

7th International Symposium on Dielectric Materials and Applications

6-8.12.2022
POZNAŃ, POLAND

ONLINE



BOOK of ABSTRACTS

ISyDMA⁷

EDITORIAL OFFICE

Biuro Organizacji Konferencji
Poznański Park Naukowo-Technologiczny
Fundacja UAM w Poznaniu
ul. Rubież 46
61-612 Poznań, Polska
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This volume has been compiled from files supplied by the Authors.

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ISBN 978-83-950380-3-7

PUBLISHER

Fundacja UAM w Poznaniu
ul. Rubież 46
61-612 Poznań, Polska
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Ministry of Education and Science
Republic of Poland

Conference Seventh International Symposium on Dielectric Materials and Applications ISyDMA'7 - a task financed from funds of the Minister of Education and Science for the „Doskonała Nauka” programme.

CONTENTS

PREFACE

ORGANIZING COMMITTEE

SCIENTIFIC COMMITTEE

SPECIAL ISSUE

HONORARY PATRONAGE

CONFERENCE TOPICS

PROGRAM

INVITED SPEAKERS

ORAL SESSION

POSTER SESSION

YOUNG SESSION

LIST OF PARTICIPANTS

PREFACE

On behalf of the Organizing Committee, I am pleased to present a book of abstracts to you containing the agenda and abstracts of oral and poster presentations submitted to the 7th International Symposium on Dielectric Materials and Applications ISyDMA'7, which will be held from Tuesday 6 to Thursday 8 December 2022.

ISyDMA is a cyclical international event addressed to materials scientists, physicists, chemists, biologists, and engineers involved in basic and applied research of dielectric materials and their innovative applications.

Previous, very successful ISyDMA editions were held in Kenitra and Rabat (Morocco 2016), Bucharest (Romania 2017), Beni-Mellal (Morocco 2018), Amman (Jordan 2019), Marrakech (Morocco 2020), Calais (France 2021).

The 2022 Conference was organized by the Institute of Molecular Physics of the Polish Academy of Sciences in cooperation with Adam Mickiewicz University and its Foundation. It will once again provide a forum for sharing ideas, presenting research findings, and discussing. We hope the meeting will strengthen contacts between Ph.D. students, students, novices, and experienced scientists from various international centers and initiate new international and multilateral cooperation. As many as 100 participants from multiple global research centers confirmed their presence.

Thank you for your scientific contribution to the Seventh International Symposium on Dielectric Materials and Applications. I look forward to showcasing and disseminating your research.

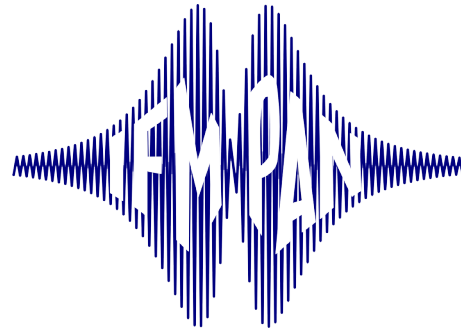
Special thanks also to the Organizing Committee and all the people that worked hard to make this event possible.

We hope that the ISyDMA conference will become more and more popular and attractive for the next young generations of researchers every year. Wishing you many fruitful discussions, pleasant intellectual experiences, and numerous citations, we invite you to the seventh edition of the ISyDMA Conference.



ISyDMA⁷

organized by
the Institute of Molecular Physics Polish Academy of Sciences



in cooperation with
Adam Mickiewicz University and its Foundation



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CONFERENCE TOPICS

The thematic scope of the conference covers a wide range of topics related to issues such as energy, environment, biotechnology, electronics, and optoelectronics. The presentations will focus on the following topics:

- Dielectric materials for electronics, photonics, and biotechnology: piezoelectrics, pyroelectrics, ferroelectrics, multiferroics, ceramics, polymers, glasses, composites and nanostructures, ionic conductors, 3D printing materials, electrocaloric materials, thermoelectrics, dielectrics for superconducting applications, bioelectrics for environmental applications and bioengineering systems, and metamaterials,
- Dielectric properties,
- Polarization phenomena,
- Electric conductivity,
- Surface and interfacial phenomena,
- Measurement techniques: impedance spectroscopy, NMR spectroscopy, Raman and IR spectroscopy, new diagnostic applications for dielectrics, advanced characterization,
- Modeling and theory,
- Dielectric devices for biotechnological and industrial applications: electricity storage, supercapacitors, electrostatic capacitors, electrolyzers, batteries.



OPENING	8.45 - 9.00	CHAIRMAN: Cyril Popov	
INVITED	9.00 - 9.40	Yasuo Cho (I-1) Statistical analysis of local C-V map data for ferroelectric thin films	
INVITED	9.40 - 10.20	Hynek Nemeč (I-2) Time domain terahertz spectroscopy: methods and application	
ORAL	10.20 - 10.40	Diouma Kobor (O-1) In situ temperature structural transitions of ferroelectric PZN-4.5PT nanoparticles thin films using synchrotron lightsource	
ORAL	10.40 - 11.00	Sana Zakaria (O-2) In the absence of sulfurization: zinc molarity effect on nontoxic and low cost CZTS thin films deposited by spin coating technique	
BREAK	11.00 - 11.30	CHAIRMAN: Hynek Nemeč (a), Mustapha Ait Ali (b)	
INVITED	11.30 - 12.10	Vid Bobnar (I-3) Designing novel inorganic and polymer systems with enhanced dielectric and electromechanical response	
ORAL	12.10 - 12.30	Zahra Ramzi (O-3a) Effect of the glass composition on the dielectric properties of strontium-phosphate-based glasses	Lahcen Ait Lamine (O-3b) DFT investigation of structural and electronic properties of zinc oxide
ORAL	12.30 - 12.50	Salma Larguech (O-4a) Electrical properties and dielectric relaxation studies in microcrystalline cellulose/multiwalled carbon nanotubes/EVA-VeoVa ternary composites	Abdellah Hbab (O-4b) Investigation of structural and electronic properties of ferroelectric phase of LiNbO ₃ using PZ and VdW-DF functionals: a DFT study
ORAL	12.50 - 13.10	Marouan Karam (O-5a) Contribution of volume and surface magnons to the study of the magnetic properties of Fe/Pt superlattices	Said Amounas (O-5b) DFT study of spontaneous polarization and refractive indices of tetragonal BaTiO ₃ and PbTiO ₃ for various pseudopotentials
ORAL	13.10 - 13.30	Mouhsine Laayati (O-6a) Synthesis and characterisation of GO/SrFe ₁₂ O ₁₉ as magnetic hybrid nanocatalyst for regioselective ring-opening of epoxides with amines under eco-friendly conditions	Meriem Boutaldat (O-6b) Simulation study of triboelectric nanogenerator for effective energy harvesting
ORAL	13.30 - 13.50	Ciril Popov (O-7a) Fabrication of diamond photonic nanostructures	Tomasz Maślowski (O-7b) Long time protonic conductivity behavior of CsH ₅ (PO ₄) ₂ crystal at high pressure
BREAK	13.50 - 15.00	CHAIRMAN: Roger M. Leblanc	
INVITED	15.00 - 15.40	Friedrich Kremer (I-4) Glassy dynamics and charge transport in (polymeric) ionic liquids	
INVITED	15.40 - 16.20	Andrzej Katrusiak (I-5) Compressibility of chemical compounds	
ORAL	16.20 - 16.40	Ilham Bouknaitir (O-8) Electrical impedance analysis of carbon dots/PMMA composite materials	
ORAL	16.40 - 17.00	Rajae Belhimria (O-9) Structural dependent electrical impedance spectroscopy behaviour of multiwalled Carbon nanotube/Graphite/Polyester ternary composites	
ORAL	17.00 - 17.20	Zineb Samir (O-10) Electrical and dielectric properties of different forms of carbon allotropes/resin epoxy composite materials near the percolation threshold	
ORAL	17.20 - 17.40	Kevin Amith Mathias (O-11) Dielectric and mechanical studies on silicone rubber particle and liquid filled composite material	

		CHAIRMAN: Yasuo Cho	
INVITED	9.00 - 9.40	Anna Gagor (I-6) The cation- and metal-controlled properties of hybrid hypophosphite perovskites	
ORAL	9.40 - 10.00	Miriam Achkar (O-12) Electrocaloric characterization of samarium doped barium titanate ceramics synthesized by sol-gel process	
ORAL	10.00 - 10.20	Layla Farhat (O-13) Measurement of the dynamic temperature response of electrocaloric effect in solid ferroelectric materials via thermorefectance	
ORAL	10.20 - 10.40	Eskilla Venkata Ramana (O-14) Processing and electrical characterization of $\text{Ba}(\text{Ti}_{0.8}\text{Zr}_{0.2})\text{O}_3-(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ lead-free piezoelectrics for energy-efficient caloric applications	
ORAL	10.40 - 11.00	Nidal Khemmou (O-15) Effect of an additive organic TE1 in improving the quality of nickel electroplating on brass	
BREAK 11.00 - 11.30		CHAIRMAN: Ashok Vaseashta (a), Friedrich Kremer (b)	
INVITED	11.30 - 12.10	Luis Cadillon Costa (I-7) Using impedance spectroscopy to characterize materials	
ORAL	12.10 - 12.30	Salma Kaotar Hnawi (O-16a) Novel organometallic complexes and their application in solar cells	Adam Ostrowski (O-16b) Proton conductivity of imidazole or 1,2,4-triazole entrapped in microporous molecular sieves
ORAL	12.30 - 12.50	Silvia Gavinho (O-17a) Electrical properties of cerium-containing Bioglass®	Yassine El Hasnaoui (O-17b) Designing of new dielectric resonator antenna fed by microstrip line with quarter wave transformer
ORAL	12.50 - 13.10	Imen Hammami (O-18a) The effect of niobium oxide on the structure, electrical and biological properties of 45S5 bioactive glass	Messaoud Hamouda (O-18b) Determination of the critical sizes of an electric discharge on a disk model
ORAL	13.10 - 13.30	Manuel Pedro Graca (O-19a) TSDC studies on bioglasses charged by the Corona discharge method	Khadija Oumghar (O-19b) Characterization of electroactive nanocomposite based on polylactidetitanium dioxide for piezoelectric β -phase improvement
ORAL	13.30 - 13.50	Paolo Negro (O-20a) $\text{MoS}_2/\text{TiO}_2$ heterojunctions for tuning the optical properties: a case study	Najoia Aribou (O-20b) Predictive model on the DC electrical conductivity of filler/matrix interphase zone of two- and three-dimensional composites
BREAK 13.50 - 15.00			

BREAK	13.50 - 15.00	CHAIRMAN: Anna Gagor (a), Luis Cadillon Costa (b)	
INVITED	15.00 - 15.40	Amina Tachafine (I-8) Microscopic and macroscopic electrical properties and impedance spectroscopy of strontium-calcium titanate materials for environmentally friendly monolithic ceramic capacitors	
POSTER	15.40 - 15.50	Marina Ciobanu (P-1a) The features of X-ray diffraction in non-stoichiometric $\text{AsS}_3\text{-GeS}_4$ glassy thin films	Asma Triki (P-1b) Interfacial polarization effect analysis of hybrid recycled cotton fibers reinforced unsaturated polyester composites
POSTER	15.50 - 16.00	Vania Ilcheva (P-2a) Synthesis, characterization and dielectric properties of $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$	Stanisław A. Rózański (P-2b) Effect of surface treatment on the dynamics of relaxation processes in confinement
POSTER	16.00 - 16.10	Eskilla Venkata Ramana (P-3a) Ferroelectric and pyroelectric characterization of promising perovskite ceramics	Ikhlass Benamara (P-3b) Numerical simulation of coffee grounds pyrolysis for biofuels production
POSTER	16.10 - 16.20	Ivan Yakovkin (P-4a) Hysteresis of surface plasmon polariton effective index induced by liquid crystal reorientation	Natalia Bielejewska (P-4b) Nanocomposite molecular films based on nanocrystalline cellulose and liquid crystals
POSTER	16.20 - 16.30	Arulmozhi Durairajan (P-5a) Li^+ and W^+ ion irradiation induced changes on the electrical properties of BaSnO_3 ceramics	Tomasz Szczepański (P-5b) Electron scattering by magnetic quantum dot in the topological insulator
POSTER	16.30 - 16.40	Bartłomiej Andrzejewski (P-6a) Electric and structural properties of ZnO-based surge arrester ceramics	Badiaa Bachiri (P-6b) Impact of bismuth iodide (BiI_3) interfacial layer on perovskite solar cell based MAPbI_3
POSTER	16.40 - 16.50	Paweł Ławniczak (P-7a) Starch-based protonic conductors	Faissal El Manjli (P-7b) An innovative approach to produce black phosphorus from red phosphorus via the addition of small amounts of iron
POSTER	16.50 - 17.00	Andrzej Hilczer (P-8a) Dielectric and magnetic response of $\text{Sr}_{1-x}\text{Nd}_x\text{Fe}_{12}\text{O}_{19}$ ($0 \leq x \leq 0.09$) hexaferrite nanoceramics	Benyamna Belkacemi (P-8b) Comparative study of AgGaSe_2 and AgGaTe_2 chalcopyrite-based solar cells
POSTER	17.00 - 17.10	Arulmozhi Durairajan (P-9a) Low temperature dielectric, magnetic and spectral behaviour of pure and Mn doped multiferroic BiFeO_3 nano ceramics	Ikhlass Benamara (P-9b) Modelling and simulation of the optical properties of zinc oxide thin films targeting the optimal configuration (ZnO/Substrate)
POSTER	17.10 - 17.20	Ruzha Harizanova (P-10a) Dielectric properties of strontium-substituted barium titanate glass-ceramics	Oleh Kozachenko (P-10b) Stress dependent photovoltaic effect in the ferroelectric $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_x\text{Ti}_{1-x}]\text{O}_3$ crystal
POSTER	17.20 - 17.30	Soud Ait Saghir (P-11a) Structural, phonon and dielectric properties calculations based on DFT and modern theory of polarization	Messaoud Hamouda (P-11b) Study of the parameters of influence on the critical conditions of the flashover
POSTER	17.30 - 17.40	Abderrahim Ait Lhaj (P-12a) Theoretical modeling of structural, electronic and optical properties of tin dioxide	Veselin Zhelev (P-12b) Study of samarium doped ceria prepared by ionic gelation method and solid state reaction synthesis

