X_xO_{3-\delta}$ (X: Cu, Ni, Fe) oxides

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One of the most popular new paths of solid oxide fuel cells (SOFCs) cathode material development is based on multicomponent modification of cobalt-based $SrCoO_{3-\delta}$ perovskites. Such oxides exhibit excellent mixed ionic-electronic conductivity and high oxygen reduction reaction activity. However, the main disadvantage of this group of oxides is the undesirably high value of a thermal expansion coefficient, caused by high Co content.

We propose a new group of perovskites with the general formula $SrCo_{0.7-x}Ta_{0.1}Mo_{0.1}Mn_{0.1}X_xO_{3-\delta}$ (where X: Cu, Fe, Ni). Studies of both structural and functional properties using methods such as XRD, SEM, DIL, and 4-probe DC, showed a strong impact of the additional elements on the characteristics of the materials. The total conductivity values reach 68.9 $S\cdot cm^{-1}$ at 376 °C and 53.2 $S\cdot cm^{-1}$ at 428 °C for base and Cu-doped materials, respectively. Additionally, X-ray absorption spectroscopy measurements were carried out. These studies allowed us to determine the oxidation state of cobalt, which indicates that for all materials element occurs in the oxidation state range of 2.68-2.91. The possibility of using the considered oxides as cathode materials in SOFC cells was also examined. The Cu-doped material turned out to be particularly interesting: using symmetrical cells with GDC as an electrolyte support a polarization resistance value of about 0.538 $\Omega\cdot cm^2$ was achieved at 700 °C for a phase-pure cathode, and as low as 0.081 $\Omega\cdot cm^2$ at 700 °C for a composite 60:40 wt% layer cathode, making the material an interesting alternative to state-of-the-art analogues.

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