		CHAIRMAN: Amina Tachafine
INVITED	9.00 - 9.40	Marinella Striccoli (I-9) Functional nanostructured materials by wet chemistry synthetic routes
INVITED	9.40 - 10.20	Mustapha Ait Ali (I-10) Chemistry of 2D-nanomaterials; silicene-siloxene: synthesis and functionalization
ORAL	10.20 - 10.40	Abdallah Nayad (O-21) Direct synthesis of dehydrogenated siloxene materials: towards the improvement of physical and electrochemical responses
ORAL	10.40 - 11.00	Younes Ouaomar (O-22) Using ANN modelling to Improve the accuracy of energy baseline models for Industrial Buildings
BREAK	11.00 - 11.30	
		CHAIRMAN: Bartłomiej Andrzejewski
YS	11.30 - 11.50	Zineb Gargar (Y-1) Grain size effects on dielectric properties of yttrium doped BaTiO ₃ ceramics
YS	11.50 - 12.10	Zakia Aribou (Y-2) Effect of organic additive on the electrodeposition of a copper deposit: electrochemical and corrosion resistance study
YS	12.10 - 12.30	Nouhaila Ferraa (Y-3) Valorization of three apatitic calcium phosphates (PTCa, HA and OCPa) as steel corrosion inhibitors in NaCl 3%: Characterization and comparison
YS	12.30 - 12.50	Yassine Nioua (Y-4) Electrical conductivity study of epoxy polymer loaded with reduced Graphene Oxide particles
YS	12.50 - 13.05	Salma Kaotar Hnawi (Y-5) Novel schiff base complexes and natural dye as sensitizers in dye sensitized solar cells
YS	13.05 - 13.20	Agata Tabero (Y-6) Imidazole-loaded KIT-6 mesoporous materials with high proton conductivity
YS	13.20 - 13.35	Tobiasz Banaszek (Y-7) Study of physicochemical properties of new composite films formed by cellulose derivatives with imidazole
YS	13.35 - 13.50	Konrad Rotnicki (Y-8) Analysis of the ionic liquid trapped in carbon matrices using FTIR, Raman and dielectric spectroscopy
BREAK	13.50 - 15.00	
		CHAIRMAN: Vid Bobnar
INVITED	15.00 - 15.40	Roger M. Leblanc (I-11) Novel carbon dot nanomaterials with dielectric and thermoelectric properties
INVITED	15.40 - 16.20	Ashok Vaseashta (I-12) Hierarchical integration of electrospinning and 3D/4D printing process for rapid prototyping
ORAL	16.20 - 16.40	Rania Lataoui (O-23) Electrical properties of La _{1-x} Sr _x FeO ₃ (0 ≤ x ≤ 0.5) ortho-ferrites by dielectric spectroscopy
ORAL	16.40 - 17.00	Oussama Oulhakem (O-24) Studying the photocatalytic properties of tungstate-based materials for water splitting
ORAL	17.20 - 17.40	Ivan Yakovkin (O-25) Orientational instability of the director in a planar flexoelectric nematic cell with easy axis gliding
CLOSING	17.40	

INVITED SPEAKERS

Statistical analysis of local C-V map data for ferroelectric thin films

Y. Hiranaga, **Y. Cho**

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Nanoscale characterization of polarization switching behavior is important in the future development of piezoelectric and ferroelectric devices. Recently, we have developed a novel probe microscopy technique for local C-V mapping based on scanning nonlinear dielectric microscopy (SNDM). This method enables detailed analysis of dynamic polarization switching behavior beyond the conventional static domain observation.

An SNDM system has an LC oscillator probe, which enables local capacitance deviation to be detected with high sensitivity. In a conventional SNDM observation, an AC bias voltage below a domain switching voltage is applied to a sample, and a nonlinear response is detected to visualize the static domain structure. On the other hand, in the novel method, the response is measured with a large-amplitude AC bias above the polarization switching voltage. For ferroelectric films, C-V curves observed in this way draw a butterfly curve, as with macroscopic measurements. By analyzing such local C-V butterfly curves, various parameters related to polarization switching can be obtained

In this talk, we will discuss the analysis of local C-V map data by a statistical approach. First, noise reduction using principal component analysis will be described in detail. Response signals obtained by local C-V measurements often show steep peak waveforms that reflect polarization inversion. When a general frequency filter is applied to such waveforms, the steepness of the peak is impaired. On the other hand, noise reduction using principal component analysis can reduce the noise component while maintaining the steepness of the peak.

In addition, we will introduce the recent progress of feature analysis in a local C-V dataset. At the previous symposium (ISyDMA'6), we extracted the features related to the net switchable polarization amount, intrinsic coercive field, and local imprint. This time, in addition to the above features, we will discuss the extraction of features focusing on the asymmetry of the C-V curves, which are considered to be related with some kind of defects including domain pinning sites.

Time domain terahertz spectroscopy: methods and applications

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Broadband coherent terahertz (THz) pulses used in time-domain THz spectroscopy enable efficient noncontact spectroscopic characterization of materials as well as imaging and tomography. Specifically, the high probing frequency permits sensing of charge transport on nanoscale distances, and thus understanding electron motion in nanostructured materials. The probing frequency is also highly pertinent for the characterization of polar lattice vibrations with lower eigenfrequency.

In this contribution, the basic methods of time-domain THz spectroscopy will be presented, including the latest developments of sub-wavelength imaging approaches. Fundamentals of data analysis will be introduced to demonstrate the potential of time-domain THz spectroscopy for the characterization of dielectric materials. We will elaborate on basic models of electrical permittivity allowing to interpret the measured THz spectra on a simple level. In inhomogeneous materials, this also implies to account for their morphology, which controls the distribution of depolarization fields and therefore also the effective response of these materials.

Designing novel inorganic and polymer systems with enhanced dielectric and electromechanical response

V. Bobnar¹, A. Matavž¹, V. Jurečič¹, Y.B. Pottathara², V. Kokol², S. Thomas³, K. Geirhos⁴, P. Lunkenheimer⁴, X. Chen⁵, Q. M. Zhang⁵

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The lecture will demonstrate, using various examples from our work, that novel materials with high dielectric and piezoelectric response, required in energy storage systems and electromechanical applications, can efficiently be developed by taking into account some basic physical phenomena:

(i) In a heterogeneous system, composed of a dielectric matrix and electrically conductive inclusions, the charge accumulated at phase boundaries acts as a large electric dipole. Using this Maxwell-Wagner polarization we have effectively increased the dielectric permittivity of PVDF-based electroactive polymers and thus substantially reduced the electric field required for their giant electrostrictive response [1]. Analogously, we have fabricated flexible, eco-friendly composites from cellulose nanofibrils and graphene oxide [2] as well as inorganic materials such as bulk all-ceramic percolative composites and core-shell structured thin films that consist of semiconducting grains separated by thin insulating grain-boundaries [3].

(ii) The electromechanical response in thin films is obstructed by the mechanical clamping of the substrate, resulting in a deterioration of the piezoelectric coefficients. We have thus developed a simple and robust method for the chemical solution deposition of highly-porous ferroelectric thin films, where the porosity-mediated release of the substrate's mechanical constraints enhances piezoelectric coefficients back to the level of bulk ceramics [4]. Moreover, we have partially filled the pores with ferromagnetic nickel ferrite and thus developed a thin-film composite that exhibits not only multiferroic but also magnetocapacitive response [5].

(iii) A significant enhancement of the dielectric breakdown strength in blends of polyetherimide with polyimide occurs due to strong electrostatic interactions between the phenyl groups of different polymer chains. These interactions strongly reduce the number of accumulated space charges, which in weak points gain higher energies when accelerated by an applied electric field and initiate the breakdown at lower electric fields. The blending of properly matched polymers thus turned out as an outstanding strategy for realizing high energy density while maintaining low dielectric losses.

References:

[1] X. Chen, T. Yang, Q. Zhang, L.Q. Chen, V. Bobnar, C. Rahn, Q.M. Zhang, *Nano Energy* 88 (2021) 106226.

[2] Y.B. Pottathara, V. Bobnar, Y. Grohens, S. Thomas, R. Kargl, V. Kokol, *Cellulose* 28 (2021) 3069.

[3] V. Bobnar, M. Hrovat, J. Holc, M. Kosec, *Ferroelectrics - Characterization and Modeling*, pp. 117-134, InTech Open Access Publisher (2011).

[4] A. Matavž, A. Bradeško, T. Rojac, B. Malič, V. Bobnar, *Applied Materials Today* 16 (2019) 83.

[5] A. Matavž, P. Koželj, M. Winkler, K. Geirhos, P. Lunkenheimer, V. Bobnar, *Thin Solid Films* 732 (2021) 138740.

Glassy dynamics and charge transport in (polymeric) ionic liquids

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Glassy dynamics and charge transport in a variety of bulk glass-forming ionic liquids (ILs) are investigated using a combination of Broadband Dielectric Spectroscopy (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR), Differential Scanning Calorimetry and Rheology. While the absolute values of the dc conductivity as well as viscosity vary over more than 11 decades with temperature and upon systematic structural variation of the ILs, quantitative agreement is found between the characteristic diffusion rates and the mechanically measured structural - relaxation. Based on Einstein, Einstein-Smoluchowski, Maxwell and Langevin relations, the link between rotational and translational diffusion in ILs is experimentally verified and universal scaling of charge transport in ionic liquids is traced back to the dominant role of Brownian dynamics. A further analysis of the dielectric spectra enables one to deduce - using the Einstein-Smoluchowski equation - diffusion coefficients in quantitative agreement with independent PFG NMR results, but in an extraordinarily broad range spanning over 13 decades.

References:

- [1] F. Kremer, A. Schönhalz (Eds.) Broadband Dielectric Spectroscopy, Springer (2003).
- [2] J.R. Sangoro, A. Serghei, S. Naumov, P. Galvosas, J. Kärger, C. Wespe, F. Bordusa, F. Kremer, Phys. Rev. E 77 (2008) 051202.
- [3] J.R. Sangoro, C. Iacob, A. Serghei, C. Friedrich, F. Kremer, Phys. Chem. Chem. Phys. 11 (2009) 913.
- [4] C. Iacob, et al. in: "Dynamics in Geometrical Confinement", F. Kremer (Ed.), Springer-Verlag (2014) ISBN 978-3-319-06099-6.
- [5] F. Frenzel, M.Y. Folikumah, M. Schulz, A.M. Anton, W.H. Binder, F. Kremer, Macromolecules 49 (2016) 2868.
- [6] F. Frenzel, R. Guterman, A.M. Anton, J. Yuan, F. Kremer, Macromolecules 50 (2017) 4022.
- [7] A.M. Anton, F. Frenzel, J. Yuan, M. Tress, F. Kremer, Soft Matter 16 (2020) 6091.

Compressibility of chemical compounds

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Compressibility and thermal expansion belong to the most basic properties of all matter. The description of these properties can be connected with the foundations of thermodynamics and of all materials sciences. The compressibility and thermal expansion of solids have the form of tensors, which reflect the symmetry, crystal structure, chemical composition and cohesion forces. Traditionally, compressibility is the inverse of the hardness of solid materials and it is considered a static property related to equilibrated systems. The hardness, bulk modulus, Young modulus, and Poisson's ratio, clearly depend not only on the material itself, but also on the mode of applying the stress. In recent decades, owing to the ingenious inventions of high-pressure devices, particularly the diamond anvil cell, as well as spectacular improvements in the measuring equipment, such as powerful radiation sources, area detectors, diffractometry, computational hardware and software, the compressibility measurements have become more frequent, their precision has increased, and they have expanded to all fields of materials sciences. Compressibility continues to be the most basic macroscopic property, but at the same time, it provides increasingly more refined characteristics pertaining to the microscopic structure. This poses new questions regarding the regime of compressibility calculations, which in traditional solid-state physics could be performed just for the monotonic compression regions of a given homogenous chemical compound. Presently, gradual chemical changes induced in chemical compounds have been observed for specific phases, without distinct phase transitions. For example, a gradual conformation change can occur in a given compound, or a charge-transfer complex gradually changes the rate of the electron transfers between the neutral and ionic states, which is reflected in the crystal compression. Other examples of possible transformations and the measurement techniques affecting the compressibility determination will be discussed [1-6].

References:

- [1] K. Roszak, A. Katrusiak, *Acta Cryst. B* 77 (2021) 449.
- [2] W. Cai, A. Gładysiak, M. Anioła, V.J. Smith, L.J. Barbour, A. Katrusiak, *J. Am. Chem. Soc.* 137 (2015) 9296.
- [3] P.A. Guńka, K.F. Dziubek, A. Gładysiak, M. Dranka, J. Piechota, M. Hanfland, A. Katrusiak, J. Zachara, *Cryst. Growth Des.* 15 (2015) 3740.
- [4] B.A. Zakharov, Y.V. Seryotkin, N.A. Tumanov, D. Paliwoda, M. Hanfland, A.V. Kurnosovg, E.V. Boldyreva, *RSC Adv.* 6 (2016) 92629.
- [5] S. Bhattacharyya, Sz. Sobczak, A. Pórolniczak, S. Roy, D. Samanta, A. Katrusiak, T.K. Maji, *Chem. Eur. J.* 25 (2019) 6092.
- [6] I.E. Collings, M. Hanfland, *Acta Cryst. B* 78 (2022) 100.

The cation- and metal-controlled properties of hybrid hypophosphite perovskites

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A perovskite crystal structure of ABX_3 formula is a common architecture for a number of organic-inorganic materials which show ferroelectric, multiferroic, photovoltaic or photoluminescent properties. Metal centers at B sites (usually Pb^{2+} , Sn^{2+} , Mn^{2+} , Cd^{2+} , Zn^{2+} etc.) are octahedrally coordinated by X ligands, which may be simple halides or more extended, formate, azide, cyanate, dicyanamide, or hypophosphite ions ($H_2PO_2^-$). The ligands act as bridging units forming 3D inorganic structure built of corner-sharing octahedra. A-site molecular cations, occupy the lattice cavities and interact via hydrogen bonds with the metal-ligand framework. The non-spherical shapes of amines, extended x-site ligands, as well as hydrogen-bond interactions between them result in unconventional octahedral tilts, columnar shifts, and unprecedented off-center shifts of cations being unique to hybrid perovskites. In this presentation, we report the results of chemical engineering on the crystal structures, phase transitions, magnetic, and photoluminescent properties in the family of hybrid hypophosphite perovskites. Metal-controlled synthesis (replacing Mn^{2+} for Cd^{2+} and Co^{2+}) tunes the physical properties, e.g. changes the ferromagnetic response and magnetic ordering temperatures, induces broadband emission, etc. Molecular cation replacement results in the structures differing in symmetry and distortion of perovskite cavities. The combination of pyrrolidinium and Cd(II) at the B site leads to a polar crystal structure, that has not been observed in any known hybrid hypophosphite [1]. The new luminescent hypophosphites with magnetic or polar order are a promising platform to design new functional materials, including light-emitting, ferroelectric, and multiferroic.

This research was supported by the National Science Centre (Narodowe Centrum Nauki) in Poland under project no. 2018/31/B/ST5/00455.

References:

[1] M. Mączka, A. Gagor, D. Stefańska, A. Pikul, Dalton Transactions 51 (2022) 352.

Using impedance spectroscopy to characterize materials

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Impedance spectroscopy is a powerful technique to characterize materials, as it permits the understanding of the charge migration and the orientation of permanent dipoles inside them. To obtain a complete dielectric response, a large range of frequencies and temperatures must be used. The different regimes of the dielectric function can be observed, and the dynamics of the relaxation processes can be found. Impedance spectroscopy can provide the measurement of the complex impedance, $Z^* = Z' - iZ''$, or derived quantities related to it. The macroscopic properties, impedance, Z^* , or the admittance, $Y^* = Z^{*-1}$, can also express the properties of a material. The interrelations between these quantities and microscopic quantities, such as complex permittivity and modulus, are simple when it is known the shape and the size of the samples.

In this talk, different examples of using impedance spectroscopy to characterize materials are presented, showing the ability of this technique. It offers performances that permit the investigation of the fundamental aspects of the electrical properties, yielding a wealth of information about the molecular motions and relaxation processes present in the materials.

Figure 1 shows a Nyquist plot, performed in a partially decomposed CsH_2PO_4 pellet. Three different relaxation processes can be identified. The high frequency (HF) process is assigned to the impedance of the CsH_2PO_4 phase, the intermediate frequency process to the relaxation from the CsPO_3 phase, while the low frequency (LF) process is assigned to the blocking electrode effect.

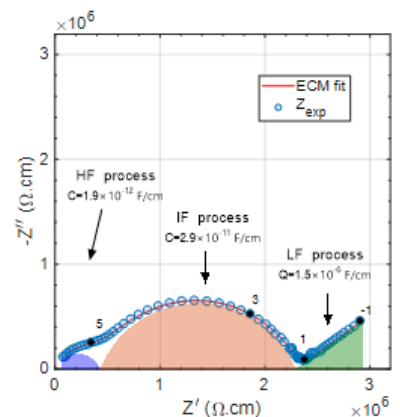


Figure 1. Nyquist plot showing the electrode polarization (LF), the relaxation from the CsPO_3 phase (IF), and the relaxation from the CsH_2PO_4 phase

This work was partially supported by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT - Portuguese Foundation for Science and Technology under the project UID/CTM/50025/2019. B.M.G. Melo acknowledges Fundação para a Ciência e Tecnologia (FCT) for the Ph.D. grant (SFRH/BD/117487/2016).

Microscopic and macroscopic electrical properties and impedance spectroscopy of strontium-calcium titanate materials for environmentally friendly monolithic ceramic capacitors

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Due to the rapid evolution of the development of telecommunication systems and advances in technologies of electronic miniaturization used in industries, an important need for high-frequency tunable components and multifunctional devices has arisen. Today, ceramic capacitors are one of the most widely used forms of capacitor used in electronic equipment. Ceramic capacitors are nowadays available in many versions including leaded disc ceramic capacitors, surface mount multilayer ceramic capacitors, MLCCs. With the progress of high-frequency technologies, the dielectric properties of materials used in electronic components, such as telecommunication devices, are of importance for satisfying conditions on the quality factor $Q = 1/\text{tg}\delta$. In this way, high-frequency systems for telecommunications have attracted great interest. Lead-based ferroelectric ceramics, such as $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT), have attracted worldwide research interest due to their high dielectric performance. However, it contains lead in regards with the European directive Restriction of Hazardous Substances, 2002/95/CE (RoHS). Accordingly, it is now necessary to implement materials without these prohibited substances, and presenting low losses, high dielectric permittivity and relatively stable properties in frequency and temperature. In particular, SrTiO_3 ceramic exhibits low dielectric losses at high frequencies. In this work, we present the dielectric study in a wide range of frequencies and temperatures of SrTiO_3 and $\text{Sr}_{0.6}\text{Ca}_{0.4}\text{TiO}_3$ ceramics in which strontium is substituted by a high calcium content (40%). We present the microscopic electrical properties of the material, studied by impedance spectroscopy, namely the different phenomena of transport, conduction and relaxation at the level of grains and grain boundaries. We also present the macroscopic dielectric properties of the bulk material and show that this material could be a real candidate for the development of environmentally friendly monolithic ceramic capacitors.

Functional nanostructured materials by wet chemistry synthetic routes

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The design of new nanostructured materials, able to join novel size dependent properties with versatile and reliable processing capabilities, represents one of the most relevant challenges in nanotechnology and material science. Wet-chemistry protocols allow synthesizing nanomaterials in a large variety of shapes, sizes and compositions with geometrically tunable chemical and physical properties. Semiconductor inorganic nanocrystals have been widely exploited as quantum optical emitters or sensitizers, thanks to their high quantum yield, chemical stability, low tendency to photobleaching and possibility to tune the optical features in a large spectral range [1,2]. Also, recently, perovskite nanoparticles and carbon dots have attracted great attention due to their very intense emission and to the low toxicity, respectively. Metal oxide nanoparticles possess interesting size- and morphology tunable properties, great physicochemical versatility, specific reactivity, and surface chemistry [3]. Such characteristics are beneficial for using the synthesized nanoparticles in several environmental applications, electronics, and energy related devices, in sensing and textile, bioimaging and nanomedicine. In addition, post-synthetic functionalization procedures allow to manipulate such nano-objects, integrating them in solid matrices, depositing or assembling on substrates, preserving their original properties, and adding new collective features. In this talk, different nanomaterial preparation synthesis in solution by colloidal, solvothermal and precipitation routes will be illustrated with particular attention to nanostructured materials for applications in energy conversion.

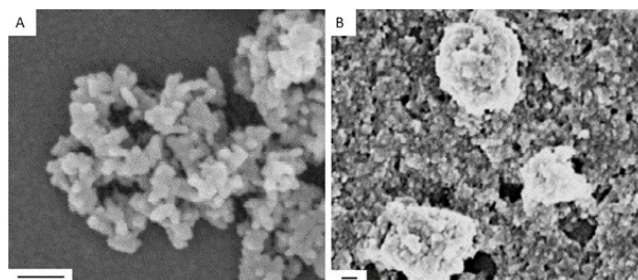


Figure 1. SEM micrographs of SnO₂ nanoparticles synthesized by solvothermal approach in presence of NaOH (A) and NH₄OH (B), respectively (scale bar 100 nm)

Funding acknowledgment: The Project IEMAP - Materiali Avanzati per l'Energia, MISE-Mission Innovation Program 2021-202 and the PON Project ARS01_00519 "BEST-4U" are grateful acknowledged.

References:

- [1] C.N. Dibenedetto, T. Sibillano, R. Brescia, M. Prato, L. Triggiani, C. Giannini, A. Panniello, M. Corricelli, R. Comparelli, C. Ingrosso, N. Depalo, A. Agostiano, M.L. Curri, M. Striccoli, E. Fanizza, *Molecules* 25 (2020) 2939.
- [2] S. Ahn, C. Ingrosso, A. Panniello, M. Striccoli, G.V. Bianco, A. Agostiano, G. Bruno, M.L. Curri, O. Vazquez-Mena, *Adv. Electron. Mater.* 8 (2022) 2100672.
- [3] M. Dell'Edera, F. Petronella, A. Truppi, L.F. Liotta, N. Galli, T. Sibillano, C. Giannini, R. Brescia, F. Milano, M. Striccoli, A. Agostiano, M.L. Curri, R. Comparelli, *Catalysts* 10 (2020) 893.

Chemistry of 2D-nanomaterials; silicene-siloxene: synthesis and functionalization

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The design of bi-dimensional (2D) materials has attracted a great attention for their remarkable physical properties in various technological applications. Since facile fabrication processes of large area nanosheets are required for practical applications, a development of soft chemical synthesis route without using conventional vacuum processes is a challenging issue. Techniques for the exfoliation of layered compounds are widely used to fabricate nanometer-thick materials, such as oxides, niobates, chalcogenides, phosphates, and graphene. Although a variety of nanosheets has been synthesized, there have been few reports of silicene, siloxene and their functionalised nanosheets. Mass production of siloxene and functionalised siloxene nanosheets can be achieved using chemical processes as an alternative route to large-scale synthesis of 2D nanomaterials under production conditions.

Silicon Nano-sheets (SiNSs), low dimensional crystalline silicon materials with their high specific surface area, makes them promising candidates for a variety of applications in nanoscience and nanotechnology. In this perspective, this work focuses on recent progress in soft chemical fabrication of 2D-nanomaterials from calcium disilicide: silicene, siloxene nanosheets and their chemical modification.

Calcium disilicide Zintl phase is by far the precursor material used for the preparation of SiNSs via topochemical deintercalation of the silicide by thermal treatment with metal chlorides and by soft chemical exfoliation of CaSi_2 in the presence of I_2 as oxidant. However, the synthesized silicene are highly unstable under ambient conditions and are prone to random oxidation and surface attachments, which make difficult its potential utilization. The surface functionalization of SiNSs, expected to be stable in air-ambient, has been recently explored lately such as fully hydrogenated SiNSs (Si_6H_6), siloxene [$\text{Si}_6\text{H}_6(\text{OH})_3$] and by modifications of layered polysilane with organic compounds; but few progresses were made in this objective. In this work, an easy and direct functionalization approach of SiNSs by exfoliation of CaSi_2 with available organic substrates is described and all new materials were successfully confirmed and characterized.

Novel carbon dot nanomaterials with dielectric and thermoelectric properties

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Carbon dots (CDs) are a group of novel carbon-based spherical nanoparticles (NPs) with diameters less than 10 nm. They are widely present in the nature and can be also synthesized using various carbon-based substances as precursors by either top-down or bottom-up approaches. They are well characterized for tunable surface functionality, excellent photoluminescence (PL), high photostability and water dispersity, good biocompatibility, and nontoxicity. Also, they display different sizes and surface chemistry depending on the preparation methods and precursors applied. Applications of CDs in drug delivery, bioimaging, sensing, and other nanotechnology fields are rapidly rising due to their aforementioned unique properties. In addition, various spectroscopic and microscopic measurements have been performed on diverse CD preparations, which revealed some typical physicochemical features of CDs. For example, UV/vis absorption spectra of CDs usually display two peaks at 250 and 350 nm, which corresponds to C=C and C=O conjugate structures, respectively. Most fluorescence emission spectra have shown an excitation-dependent PL emission of CDs, which arouses a debate regarding the PL mechanism of CDs. The spherical morphologies of different CDs are studied through a combination of atomic force microscopy (AFM) and transmission electron microscopy (TEM) to obtain the three-dimensional data. As for the structural analysis of CDs, Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, X-ray diffraction (XRD), small-angle X-ray scattering (SAXS), and thermogravimetric analysis (TGA) have all been utilized to investigate the surface functionalities and core structures. Considering the abundant functionalities such as -COOH and -NH₂, distinct CDs were conjugated via an amidation reaction mediated by EDC and NHS to explore the construction of large multifunctional carbon-based nanostructures. Also, zeta potential studies show most CDs carry negative charge on the surface, which inspires numerous research on the electrical or dielectric properties of CDs.

References:

- [1] C.Y. Oztan, B. Hamawandi, Y. Zhou, S. Ballikaya, M.S. Toprak, R.M. Leblanc, V. Coverstone, E. Celik, *Journal of Alloys and Compounds* 864 (2021) 157916.
- [2] R.K. Shukla, J. Mirzaei, A. Sharma, D. Hofmann, T. Hegmann, W. Haase, *RSC Advances* 5 (2015) 34491.

Hierarchical integration of electrospinning and 3D/4D printing process for rapid prototyping

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Electrospinning is an effective and versatile technique used to produce porous structures ranging from submicron to nanometer diameters. Using a variety of high-performance polymers and blends, several porous structure configurations have become possible for applications in tactile sensing, energy harvesting, filtration, and biomedical applications, however, the structures lack mechanical complexity, conformity, and desired three-dimensional single/multi-material constructs necessary to mimic desired structures. A simple, yet versatile, strategy is through employing digitally-controlled fabrication of shape-morphing by combining two promising technologies, viz., electrospinning and 3D printing/additive manufacturing process. Using hierarchical integration of configurations, elaborate shapes and patterns are printed on mesostructured stimuli-responsive electrospun membranes, modulating in-plane and interlayer internal stresses induced by swelling/shrinkage mismatch, and thus guiding morphing behaviors of electrospun membranes to adapt to changes of the environment. Recent progress in 3D/4D printing/additive manufacturing processes includes materials and scaffold constructs for tactile and wearable sensors, filtration structures, sensors for structural health monitoring, biomedical scaffolds, tissue engineering, and optical patterning, among many other applications to support the vision of synthetically prepared material systems that mimic many of the structural aspects with digital precision. A novel technology called 3D jet writing was recently reported that catapults electrospinning to adaptive technologies for the manufacturing of scaffolds according to user-defined specifications of the shape and size of both the pores and the overall geometric footprint. This chapter reviews the hierarchical synergy between electrospinning and 3D printing as part of precision micromanufacturing for rapid prototyping of structures that are likely to evolve next-generation structures into reality.

ORAL SESSION

In situ temperature structural transitions of ferroelectric PZN-4.5PT nanoparticles thin films using synchrotron lightsource

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The $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ -4.5 PbTiO_3 (PZN-4.5PT) single crystals showed very large ferroelectric and piezoelectric properties compared to traditional ferroelectric ceramics (BaTiO_3 and PZT) used as active material in medical imaging, detection and sonars. However, despite these excellent properties, the greatest difficulty to use PZN-4.5PT single crystals on electronic devices is to achieve them in thin layers form related to the difficulty to make them as ceramic material. To overcome this difficulty, we successfully fabricated thin films by dispersing their nanoparticles in a matrix gel that can maintain at least their bulk properties. After this size reduction at nanoscale and the annealing process following the deposition, phases changes and structural transformations occurred. SEM images show some agglomeration at the surface of the silicon substrate and non-identified microstructural phases which could be at the origin of their excellent properties.

In this paper we use the combined USAXS/SAXS/WAXS instrument at 9ID beamline at APS-ANL for in situ characterization of undoped and 1% Mn doped PZN-4.5PT inorganic perovskite nanoparticles thin films deposited on nanostructured silicon to understand the phases transitions and determine the observed microcrystal's structure. The sample was annealed from ambient to 1000 °C. The results revealed structure changes of the nanoparticles thin films which could be explained by the new phase that can be assigned to the $\text{Pb}_3(\text{PO}_4)_2$ based component. The peak at 31° indicates the presence of the rhombohedral phase perovskites assigned to the nanoparticles. XRD spectra, Raman and EDX mapping are compared to the WAXS results. WAXS characterization permitted to identify many transitions during thermal annealing like dehydration or dihydroxylation of phosphorus gel -OH bonds and internal water. Two most important peaks were identified at q values around 3.8 and 5.8 Å^{-1} while q 1.84 at 542 °C and 1.94 at 563 °C correspond to the formation of SiP_2O_7 .

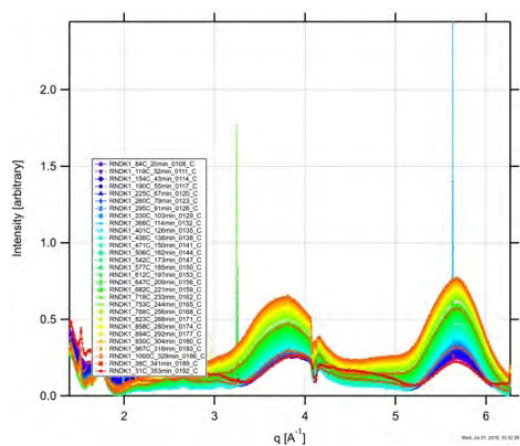


Figure 1. In situ WAXS curves from ambient to 1000 °C

References:

[1] R. Ndioukane, M. Touré, D. Kobor, L. Motte, J. Solard, L. Lebrun, J. Mod. Phys. 10 (2019) 613.

In the absence of sulfurization: zinc molarity effect on nontoxic and low cost CZTS thin films deposited by spin coating technique

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Quaternary kesterite $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) compound have been deposited with different Zn concentrations varying from 0.5 M to 2.5 M by spin coating technique. The effect of copper concentration on the film's structural, morphological, and optical characteristics was investigated.

The structural studies show that as Zn concentration increases, more intense and sharper diffraction peaks (112), (200), and (312) of the kesterite crystal structure are observed. Scanning electron microscope coupled with energy dispersive X-ray analyzer (EDX) has used to identify the existence of spherical morphology and confirmed the elemental composition present in the prepared films. Accordingly, the film composition and structural property were varying with Zn molarity: at relatively high Zn molarity ZnS secondary phase is formed. Derivation approach is used to determine the gap energy of the samples, that was varying slightly between 1.46 eV and 1.58 eV depending on Zn molarity, whereas the conductivity is reduced with the increase of Zn molarity due to the development ZnS secondary phase. By injecting the solar cell (CZTS/ZnS/S:ZnO) in SCAPS 1D using the parameters determined in this work, a theoretical efficiency of 10.98% was attained.

The theoretical simulation supported the experimental finding under the chosen synthesis circumstances, indicating that the synthesized material is a potential candidate for use as an absorber layer in solar cells.

Effect of the glass composition on the dielectric properties of strontium-phosphate-based glasses

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Phosphate glasses have been extensively investigated in recent years in view of their interesting possibilities for wide applications. P_2O_5 is one of the four classic Zachariasen glass forming oxides (along with SiO_2 , GeO_2 and B_2O_3) [1]. Phosphate based glasses have attracted much more attention than other oxide glasses. This attraction is due to their technological and biological applications as well as unique physical properties such as semiconducting properties, simple structure, strong glass forming characteristic, UV transmission and optical features, low melting point and glass transition temperatures, large thermal expansion coefficients, and biomedical compatibility [2-3].

Glass samples in the system $70P_2O_5-(30-x)SrO-xBi_2O_3$ ($0 \leq x \leq 20$ mol%) were successfully prepared via melt-annealing route. X-ray diffraction (XRD) data reveal the amorphous nature of examined glasses. The fourier transform infrared (FT-IR) spectroscopy was used to verify local structure of glass-network. The density and the glass transition temperatures (T_g) of the glasses increases with the increasing amount of Bi up to 10 mol% Bi_2O_3 , and then monotonically decreases. Some optical parameters such as indirect allowed optical band gap, Urbach energy, and refractive index were evaluated from the absorption spectra. On the other hand, Dielectric parameters such as dielectric constant ϵ' , dielectric loss ϵ'' and ac conductivity of the investigated glasses have been evaluated.

References:

- [1] R.L. Christensen, A. Faksh, J.A. Meyers, I.D.W. Samuel, P. Wood, R.R. Schrock, K.C. Hultzs, J. Phys. Chem. A 108 (2004) 8229.
- [2] A. Pedone, X. Chen, R.G. Hill, N. Karpukhina, J. Phys. Chem. B 122 (2018) 2940.
- [3] L.F.P. Pereira, K. Bodiang, E.H.M. Nunes, F.O. Mear, L. Delevoeye, L. Montagne, J. Phys. Chem. C 122 (2018) 15886.

DFT investigation of structural and electronic properties of zinc oxide

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The present work is devoted to the investigation optimized structure, electronic band structure, total and partial density of states, respectively DOS and PDOS, as well as optical properties of bulk wurtzite phase of zinc oxide (ZnO). The optical refractive indices have been studied for both ordinary and extraordinary polarization of the incident light. The calculations, which are based on the density functional theory, are performed by using Quantum Espresso code.

The lattice constants *a* and *c* of the wurtzite phase of ZnO single crystals were found to be 3.18 Å and 5.04 Å, respectively; these values are in reasonable agreement with the experimental values, which are 3.25 Å and 5.20 Å as reported by Kisi et al. [1]. Moreover, the obtained electronic band structure (Figure 1), DOS and PDOS confirm the semiconducting behavior and direct band gap nature of this material; they show also that the top of the valance band is dominated by the O_{2p} state whereas the bottom of the conduction band is dominated by the Zn_{4s} state. Furthermore, it was found that the use of the local density approximation (LDA) leads to an underestimated value of the gap energy, which was found to be 0.79 eV. To remedy this underestimation, the Hubbard-U correction for both 3d and 2p states of Zn and O atoms was considered. Thereby, the energy gap was recalculated to be 3.14 eV with a deviation of 6.21% compared to the experimental value, which is 3.37 eV [2].

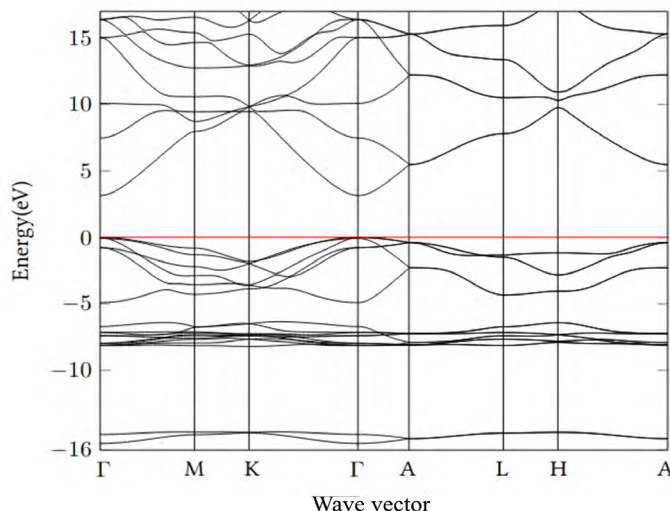


Figure 1. Electronic band structure the wurtzite phase of ZnO single crystals

References:

- [1] E.H. Kisi, M.M. Elcombe, Acta Crystallographica Section C 45 (1989) 1867.
- [2] C.F. Klingshirn, B.K. Meyer, A. Waag, A. Hoffmann, J. Geurts, Zinc oxide: From fundamental properties towards novel applications, pp. 1–5, Springer (2010).

Electrical properties and dielectric relaxation studies in microcrystalline cellulose/multiwalled carbon nanotubes/EVA-VeoVa ternary composites

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Dielectric measurements were carried out on a vinyl resin matrix (EVA/VeoVa) and its composites reinforced with microcrystalline cellulose (MCC) and multiwalled carbon nanotubes (MWCNT) in a ratio of 3:1. The composites VR/MCC/MWCNT0.2 and VR/MCC/MWCNT0.5 have weight fractions of 0.2% and 0.5%, respectively. An Alpha Dielectric/impedance Analyzer (Novocontrol) was used to conduct dielectric studies in isothermal runs with frequencies ranging from 0.1 Hz to 1MHz and temperatures ranging from 30 °C to 130 °C.

The ac conductivity analysis was accomplished according to the following equation: $\sigma_{ac}(\omega) = [\sigma_s / (1 + \tau^2 \omega^2)] + [(\sigma_\infty \tau^2 \omega^2) / (1 + \tau^2 \omega^2)] + A\omega^s$. Figure 1a gives an illustration of the obtained fitting at the temperature 110 °C for the matrix and its composites. The temperature dependence of s reveals an increasing behavior with increasing temperature for the matrix, as depicted in Figure 1b. Its values remain less than 1 for temperatures lower than 125 °C. So ac conductivity mechanism is attributed to the short-range hopping assisted by small polaron. However, for temperatures higher than 120 °C s is higher than 1 and then the mechanism conduction becomes attributed to the localized orientation hopping assisted by the small polaronic hopping. Similar tendency is obtained for both composites but with temperature range variation of the appearance of each mechanism. The recourse to the complex impedance analysis allows separating the bulk from the interfacial properties. Taking into account the dielectric relaxation identification originating from the heterogeneous structure of the samples, the associated electrical response is given by an equivalent circuit composed by four parallel combinations of resistance and constant phase element impedance (R//ZCPE) or resistance and capacitance (R//C) for composites, as can be seen in Figure 1c. The decreasing tendency of the semicircle diameter with increasing weight fraction is attributed to the dc conductivity enhancement.

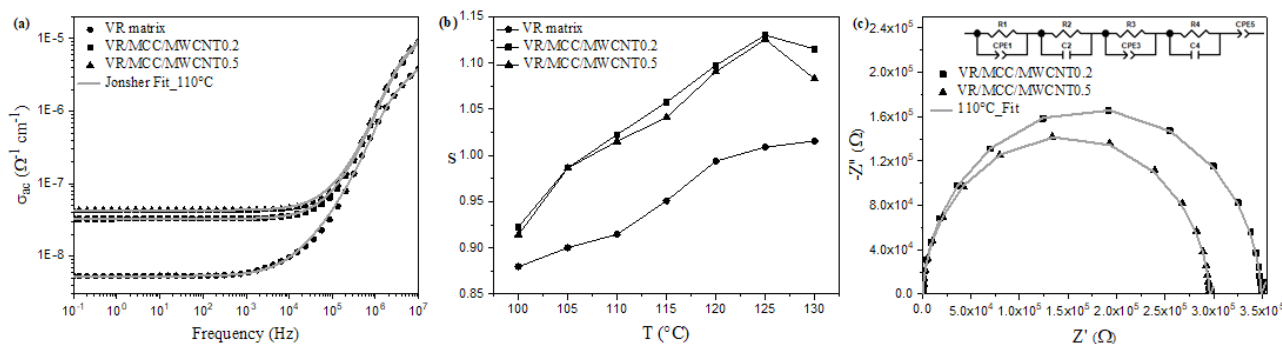


Figure 1. Non-linear fitting of the ac conductivity at 110 °C (a), Temperature dependence of the exponent s (b), Electrical impedance spectra, modeling result and respective equivalent circuit at 110 °C

Investigation of structural and electronic properties of ferroelectric phase of LiNbO_3 using PZ and VdW-DF functionals: a DFT study

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Lithium niobate (LiNbO_3) has attracted a great interest as a future functional material and frequently used in many technological applications due to its excellent ferroelectric, photorefractive, electrooptic, piezoelectric, nonlinear-optical properties. This material occurs in two phases depending on the temperature: the first one, which is a ferroelectric phase with space group $R3c$, is stable below the curie temperature $T_c = 1210^\circ\text{C}$ while the second one, which is a paraelectric phase with the same space group, is stable above the temperature T_c [1]. In the present work, structural and electronic properties of the ferroelectric phase of LiNbO_3 single crystals have been theoretically investigated using (i) a standard local functional of type Perdew-Zunger (PZ) and (ii) a nonlocal functional of type Van der Waals density function (vdW-DF) within the framework of the density functional theory (DFT) as implemented in Quantum Espresso [2]. The obtained values of the optimized lattice parameters are in a good agreement with the experimental ones. Our calculated values of gap energy are 2.62 eV and 2.78 eV, respectively for the functionals PZ and vdW-DF. These values present an underestimation compared to the experimental value, which is 3.78 eV [3], but they are in good agreement with other DFT-based calculations. Furthermore, the analysis of the total density of state (DOS) and partial density of state (PDOS) show that the conduction and valence band are mainly composed niobium and oxygen orbitals while the lithium has a weak contribution in both conduction and valence bands.

References:

- [1] K. Toyoura, M. Ohta, A. Nakamura and K. Matsunaga, Journal of Applied Physics 118 (2015) 064103.
- [2] P. Giannozzi et al., Journal of Physics: Condensed Matter 21 (2009) 395502.

Contribution of volume and surface magnons to the study of the magnetic properties of Fe/Pt superlattices

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The work presented in this paper is a contribution to the study of the properties of magnons created in “bulk” and “surface” in Fe/Pt single magnetic multilayer systems. This study is based on the calculation of the excitation spectrum $E(k)$ and the spin magnetization $M(T)$ using the Heisenberg model treated by Green's function method. We have highlighted the existence of two types of population: magnons created on surface and in bulk. Each of these two populations is characterized by a creation gap $E_g^{s,b}$, a lifetime $\tau_{s,b}$, and a permitted bandwidth $W_{s,b}$. The comparison of the calculated and measured magnetization [1] is very satisfactory justifying thus our working hypotheses.

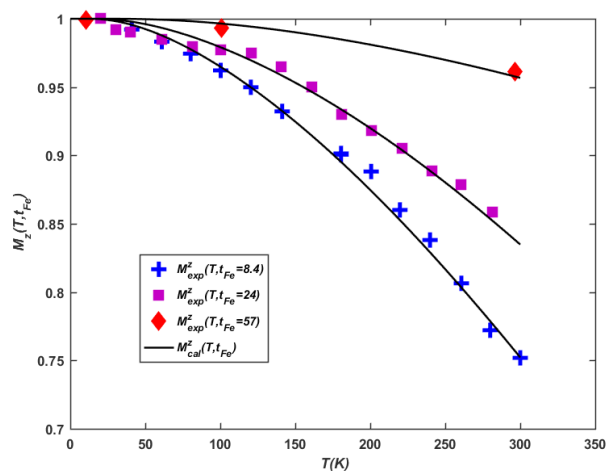


Figure 1. variation of the thermal magnetization $M(T,t)$ of the different thicknesses of the magnetic layer t_{Fe}

References:

- [1] R. Elkabila, K. Benkiranea, H. Lassri, M. Abidb A. Hamdouna, A. Berradad, R. Krishnane, Physica A 358 (2005) 142.

DFT study of spontaneous polarization and refractive indices of tetragonal BaTiO₃ and PbTiO₃ for various pseudopotentials

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Ferroelectric and optical properties are among the most determining properties that help to choose suitable ferroelectric materials for technological applications such as capacitors, ferroelectric and holographic memories, electro-optical modulators, etc. In this study, we focus on the spontaneous electrical polarization and refractive indices of tetragonal barium titanate (BaTiO₃) and lead titanate (PbTiO₃) single crystals by using density functional theory (DFT) and considering various exchange-correlation functionals (PZ, PW91, BLYP, PBE, B86BPBE, etc.) as implemented in Quantum Espresso.

The calculated values of the spontaneous polarization, which depend on the exchange-correlation functional used, range between 0.27 and 0.65 C/m² for BaTiO₃, and between 0.57 and 0.85 C/m² for PbTiO₃. For the refractive indices, the calculated values range between 2.3 and 2.9 for BaTiO₃, and between 2.7 and 3.3 for PbTiO₃. The analysis of the results obtained shows that they present a satisfactory agreement with the experimental measurements [1,2] as well as with the previous theoretical calculations.

References:

- [1] D.I. Bilc, R. Orlando, R. Shaltaf, G.M. Rignanese, J. Íñiguez, Ph. Ghosez, Physical Review B 77 (2008) 165107.
- [2] H. Chaib, L.M. Eng, T. Otto, Journal of Physics: Condens. Matter 17 (2005) 161.

Synthesis and characterisation of GO/SrFe₁₂O₁₉ as magnetic hybrid nanocatalyst for regioselective ring-opening of epoxides with amines under eco-friendly conditions

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Herein, a highly efficient magnetically separable hybrid GO/SrFe₁₂O₁₉ nanocomposite was synthesized via dispersing M-type strontium hexaferrite (SrFe₁₂O₁₉) on graphene oxide (GO) sheets. First, SrFe₁₂O₁₉ nanoparticles (NPs) and GO sheets were prepared via chemical coprecipitation and chemical oxidation of graphite powder, respectively. Chemically reduced GO (rGO) and rGO/SrFe₁₂O₁₉ were also prepared for a comparison purposes.

Thereafter, the prepared nanostructured materials were explored by XRD, FTIR, Raman, FESEM-EDX, BET, and Zeta-Sizer analyses. All the characterizations confirm the nanoscale and the high stability structures of the prepared materials. The prepared hybrid magnetic nanocomposite GO/SrFe₁₂O₁₉ exhibited a high surface area value resulting in a high catalytic activity and selectivity for the epoxide ring-opening with amines in neat water. Moreover, the use of hybrid GO/SrFe₁₂O₁₉ compared to the pure SrFe₁₂O₁₉ and GO sheets is of great interest for using environmentally benign heterogeneous nanocatalysts, for the synthesis of β-amino alcohols, with excellent recyclability under eco-friendly conditions.

In addition, a mechanistic study was performed through density functional theory (DFT) calculations and Parr functions to explain the observed reactivity and selectivity of SrFe-GO nanocatalyst in epoxide ring-opening reaction.

Simulation study of triboelectric nanogenerator for effective energy harvesting

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In the past few decades, energy-harvesting devices for producing electricity from different energy sources have been developed with the aim of resolving the global energy crisis, including portable, wearable generators and self-powered electronics [1,2]. The energy sources that are insensitively studied are solar, thermal, and mechanical energies. Among these sources, mechanical energy is one of the most universally existing, diversely presenting but usually wasted energies in the natural environment, which has attracted a lot of effort in developing the energy harvesting techniques based on different effects and mechanisms. There are a lot of new technologies that are working to develop small and portable energy harvesters for electronic devices such as triboelectric nanogenerators (TENGs) [3]. This paper investigates a new TENG based on different triboelectric films a simulation was performed by using COMSOL in order to investigate the principle of the electricity generating of this model. For the chosen parameters, the maximum reported output power for an optimal resistance load of 795 MΩ is 493 μW in the case of Mica-PET films.

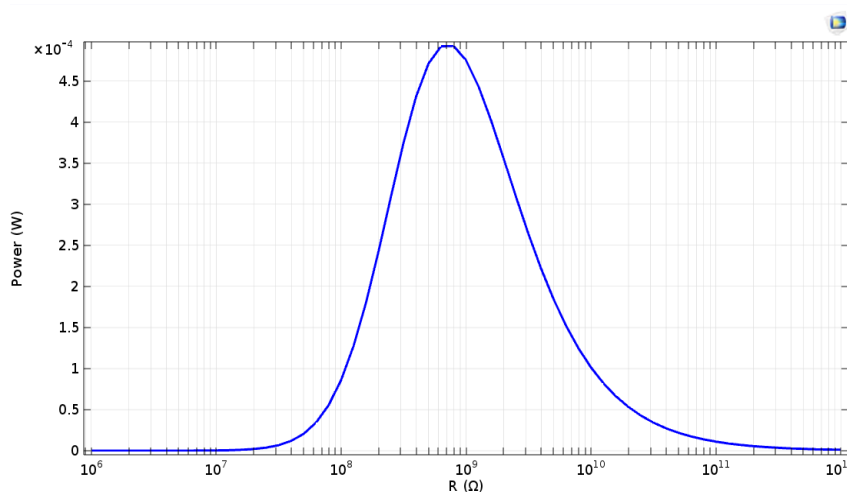


Figure 1. Variation of the electric power of the TENG based Mica/PET as a function of load resistances

References:

- [1] A. Mahmud, A.A. Khan, S. Islam, P. Voss, D. Ban, Nano Energy 58 (2019) 112.
- [2] S.M. Zhu, A.F. Yu, G.Y. Yu, Y.D. Liu, J.Y. Zhai, W. Dai, E. Luo, Appl. Phys. Lett. 111 (2017) 153901.
- [3] J.Luo, Z.L. Wang, EcoMat 2 (2020) e12059.

Fabrication of diamond photonic nanostructures

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Diamond is a material with a number of outstanding mechanical, optical, electrical and chemical properties. In the last decade it has additionally attracted the attention of scientists due to the promising properties of the color centers in its crystal lattice such as the nitrogen-vacancy (NV) and the silicon-vacancy (SiV) centers which can find applications in quantum information technology. In order to increase the collection efficiency of the photons emitted by the color centers they should be incorporated in photonic structures. We demonstrate the fabrication of several types of single-crystal diamond (SCD) photonic nanostructures, namely nanopillars, thin membranes and photonic crystals (see Figure 1). Nanopillars with diameters down to 50 nm were prepared by electron beam lithography (EBL) and inductively coupled plasma reactive ion etching (ICP-RIE) with oxygen [1-3]. NV color centers were incorporated in the diamond nanopillars by nitrogen implantation in monocrystalline diamond prior the structuring. The SiV centers were introduced in the diamond crystal lattice by short overgrowth of already structured nanopillars incorporating Si atoms etched from the substrate on which the diamond samples were placed. SCD in a form of thin membranes is a particularly promising for the fabrication of high-quality photonic devices. We report on the fabrication process of SCD membranes with various diameters (500 μm - 1 mm) and thickness (3 - 5 μm down to 500 - 600 nm), exhibiting a low surface roughness down to 0.2 nm on a small area scale, applying ICP-RIE. For SCD samples with an initial rms surface roughness of ~ 1.5 nm a significant roughness reduction was achieved by using two distinct Ar/Cl₂ etching recipes as a planarization step before the actual structuring process, comprised out of alternating Ar/Cl₂ + O₂ etching steps. By a variation of etching parameters, an enhanced planarization of the surface was obtained, due to a low etch rate of a few nm/min and the Ar/Cl₂ chemistry, which rather smoothens out the groove profile, introduced by the polishing procedure, instead of transferring it during the etching. These planarized SCD membranes are successfully bonded via van der Waals forces on plane cavity mirrors and optically characterized in a fiber-based Fabry-Pérot microcavity system regarding their mode structure and finesse [4]. Finally, we demonstrate the fabrication of 2D photonic crystals in SCD membranes by EBL and ICP-RIE.

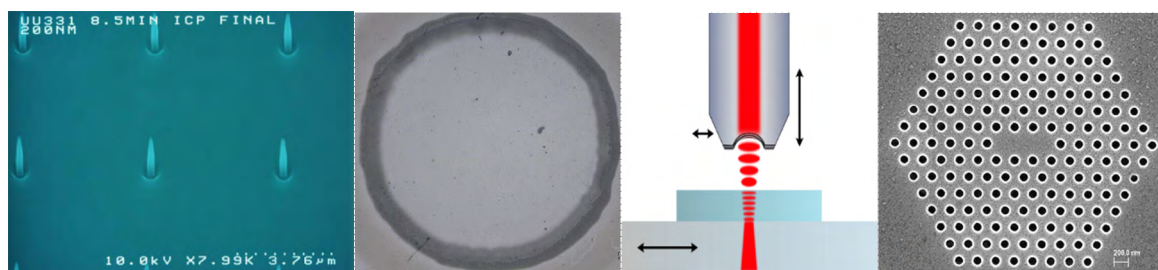


Figure 1. SCD photonic nanostructures: (left) nanopillars, (middle) thin membrane in Fabry-Pérot microcavity and (right) 2D photonic crystal

Funding acknowledgment. The authors would like to thank the German Federal Ministry of Education and Research (BMBF) for the financial support under Projects QR.X and DIQTOK.

References:

- [1] N. Felgen, B. Naydenov, F. Jelezko, J.P. Reithmaier, C. Popov, *Phys. Stat. Sol. A* 215 (2018) 1800371.
- [2] N. Felgen, A. Schmidt, B. Naydenov, F. Jelezko, J.P. Reithmaier, C. Popov, *Quantum Information Technology and Sensing Based on Color Centers in Diamond*. In *Advanced Nanotechnologies for Detection and Defence Against CBRN Agents*, Eds. P. Petkov, D. Tsiulyanu, C. Popov, W. Kulisch, Springer, pp. 193-214 (2018).
- [3] K. Volkova, J. Heupel, S. Trofimov, F. Betz, R. Colom, R.W. MacQueen, S. Akhundzada, M. Reginka, A. Ehresmann, J.P. Reithmaier, S. Burger, C. Popov, B. Naydenov, *Nanomaterials* 12 (2022) 1516.
- [4] J. Heupel, M. Pallmann, J. Körber, R. Merz, M. Kopnarski, R. Stöhr, J.P. Reithmaier, D. Hunger, C. Popov, *Micromachines* 11 (2020) 1080.

Long time protonic conductivity behavior of $\text{CsH}_5(\text{PO}_4)_2$ crystal at high pressure

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The $\text{CsH}_5(\text{PO}_4)_2$ salt is close relative to well known, as one of the promising materials for practical applications, the proton conductive CsH_2PO_4 salt. The compound has a unique H-bond network in which PO_4^{3-} anions are linked via O...O bonds at all corners of the phosphate tetrahedra forming $(\text{H}_2\text{PO}_4)_\infty$ layers in the [100] direction. The layers are linked together due to electrostatic interaction with Cs^+ and due to H-bonds. The considerably stronger H-bond network in the $\text{CsH}_5(\text{PO}_4)_2$ prompts for a higher superprotonic transition temperature. However, due to the relatively weak bonding between the $\{[\text{H}_2\text{PO}_4]\}_\infty$ planes in the [100] direction of the $\text{CsH}_5(\text{PO}_4)_2$ structure, the bonds between the planes become thermally broken, and the crystal melts before the H-bond network rearranges via the water release into an open structure typical of the superprotonic phase.

We examined, using impedance spectroscopy, the proton conducting crystal $\text{CsH}_5(\text{PO}_4)_2$ to check whether subtle changes in the crystal structure and proton dynamics caused by external pressure induce the superionic phase in the crystal. The ac conductivity was measured, in the frequency range from 100 Hz to 1 MHz, at temperatures $200 \text{ K} < T < 420 \text{ K}$ and pressures $0.1 \text{ MPa} < p < 360 \text{ MPa}$.

At fixed thermodynamic conditions ($p = 170.7 \text{ MPa}$, $T = 417 \text{ K}$) the protonic conductivity of $\text{CsH}_5(\text{PO}_4)_2$ crystal along the direction of small conductivity exhibits an unexpected and noticeable evolution in time (see Figure 1). The conductivity is approximately constant for short times, less than 10 hours. Next, for times up to 300 hours, comes a period of conductivity growth which saturates at ten times its initial value. This growth occurs in a highly randomized way where large jumps are followed by significant falls. Further observation shows a slow descent of conductivity. This process is reversible.

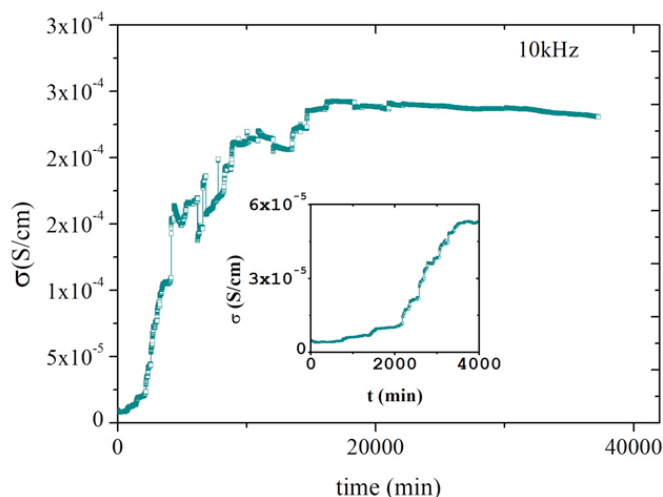


Figure 1. The time evolution of $\text{CsH}_5(\text{PO}_4)_2$'s protonic conductivity at $p = 170.7 \text{ MPa}$, $T = 417 \text{ K}$

To explain this phenomenon, we propose that weak metastable bonds between planes of high conductivity may emerge and form a percolation path perpendicular to these planes. Each such path is then a source of the disorder leading to an increase of interplane bonds and, as such, the growth of new percolation paths. We justify this picture by the numerical calculations in the 3-dimensional model of protonic conductivity and reproduce the observations qualitatively.

Electrical impedance analysis of carbon dots/PMMA composite materials

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The AC electrical conductivity of carbon dots (C.dots) in Poly(methyl methacrylate) (PMMA) polymer composites has been studied from 200 to 390 K in the frequency range from 100 Hz to 1 MHz as a function of the filler volume fraction, above the percolation threshold. We have shown that the AC conductivity follows a power law in frequency, $\sigma_{AC}(\omega) \propto \omega^s$, at high frequency, where s depends on the temperature. This behavior was explained in terms of the correlated barrier hopping model. Finally, the complex impedance and Nyquist plots of the C.dots/PMMA composites are analyzed by using equivalent circuit models, which includes a constant phase element (CPE). The analysis gathered here, aims to contribute to the understanding of the enhanced dielectric properties of low-conducting polymer composites, filled with C.dots particles.

Structural dependent electrical impedance spectroscopy behaviour of multiwalled Carbon nanotube/Graphite/Polyester ternary composites

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The purpose of the present study is to identify the relationship between the electrical and structural characteristics of ternary composites, prepared by adding with multi-walled carbon nanotubes (MWCNT) and graphite (Gr) as conductive fillers to an insulating pPolyester matrix. The structural characterization of these ternary composites was performed using small-angle neutron scattering (SANS) and infrared (IR) and Raman spectroscopies. Electrical measurements were carried out in a frequency range from 100 Hz to 1 MHz and in the temperature range from 200 K to 380 K. The frequency dependence of the alternating conductivity (AC) obeys the Jonscher's power law. The temperature dependence of AC conductivity indicates that the electrical conduction in the material is a thermally activated process. The critical behavior of the DC electrical conductivity and electrical resistivity as a function of the temperature indicates a strong positive temperature coefficient and a negative temperature coefficient of resistivity (PTCR/NTCR) below and above the critical temperature T_c , respectively. The percolation threshold of the MWCNT/Gr/Polyester composite is much lower than that of either the MWCNT/Polyester or Gr/Polyester composite. Furthermore, the analysis of the temperature dependence of DC conductivity using the Arrhenius equation indicated that the addition of MWCNT and Gr into Polyester matrix decrease the activation energies.

Electrical and dielectric properties of different forms of carbon allotropes/ resin epoxy composite materials near the percolation threshold

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This work presents the electric and dielectric response of four series of polymer composites in a various content of reduced Graphene Oxide (rGO), Carbon Nanotubes (CNT) and Carbon Black (CB) inclusions, using impedance spectroscopy in the frequency range between 200 Hz and 1 MHz. Percolation theory is used to describe the mechanisms of electronic transport in these heterogeneous materials [1]. We have determined the critical exponents which describe the behaviors of the dielectric constant, near the percolation threshold, as functions of the frequency. The experimental values of the critical exponents are in agreement with those given in the literature. Furthermore, the complex impedance spectra and Bode diagrams of these composites, near the percolation threshold, were carefully analyzed by using equivalent circuit models, which includes a constant phase element (CPE) [2]. Finally, the Cole-Cole representation was used to interpret the impedance spectra of all composites series [3].

References:

[1] D. Stauffer, A. Aharony, Introduction to Percolation Theory (1992).

[2] J.R. Macdonald, Annals of Biomedical Engineering 20 (1992) 289.

[3] J.R. Macdonald, Impedance Spectroscopy-Emphasizing Solid Materials and Systems, Wiley, New York (1987).

Dielectric and mechanical studies on silicone rubber particle and liquid filled composite material

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The objective of the present study is to develop soft dielectric material to be used in sensors and actuators. The capacitive sensors and actuators made up of the soft dielectric material need to possess higher dielectric permittivity and lower stiffness [1]. The modulus of elasticity is in essence stiffness of the material. In this regard Silicone Rubber (SR) composites are prepared made of strontium titanate particles in three different volume percentages namely 5, 7.5, and 10. The composite samples developed are subjected to dielectric and mechanical testing. In dielectric testing, properties like dielectric permittivity, dissipation factor, and ac conductivity are studied. In mechanical testing, the modulus of elasticity in compression is studied. It is found that the dielectric permittivity of SR composites improved as the volume percentage of strontium titanate particles increased. But the modulus of elasticity also increased with an increase in the volume percentage of particles.

The SR composite made of 7.5 % volume of strontium titanate particles exhibited better properties and is selected for possible further improvement of properties. To achieve this objective, the silicone rubber composites made up of strontium titanate particles and glycerol liquid with three volume percentages namely 12.5, 17.5, and 22.5 are developed and tested. It is found that, as SR composites made up of strontium titanate particles filled with increased glycerol, the dielectric permittivity increased and the modulus of elasticity decreased as shown in Figure 1. The SR composite made of 7.5% volume of the particle and 15% of glycerol, the dielectric permittivity improved by 94%, and the modulus of elasticity reduced by 24% compared to SR composite with 7.5% volume of particles. This study suggests that the novel material developed is a potential material suited for soft dielectric sensors and actuators.

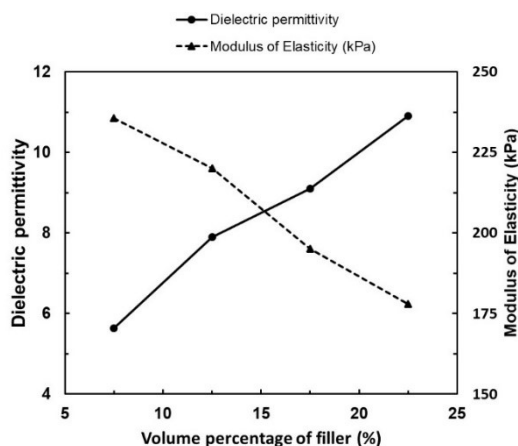


Figure 1. Variation of dielectric and mechanical properties with filler loading

References:

[1] L.J. Romasanta, M.A. Lopez-Manchado, R. Verdejo, Progress in Polymer Science 51 (2015) 188.

Electrocaloric characterization of samarium doped barium titanate ceramics synthesized by sol-gel process

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Several technologies based on solid-state refrigeration are being developed as alternative to the vapor compression refrigeration. One of these alternatives is the electrocaloric refrigeration. Electrocaloric effect (ECE) is a physical phenomenon present in polar materials and requires the application and removal of external electric field. This, results in an adiabatic reversible change of temperature or an isothermal variation of entropy [1]. Nowadays, the majority of the studied electrocaloric materials are ferroelectric, since they have a very important ECE near phase transition.

ECE is extensively studied in ceramics. The most studied ceramics are of the perovskite (ABO_3) type, in particular lead-based materials. As the use of lead is being prohibited in a growing number of countries, these materials can be substituted by perovskite materials based on barium titanate ($BaTiO_3$), which are among the most widely recognized lead-free ferroelectric material for its excellent dielectric and ferroelectric properties [2]. However, it has a relatively high transition temperature (130 °C) and an ECE that can be exploited over a very restricted temperature range. These drawbacks prevent its exploitation for practical reasons. To overcome this, various ionic doping of $BaTiO_3$ were adopted to broaden the peak of the ECE and to modify its position towards room temperature [3].

Studies of the ECE on samarium-doped barium titanate (BTO-Sm) are very rare. To our knowledge, a single electrocaloric study on BTO-Sm with 4% samarium concentration ($Ba_{0.94}Sm_{0.04}TiO_3$) synthesized by solid-state reaction method was carried out. The results revealed that the substitution led to a large ECE coefficient ($\Delta T/\Delta E \approx 0.3 \text{ K}\cdot\text{m}/\text{MV}$) [3]. In the current study, $Ba_{1-x}Sm_xTiO_3$ ($0 \leq x \leq 0.06$) was synthesized by sol-gel method. Structural, electrical, thermal and electrocaloric properties are measured. The results of the ECE showed that the substitution led to a decrease in the maximum transition temperature at which the ECE occurs and to a widening of the temperature range where the ECE may be exploited.

References:

- [1] T. Correia, Q. Zhang, Electrocaloric materials. *New Generation of Coolers*, 34, pp.1-12, Springer (2014).
- [2] Y. Bai, K. Ding, G.P. Zheng, S.Q. Shi, J.L. Cao, L. Qiao, *AIP Advances* 2 (2012) 022162.
- [3] F. Han, Y. Bai, L.J. Qiao, D. Guo, *Journal of Materials Chemistry C* 4 (2016) 1842.

Measurement of the dynamic temperature response of electrocaloric effect in solid ferroelectric materials via thermoreflectance

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Electrocaloric (EC) effect is defined as the adiabatic temperature or isothermal entropy changes, induced by an electric field, of a dielectric material. For thin films, indirect measurement is frequently used to quantify the electrocaloric effect [1], direct methods suitable for these types of films are rare. Indeed, given the low mass of the electrocaloric film relative to the mass of the substrate, the small quantity of heat generated is quickly dissipated towards the substrate and the temperature variations of the assembly is very low. However, the use of the indirect method always leaves room for suspicions, given the limits of application of Maxwell's relations. It is, therefore, imperative to study these materials using instruments offering high resolution.

In this study, we propose a characterization method based on modulated thermoreflectance technique for measuring directly the EC effect. First, the EC response in BaTiO₃-based multilayer ceramic capacitors (MLC) with Y5V specification was measured using the thermoreflectance set-up. This MLC was chosen because it is widely used and studied in the literature [2,3] and was used, in our study, to calibrate our measurements. We noticed that the MLC EC temperature responses depend on the operation voltage frequency, thus we considered three frequency range using square voltage waveform. It was found that, three distinct types of EC temperature variation responses were observed depending on the waveform frequency range.

Further, the same study was implemented on P(VDF-TrFE) 55/45 thin films, where the frequency dependence of the EC response in these films was investigated. In addition, the temperature variation at the surface of the thin film of polymer with a thickness of 1.7 μm was also measured via thermo reflectance. The data reveal a large EC effect occurring at room temperature where a surface temperature change $\Delta T = 1.144$ °C was induced under a field of 83.33 MV/m.

Acknowledgment: We are grateful to the Université du Littoral Côte d'Opale and the National Council for Scientific Research in Lebanon for the support of this work.

References:

- [1] B. Neese, B. Chu, S.-G. Lu, Y. Wang, E. Furman, Q.M. Zhang, Science 321 (2008) 821.
- [2] R. Faye, T. Usui, A. Torello, B. Dkhil, X. Moya, N.D. Mathur, S. Hirose, E. Defay, Journal of Alloys and Compounds 834 (2020) 155042.
- [3] S. Kar-Narayan, N.D. Mathur, Journal of Physics D: Applied Physics 43 (2010) 032002.

Processing and electrical characterization of $\text{Ba}(\text{Ti}_{0.8}\text{Zr}_{0.2})\text{O}_3-(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ lead-free piezoelectrics for energy-efficient caloric applications

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Ferroelectric oxides during phase transitions exhibit a large change in isotropic entropy and adiabatic temperature under the action of an electric field. Such an effect is larger and short-lived in materials of first-order compared to those with second-order. Lead-based $\text{Pb}(\text{Zr,Ti})\text{O}_3$, $\text{Pb}(\text{Mg,Nb})\text{O}_3$, etc. have exhibited excellent electrocaloric properties both in bulk and thin-film forms. However, recently there has been an intense investigation for cleaner energy with environment-friendly piezoelectrics having potential on par with the lead-based ones. In this regard, lead-free oxides having morphotropic phase boundary and polymorphic transitions have emerged as candidates for a variety of applications.

Our presentation discusses important observations obtained in the research of $\text{Ba}(\text{Ti}_{0.8}\text{Zr}_{0.2})\text{O}_3-(\text{Ba}_{0.7}\text{Ca}_{0.3})\text{TiO}_3$ (BCZT) piezoelectrics possessed by the laser-heated-pedestal growth (LHPG) in comparison with polycrystalline ceramics. We have grown BCZT fiber crystals by controlling process parameters of LHPG and obtained functionally graded materials. Detailed structure, morphology, composition, and electrical characterization of BCZT oxides are presented with a focus on caloric applications. We found a subtle change in composition and orientation has greater effects on bulk polarization and electrocaloric potential. Local changes to the piezoelectric response of BCZT fibers vis-à-vis bulk ceramics were investigated using atomic force microscopy and evident changes in morphology, as well as polar-nano-regions, have been observed. The correlations between theoretical and experimentally observed caloric properties are presented. The electrocaloric property of the studied materials is presented in Figure 1.

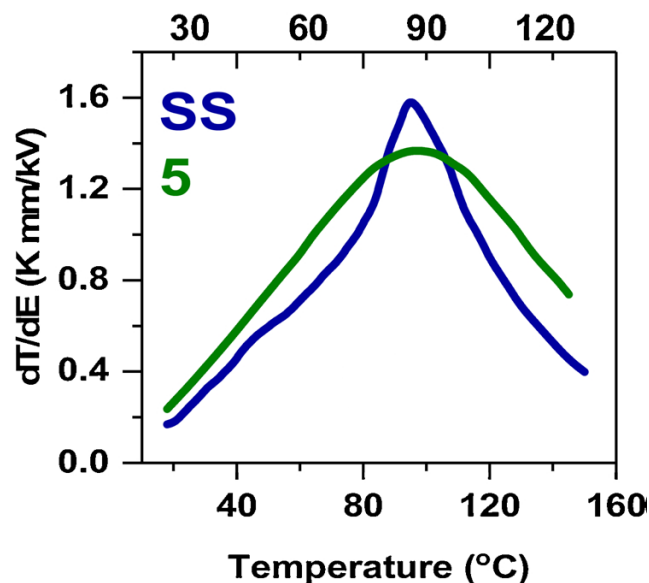


Figure 1. Electrocaloric responsivity of BCZT ceramic (SS) and fiber crystal (5). Calculated theoretically, based on the direct electrocaloric measurements

This work was developed within the scope of the project 032-88- ARH/2018 (EVR) financed by national funds (OE) through the Portuguese Foundation for science and technology (FCT), in the scope of the framework contract foreseen in the numbers 4, 5 and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19.

References:

- [1] E.V. Ramana, N.M. Ferreira, A. Mahajan, D.M. Tobaldi, I. Bdkin, B. Rozic, Z. Kutnjak, M.A. Valente, J. Eur. Ceram. Soc. 41 (2021) 6424.
- [2] E. Venkata Ramana, F. Figueiras, A. Mahajan, D.M. Tobaldi, B.F.O. Costa, M.P.F. Graça, M. A. Valente, J. Mater. Chem. C 4 (2016) 1066.

Effect of an additive organic TE1 in improving the quality of nickel electroplating on brass

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Nickel plating on brass is a technique widely used in various industrial activities. The different deposition processes are relatively complex and depend on several factors such as PH, temperature and bath composition. [1] Nickel plating in watt baths is frequently used in large surface treatment industries due to the appearance and stability of the deposit over time.

In order to improve the quality of nickel deposition on brass, a comparison of nickel plating by the Watts bath with an electrolytic nickel bath mixed with an organic additive proposed.

Cyclic Voltametry, Corrosion behaviour of nickel coatings and characterization of the deposits by (SEM) and metallurgical optical microscope were carried out.

The results obtained show the appearance of cracks and micrograins on the surface of the nickel deposit made in the Watts bath. On the other hand, the proposed bath gives a better quality of the deposit, addition of the organic adjuvant allows the homogeneity and brightness of the nickel deposit to be maintained.

References:

[1] N.P. Wasekar, P. Haridoss, S.K. Seshadri, G. Sundararajan, Surface and Coatings Technology 291 (2016) 130.

Novel organometallic complexes and their application in solar cells

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Transition metal complexes continue to attract the attention of many research teams around the world, whether academic or industrial. They have found a range of energy applications, for example, as light-to-electricity signal converters in organic light-emitting diodes and dye-sensitized solar cells, energy storage, and potentially conductive thermoelectric materials.

Efforts to produce an alternative to Ru-based dyes are ongoing and so in this research we investigated complexes of vanadium, cobalt and copper with a water-soluble Schiff base. These complexes have been synthesized and evaluated as possible dyes in DSSCs.

Proton conductivity of imidazole or 1,2,4-triazole entrapped in microporous molecular sieves

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Proton conductors, as materials for proton-exchange membranes in fuel cells, have been extensively studied over the last decades. Because of susceptibility to dehydration of commonly used Nafion compound, special attention is focused on materials, in which the conductivity does not require the participation of water and exhibit efficient proton transfer at moderate temperatures.

The solid state azoles, such as imidazole or 1,2,4-triazole exhibit very low proton conductivity ($\sim 10^{-8}$ Scm⁻¹) at room temperature. However, the mobility of azole molecules is much higher above its melting point and consequently the conductivity increases above 10^{-3} Scm⁻¹. The increase of the mobility at room temperature can be also attained by imidazole dispersion in porous matrices, such as various types of MOF's and inorganic or polymeric materials [1-7].

The main aim of our study was to prepare novel conducting materials based on composites of imidazole anchored in zeolites or zeotypes. These molecular sieves are thermally and chemically more stable than MOFs or polymers. The well-ordered and uniform crystalline porous structure of zeolites and zeotypes enables the guest molecules to be accommodated in a desired place and environment.

In our studies, we have chosen several types of zeolites differing in volume as well as pore size. We examined the influence of azoles concentration and the impact of different acidity of applied matrices (different framework Si/Al ratio) on the conductivity properties of the resulting composites.

The composites studied by us were characterized by means of typical physicochemical techniques: FTIR, PXRD, thermal analysis, ammonia TPD, BET, elemental analysis, and SEM. The conductivity measurement was performed by means of impedance spectroscopy.

As a result, we obtained thermally and time-stable composites with a relatively high proton conductivity comparable to the values of azoles in the molten phase.

We have shown how conductivity depends on azole concentration and mobility, porosity parameters and the chemical nature of matrices, and the preparation method. Based on the results obtained, we have proposed the mechanisms of the proton conductivity of studied composites [8-10].

References:

- [1] S. Bureekaew, S. Horike, M. Higuchi, M. Mizuno, T. Kawamura, D. Tanaka, N. Yanai, S. Kitagawa, *Nat. Mater.* 8 (2009) 831.
- [2] N. Hojo, T. Yamamoto, Y. Okada, J. Niikura, *ECS Trans.* 11 (2007) 123.
- [3] Y. Ye, L. Zhang, Q. Peng, G.-E. Wang, Y. Shen, Z. Li, L. Wang, X. Ma, Q.-H. Chen, Z. Zhang, S. Xiang, *J. Am. Chem. Soc.* 137 (2015) 913.
- [4] S. L. Li, Q. Xu, *Energy Environ. Sci.* 6 (2013) 1656.
- [5] T. Homburg, C. Hartwig, H. Reinsch, M. Wark, N. Stock, *Dalton Trans.* 45 (2016) 15041.
- [6] E. Eisbein, J. O. Joswig, G. Seifert, *J. Phys. Chem. C* 118 (2014) 13035.
- [7] S. Liu, Z. Yue, Y. Liu, *Dalton Trans.* 44 (2015) 12976.
- [8] A. Jankowska, A. Zalewska, A. Skalska, A. Ostrowski, S. Kowalak, *Chem. Commun.* 53 (2017) 2475.
- [9] A. Jankowska, A. Ostrowski, M. Zieliński, S. Kowalak, *Microporous Mesoporous Mater.* 274 (2019) 33.
- [10] A. Jankowska, A. Ostrowski, S. Kowalak, *Microporous Mesoporous Mater.* 298 (2020) 110059.

Electrical properties of cerium-containing Bioglass®

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The use of dental implants is increasing due to the limitations of removable prosthetics and the need for alternative devices that consider aesthetics. In addition, dental implants are considered to be the only restorative technique that preserves and stimulates natural bone. The dental implants market is expected to expand at an annual growth rate of 11.0% between 2021 and 2028 [1]. However, even with the excellent results that dental implants provide, mechanical, technical, and biological complications can still occur. There are failures associated with host factors such as systemic disease; factors related to surgical trauma; factors related to inadequate design that becomes evident with force cycles applied over time, and mainly due to infections such as peri-implantitis [2,3].

Peri-implantitis is considered the most challenging biological difficulty in implantology, as the disease can progress and result in implant loss. It affects 13% of implants and 19% of patients and its incidence tends to increase from 0.4 to 43.9% within 3-5 years. Thus, prevention of disease and promotion of the various biological events that occur at the implant-body interface is crucial in clinical dental practice [4-6].

It has been reported that the use of bioglass as an implant coating can stimulate tissue integration and accelerate implant regeneration [7-9]. Bioglass also has the ability to store surface charge thereby increasing osteoconduction by charging its surface with negative electrical charges [10]. In addition to these properties, antibacterial activity, antioxidant effect, anti-inflammatory effect can be promoted by the insertion of cerium into the bioglass network [11-13].

In this work, bioglass with 0.25%, 0.5, 1 and 2% mol of CeO was synthesized by melt-melting and morphological and electrical properties were analyzed. The electrical behavior was measured by ac and dc approaches in bulk and pellets.

References:

- [1] www.grandviewresearch.com Dental Implant Market Size, Share & Trends Analysis Report By Implants Type (Titanium, Zirconium), By Region (North America, Europe, Asia Pacific, Latin America, MEA), And Segment Forecasts, 2021 – 2028 (2021).
- [2] J. Přikrylová, J. Procházková, Š. Podzimek, *Biomed Res. Int.* 10 (2019) 2519205.
- [3] A. Hanif, S. Qureshi, Z. Sheikh, H. Rashid, *European Journal of Dentistry* 11 (2017) 135.
- [4] <https://www.efp.org/dental-implants/peri-implant-diseases/>
- [5] D. Hashim, N. Cionca, *Current Oral Health Reports* 7 (2020) 262.
- [6] A. Hanif, S. Qureshi, Z. Sheikh, H. Rashid, *European Journal of Dentistry* 11 (2017) 135.
- [10] M. Cerruti, *Phil. Trans. R. Soc. A* 370 (2012) 1281.
- [11] A. Anesi, G. Malavasi, L. Chiarini, R. Salvatori, G. Lusvardi, *Materials (Basel)* 15 (2020) 2297.
- [12] S. Raimondi, A. Zambon, R. Ranieri, F. Fraulini, A. Amaretti, M. Rossi, G. Lusvardi, *J. Biomed. Mater. Res. A* 110 (2022) 504.
- [13] G. Malavasi, R. Salvatori, A. Zambon, G. Lusvardi, L. Rigamonti, L. Chiarini, A. Anesi, *Materials (Basel)* 12 (2019) 594.

Designing of new dielectric resonator antenna fed by microstrip line with quarter wave transformer

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Dielectric resonator (DR) antenna fed by microstrip line with quarter wave transformer is designed with marble as dielectric resonator that printed on FR4 Epoxy substrate having relative permittivity of 4.4 and thickness of 1.8 mm. The dielectric constant of marble is formulated with finite dimensions in order to investigate its effect on the antenna performance around frequency of 28 GHz which already gave suitable result in our published work [1]. The designed geometry of the antenna has been optimized basis on the electromagnetic solver HFSS software to achieve a return loss value less than -10 dB with reasonably gain and directivity. Significant improvement on impedance bandwidth which is 2.25 GHz is achieved at the band of 26.86 - 29.11 GHz. The results showed that the marble is an effective material for the antenna structure offering simplicity in design.

Reference:

[1] Y. El Hasnaoui, T. Mazri, *Advances in Materials and Processing Technologies* 6 (2020) 1.

The effect of niobium oxide on the structure, electrical and biological properties of 45S5 bioactive glass

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In recent decades, the requirement for implantable medical devices increased. The placement of those implants is usually associated with bacterial infections, leading to the death of bone tissue surrounding the implant and thus its failure. The objective of this work is to solve the problem related to this implant infections issue, by developing an antibacterial biomaterial for implant coatings. In this context, a series of 45S5 bioglasses modified by the incorporation of different amounts of niobium oxide (Nb_2O_5), from 0 to 8 mol%, were synthesized by the melt-quenching technique. The structural feature of the glasses accessed by XRD, FTIR, did not change with the incorporation of Nb_2O_5 . The biocompatibility of bioactive glasses with human osteosarcoma SAOS-2 cells was evaluated. The results showed that the produced bioactive glasses are viable and have high potential for nanobiomedical applications. It is also known that the electrical characteristics of these biomaterials influence their osseointegration ability. Thus, knowing the electrical and dielectric characteristics of Nb_2O_5 , a first study on the electrical properties of these bio-glasses was also performed. Therefore, by the impedance spectroscopy method, in the frequency range from 10^2 to 10^6 Hz and over the temperature range of 200 to 400 K, the effects of Nb_2O_5 on charge transfer mobility were investigated.

Determination of the critical sizes of an electric discharge on a disk model

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The goal of this work is to determine the critical sizes of flashover. The experimental work at summer carried out on a new model of laboratory called model disc, similar to a true insulator of lines, in its form and pollution: it is an insulating disc polluted of the two faces. We carried out a series of experiments to determine the critical voltage and current in various positions of the starting point of the discharge on surface electrolyte. The interpretation of the results experiments which, enabled us to say that the voltage is the size which has a great influence on the evolution of the discharge of flashover on this model disc, on the other hand, it is the current which plays the role for the model with simple geometry.

Considering the problems of the discontinuity of the streamlines, we usefully judged to work out a new model of laboratory which presents a continuity in the lines of current. This model is valid to act an intermediate between the models with simple geometry of laboratory and a real insulator. It is a disc polluted on both sides (upper and lower).

It better represents geometrically and electrically a real insulator. On the latter we carried out a series of experiments to determine the critical magnitudes of the flashover.

References:

- [1] K. Benchaïb, Etude des conditions favorables du contournement des isolateurs haute tension pollués université USTO Oran, 1985.
- [2] S. Flazi, H. Hadi, K. L. Rabah, M. Hamouda and A. Boudjella, 2001 Annual Report Conference on Electrical Insulation and Dielectric Phenomena (2001) 593.
- [3] S. Flazi, M. Hamouda "Influence of the electric field to the neighbourhood of the discharge on its propagation to flashover" ELECO'99, Turkey.
- [4] M.E.A Slama, A. Beroual, Advances in Electrical and Electronic Engineering 13 (2015) 74.
- [5] M. Bouhmama, S. Flazi, F. Miloua, Y. Bellebna, A. Tilmatine, Journal of Electrical Engineering 17 (2017) 446.
- [6] S. Benharat, Etude du Comportement de la barrière isolante en vue de son optimisation, Thèse d'état, USTHB, Algérie 2021.

TSDC studies on bioglasses charged by the Corona discharge method

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Dental implants have been shown to replace missing teeth successfully over the long term. However, there may still be some issues that prevent osseointegration that leads to implant rejection. According to reports, the use of bioglass as a coating can help the dental implant work better given that it can boost tissue integration. Additionally, it is suggested that the surface of the bioglass is charged and/or polarized the effectiveness of osseointegration is promoted. In this work, the influence of particle size, corona discharge temperature and time in 45S5 bioglass pressed disks. The samples, from the various milling cycles, were structurally analyzed and evaluated according to the particle size reduction. TSDC experiments were done to verify the charge accumulation. It was verified that the temperature that would store the bigger amount of charge is 200 °C. This dielectric study was confronted with the analysis of the bioactivity data, which shows that the formation of the apatite layer is accelerated by the presence of negative charges on the bioglass samples.

FEDER funds through the COMPETE 2020 Program and National Funds through FCT-Portuguese Foundation for Science and Technology under the project UID/CTM/50025/2020, S.R. Gavinho acknowledges FCT-Portuguese Foundation for Science and Technology for the PhD grant (SFRH/BD/148233/2019).

Characterization of electroactive nanocomposite based on polylactide-titanium dioxide for piezoelectric β -phase improvement

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The application of flexible piezoelectric nanocomposite films in autonomous nano-systems, sensors, and portable electronics has piqued the curiosity of researchers [1].

The purpose of this paper consists the influence of titanium dioxide nanoparticles on polylactic acid crystal structure, unique crystallization, mechanical behavior, and considerable increase in piezoelectricity has been observed. The solvent casting approach was used to create polylactic acid/titanium dioxide (PLA/TiO₂) nanocomposite films with varying concentrations of titanium dioxide. Polarized optical microscope (POM), Fourier transformed infrared (FTIR), and X-ray diffraction analyses were used to analyze the various samples. POM pictures show that titanium dioxide nanofillers are distributed uniformly into the PLA matrix (see Figure 1). FTIR and XRD analyses verified the existence of β phase in nanocomposites as well as an increase of their piezoelectric characteristics. These electroactive nanocomposite might be a good candidate for energy harvesting applications [2].

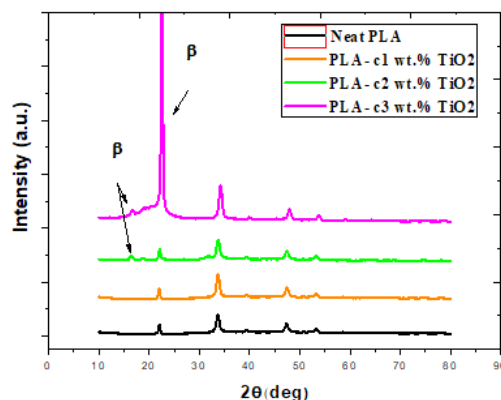


Figure 1. X-ray diffraction of PLA/TiO₂ nanocomposite

References:

- [1] K. Oumghar, N. Chakhchaoui, R. Farhan, A. Eddiai, M. Meddad, O. Cherkaoui, L. Van Langenhove, IOP Conference Series: Materials Science and Engineering 948 (2020) 012024.
- [2] A. Eddiai, M. Meddad, K. Sbiaai, Y. Boughaleb, A. Hajjaji, D. Guyomar, Optical Materials 36 (2013) 13.

MoS₂/TiO₂ heterojunctions for tuning the optical properties: a case study

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In recent years, two-dimensional semiconductor heterojunctions have received wide attention due to their novel properties and challenging applications. Among these, many MoS₂/TiO₂-based heterostructures of different dimensionality, made by MoS₂ microflowers, nanotubes, nanobelts, nanosheets, or quantum dots decorating shape-tailored TiO₂ nanoparticles (NPs), have been investigated extensively [1-3]. However, notwithstanding the great interest in MoS₂/TiO₂ systems, there is a limited number of studies concerning the in situ growth of MoS₂ on different shape-tailored anatase TiO₂ nanostructures [4].

Well-defined MoS₂ slabs on shape-tailored anatase TiO₂ structures, i.e., nanosheets and bipyramidal TiO₂ nanoparticles, having a different ratio/extension of (101), (001) co-exposed surfaces, are prepared by the *in situ* method. The peculiar properties of the obtained MoS₂/TiO₂ heterostructures are investigated by several techniques including transmission electron microscopy (TEM), spectroscopic methods (UV-Vis, FTIR, Raman spectroscopies) and XRD analysis, to highlight the role played by morphology, structure, stacking order, and defectivity of the MoS₂ slabs in enabling higher efficiency for many application fields, including photocatalysis and optical processes. In this regard, the relationship between the morphology/structure and vibrational/optical properties of TiO₂ anatase bipyramidal nanoparticles, mainly exposing {101} facets, decorated with MoS₂ slabs, is discussed and the obtained results are compared. In addition, the role of the different facets in affecting the distribution and the dispersion of MoS₂ slabs, together with the investigation of the surface sites on the main exposed faces, is highlighted. It will be shown that heterostructures obtained by the in situ strategy, are made of highly dispersed MoS₂ nanosheets, which are strongly anchored on TiO₂ surfaces, thus preventing self-aggregation phenomena from occurring.

TEM images of MoS₂-decorated TiO₂ nanosheets and TiO₂ bipyramids are illustrated (Figure 1a, c) together with TiO₂ lateral sizes and MoS₂ stacking order (Figure 1b, d). UV-Vis spectra of MoS₂/TiO₂ nanosheets and MoS₂/TiO₂ bipyramids are compared with UV-visible spectra of pure TiO₂ nanosheets and bipyramids, as references.

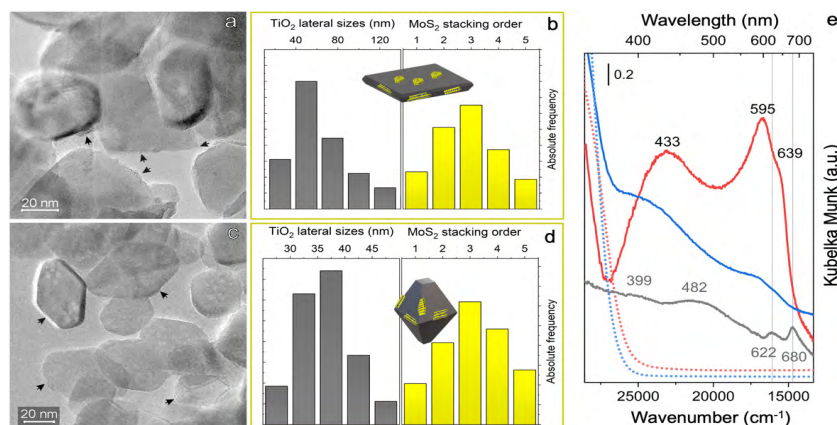


Figure 1. TEM images of: (a) MoS₂/TiO₂ nanosheets and (c) MoS₂/TiO₂ bipyramids; TiO₂ dimensions (grey histograms) and MoS₂ stacking order (yellow histograms) for: (b) MoS₂/TiO₂ nanosheets, and (d) MoS₂/TiO₂ bipyramidal nanoparticles; (e) UV-Vis spectra of MoS₂/TiO₂ nanosheets and MoS₂/TiO₂ bipyramids compared with reference materials (TiO₂ nanosheets/bipyramids, bulk MoS₂)

References:

- [1] S.G. Kumar, L.G. Devi, J. Phys. Chem. A 115 (2011) 13211.
- [2] J. Wan, S. D. Lacey, J. Dai, W. Bao, M.S. Fuhrer, L. Hu, Chemical Society Reviews 45 (2016) 6742.
- [3] J. Wang, K. Fu, X. Zhang, Q. Yin, G. Wei, Z. Su, Journal of Materials Chemistry C 9 (2021) 8466.
- [4] R. Santalucia, P. Negro, T. Vacca, F. Pellegrino, A. Damin, F. Cesano, D. Scarano, Catalysts 12 (2022) 1414.

Predictive model on the DC electrical conductivity of filler/matrix interphase zone of two- and three-dimensional composites

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Several DC electrical conductivity models have been proposed to explain the properties of the heterogeneous materials constituted by conductive particles in an insulating matrix. The experimental values of the DC electrical conductivity were compared to those obtained by using different mixing laws [1-2]. We show that effective medium theories correctly account for the experimental results at low conducting particle concentrations [3]. At concentrations higher than a few percent, these laws fail to interpret experimental results [4] and all tentative results must take into account parameters such as the volume, concentration and intrinsic conductivity of interphase zone. In this work, A three-phase predictive model is presented based, on the Voigt and Reuss modified model which describes the DC electrical conductivity of a wide variety of binary mixtures. Three series of two- and three-dimensional composites in a various content of Graphene Oxide (GO), Carbon Nanotubes (CNT) and Carbon Black (CB) inclusions have been investigated, at room temperature, taking into account the role of interphase zone existing between the macromolecular chains and the fillers. The fitting of experimental data using the Voigt and Reuss modified model provides to estimate the volume, concentration and intrinsic conductivity of interphase zone, depending on macromolecular network chains used in each series.

References:

- [1] L.K.H. van Beek, in: J.B. Birks (Ed.), Progress in Dielectrics, Vol. 7, p. 69, Heywood, London, (1967).
- [2] N. Uvarov, Solid State Ionics 136-137 (2000) 1267.
- [3] N. Aribou, Y. Nioua, I. Bouknaitir, M. El Hasnaoui, M.E. Achour, L.C. Costa, Polymer Composites 40 (2017) 346.
- [4] Y. Nioua, N. Aribou, S. Boukheir, M.E. Achour, L.C. Costa, J. Reinf. Plast. Compos. (2020) 1-7.

Direct synthesis of dehydrogenated siloxene materials: towards the improvement of physical and electrochemical responses

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Silicon (Si) materials has emerged as the next reliable and abundant materials for energy storage due to its well-known physical properties. As promising anode materials, the theoretical capacity of Si is expected to reach $4200 \text{ mAh}\cdot\text{g}^{-1}$ for Lithium-ion Battery (LiB) [1]. However, in practical, a huge volume change of Si after lithiation and delithiation along as a drastic loss of the specific capacity constitute an issue to resolve.

Layered 2D siloxene materials (LSM), bearing -H and -OH functional groups, obtained by soft-chemical synthesis of calcium disilicide (CaSi_2) has attracted recently a lot of attention in energy storage [2]. The layered geometry of such nanomaterials can be potentially prevent the volume change upon (de)lithiation. Recently, a report has found a capacity of 1669 and $579 \text{ mAh}\cdot\text{g}^{-1}$ in the first discharge and first charge, respectively, giving an initial coulombic efficiency (CE) of 34.5% [3].

In order to prevent the reactivity of the anode material with the solvent, LSM have been modified in situ with an additive at different percentages to avoid the formation of Si-H bonds. The dehydrogenation of LSM has been confirmed by FT-IR spectrum while the XRD pattern showed the formation of a suboxide amorphous SiO_2 . The scanning electronic microscopy confirmed the obtained 2D nanosheets and optical studies showed almost the same direct band gap energy compared with LSM. Dielectric studies has revealed a larger charge transfer resistance with 5% of additive (LSM-Add5%) along as a lower dielectric loss, compared to others. In addition, the electrochemical performances of the new materials as anodes in LiB have been performed in comparison with the LSM. The results proved that greater performances are obtained with the dehydrogenated LSM which exhibited a higher delivered specific capacity, a better capacity of Li retention and a better coulombic efficiency (Figure 1).

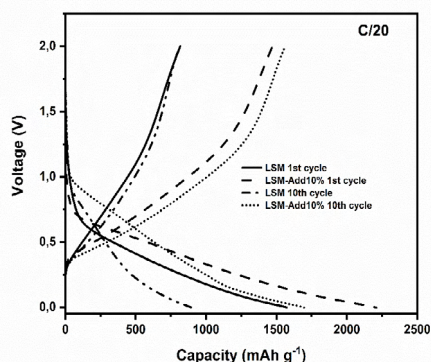


Figure 1. Charge-Discharge profile of LSM and LSM-Add10% at C/20

References:

- [1] M.N. Obrovac, L. Christensen, D.B. Le, J.R. Dahnb, J. Electrochem. Soc. 154 (2007) A849.
- [2] Y. An, Y. Tian, C. Wei, Y. Zhang, S. Xiong, J. Feng, Y. Qian, Energy Storage Mater. 32 (2020) 115.
- [3] R. Gao, J. Tang, K. Terabe, X. Yu, T. Sasaki, A. Hashimoto, K. Asano, M. Suzuki, K. Nakura, Chem. Phys. Lett. 730 (2019) 198.

Using ANN modelling to Improve the accuracy of energy baseline models for Industrial Buildings

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Corporate citizens in different sectors are now going green. They are firmly applying systems to maintain and improve the quality of environment in the long run. Not only because Businesses have a prime responsibility towards the environment, but also because they can “gain competitive advantage”, inter alia, by reducing energy cost. When considering the value of energy efficiency as the most cost-effective way to reduce pollution, the opportunities are even greater in this field. There have been recent research that have investigated the potential to reduce greenhouse gas emissions by enhancing industrial energy efficiency [1,2].

Unfortunately, the business case evaluation, penalized by the complexity and accuracy of energy business model is one among several major barriers.

This paper presents a contribution that will highlight how to set simplified and accurate models through the application of Artificial Neural Networks (ANNs) in the industrial environment. The neural network model is compared with the linear regression to prove that ANNs are more efficient and more promising as far as forecasting accuracy and simplicity are concerned.

References:

- [1] S. Broberg Viklund, M.T. Johansson, Energy Conversion and Management 77 (2014) 369.
- [2] Z. Utlu, U. Parali, Energy Conversion and Management 74 (2013) 308.

Electrical properties of $\text{La}_{1-x}\text{Sr}_x\text{FeO}_3$ ($0 \leq x \leq 0.5$) ortho-ferrites by dielectric spectroscopy

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This study focuses on the effect of Sr substitution on dielectric properties of LaFeO_3 ortho-ferrite. The analyzed ceramics $\text{La}_{1-x}\text{Sr}_x\text{FeO}_3$ with $x = 0 ; 0.1 ; 0.2 ; 0.3 ; 0.4$ and 0.5 have been synthesized by solid-state reaction method. Rietveld analysis of X-ray diffraction (XRD) data shows orthorhombic structure with Pnma space group for all samples. Scanning electron microscopy (SEM) micrographs show that the average grain size varies with the Sr substitution rate. Ac conductivity (σ') analysis has shown that the hopping process happened through long distance for $x = 0 ; 0.1 ; 0.2$ and 0.3 whereas it occurred between neighboring sites for $x = 0.4$ and 0.5 . Complex impedance analysis has evidenced the morphology effect on the dielectric response of $\text{La}_{1-x}\text{Sr}_x\text{FeO}_3$ ($0 \leq x \leq 0.5$) solid solutions. Indeed, different electrical equivalent circuits have been established according to the obtained Nyquist plots. Accordingly, contribution of grains and grain boundaries to ac conductivity has been probed. This analysis has revealed that grain boundary contributions rely on structural distortion of the ceramic. The $\text{La}_{0.5}\text{Sr}_{0.5}\text{FeO}_3$ ceramic exhibits the highest increase in charge transferred electron concentration according to its O 2p bandwidth (W) with the smallest grain morphologies. The ac conductivity is then ensured by the mediation of grain boundary which does not act as barrier for electron transport.

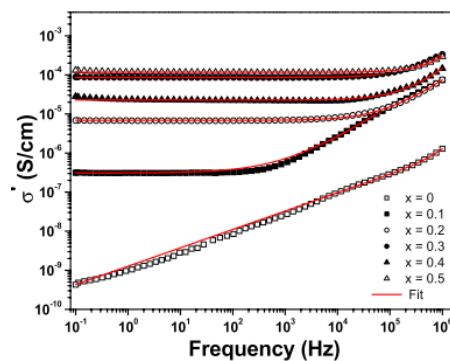


Figure 1. Frequency dependence of ac conductivity (σ') for $\text{La}_{1-x}\text{Sr}_x\text{FeO}_3$ ($0 \leq x \leq 0.5$) ortho-ferrites

Studying the photocatalytic properties of tungstate-based materials for water splitting

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Tungsten trioxide continue to attract a lot of attention for its promising properties in photocatalysis [1], photo electrochemistry [2] and photocchromism [3]. A particular interest was devoted to tuning its electronic structure and optical gap in order to enhance the photocatalytic performance in hydrogen production as well as in advanced oxidation process. One of the alternatives is the intercalation of water molecule into tungsten oxide structure. In this communication, three varieties of tungsten trioxide: tungsten oxide (WO_3), tungstite ($\text{WO}_3 \cdot \text{H}_2\text{O}$) and hydrotungstite ($\text{WO}_3 \cdot 2\text{H}_2\text{O}$) were prepared and characterized by PXRD, FTIR, RAMAN, reflectance spectroscopy, and STEM. The structures of intercalated materials were refined using Rietveld method and the electronic properties such as gap energy, conduction band and valence energies were estimated from UV-visible spectroscopy. The obtained results show that the introduction of water molecules into tungsten oxide structures reduces the gap energy from 3 eV to 2.46 eV for tungstite and 2.62 for hydrotungstite. These results were explained using crystallographic data that are suggesting the distances between two adjacent layers of WO_6 in tungstite and hydrotungstite are larger than in WO_3 is less important in comparison with $\text{WO}_3 \cdot 2\text{H}_2\text{O}$ and $\text{WO}_3 \cdot \text{H}_2\text{O}$. This result is an evidence of new alternative of band-gap engineering through intercalation.

References:

- [1] O. Oulhakem, H. Zahdi, M. Belaïche, S. Laalioui, Z. Naimi, B. Ikken, K.B. Alaoui, Z. Sekkat, Microporous Mesoporous Mater. 335 (2022) 111784.
- [2] M. Rodríguez-Pérez, C. Chacón, E. Palacios-González, G. Rodríguez-Gattorno, G. Oskam, Electrochim. Acta 140 (2014) 320.
- [3] C.O. Avellaneda, L.O.S. Bulhões, Solid State Ionics 165 (2003) 117.

Orientalional instability of the director in a planar flexoelectric nematic cell with easy axis gliding

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The orientational instability of the director in a planar cell of a flexoelectric nematic liquid crystal (NLC) in a constant electric field oriented perpendicular to the cell plane is theoretically studied [1]. On the surface of one of the polymer substrates, the direction of the axis of easy orientation of the director can change. This change is due to the effect of its original orientation, the liquid crystal and the electric field on the axis of easy orientation of the director. The effect of the electric field is manifested in the reorientation of the elastic parts of the polymer molecules of the substrate due to the interaction of the intrinsic or induced dipole moments with the electric field. The corresponding contribution to the free energy of the NLC cell is considered to be linear or quadratic with respect to the electric field strength, respectively.

It was established that the orientational instability of the director has a threshold in the case of quadratic coupling of the electric field with the axis of easy director orientation and is threshold less in the case of a linear coupling. The temporal behavior of the director's field in the volume of the NLC after switching the electric field on with the subsequent transition of the system to a stationary state (Fig. 1) and a return to the initial homogeneous state after the voltage is turned off was considered. The influence of the values of the system parameters, in particular, the values of the flexoelectric coefficients of the NLC, was studied. It was established that an increase in the values of the flexoelectric coefficients and the coupling parameter of the electric field with the gliding easy axis leads to an increase in the deformations of the director's field and to a decrease in the threshold voltage.

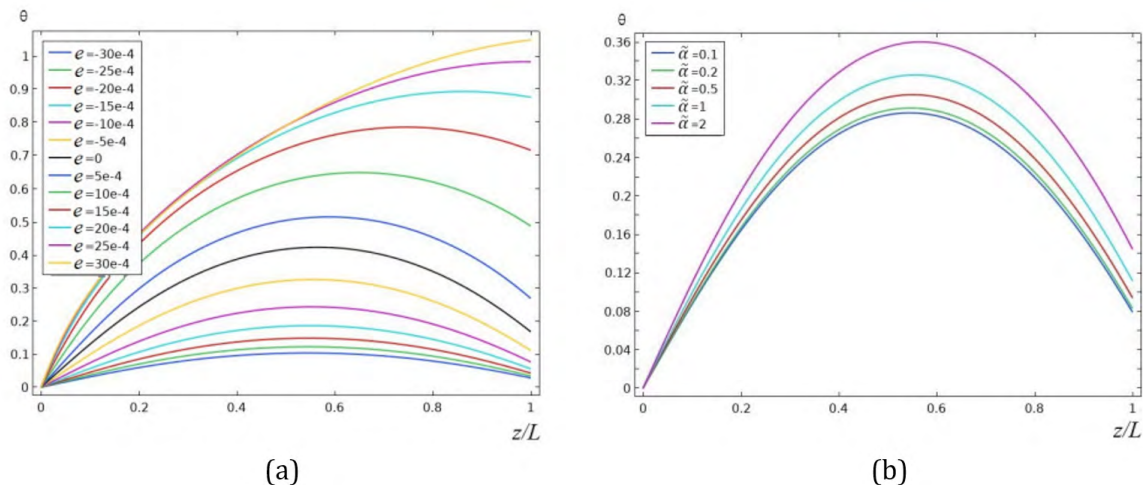


Figure 1. Stationary dependences of the director deviation angle θ on the cell thickness.
(a) $\tilde{\alpha} = \alpha / \sqrt{\epsilon_0 \epsilon_a K_1} = 1$ - the coupling parameter between the electric field and the easy axis,
(b) $e = e_{11} + e_{33} = -5 \times 10^{-4} \text{ dyn}^{1/2}$ - the sum of the flexoelectric coefficients.

The time for the system to reach a stationary state and the characteristic times of switching on and off were calculated, and their dependence on the system parameters was investigated. An increase in the value of the applied voltage leads to an increase in the value of the turn-on time in the case of positive values of the sum of the flexoelectric coefficients of the NLC and to a decrease in the turn-on time for negative values. The conducted theoretical research expands the concept of electrically induced reorientation of NLC cell on the substrate of which the conditions for the director are changed by an electric field.

References:

[1] I.I. Yakovkin, A.I. Lesiuk, M.F. Ledney, V.Yu. Reshetnyak, Journal of Molecular Liquids 363 (2022) 119888.

POSTER SESSION

The features of X-ray diffraction in non-stoichiometric $\text{AsS}_3\text{-GeS}_4$ glassy thin films

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XRD patterns of thin solid films based on non-stoichiometric chalcogenide glasses (ChG) from the pseudo-binary system $(\text{GeS}_4)_x(\text{AsS}_3)_{1-x}$ have been investigated, paying a special attention to first sharp diffraction peak (FSDP), ascribed to the middle range order (MRO) of the glassy material. The films have been grown by “flash” evaporation of the powder from previously synthesized ChG, in vacuum (10^{-5} Torr), onto mono-crystalline silicon substrates. The morphology and elemental composition of the films have been examined using SEM and EDX spectroscopy. Structural investigations were performed by grazing incidence XRD using $\text{Cu}_{K\alpha}$ radiation. Fig. 1 shows the XRD patterns of the $(\text{GeS}_4)_x(\text{AsS}_3)_{1-x}$ thin films, which are typical for glassy state, without traces of crystalline phases. Unlike the diffraction patterns of the initial ChG bulk samples, thoroughly studied in previous work [1], a boosting increase of intensities of the FSDP of all films occurs.

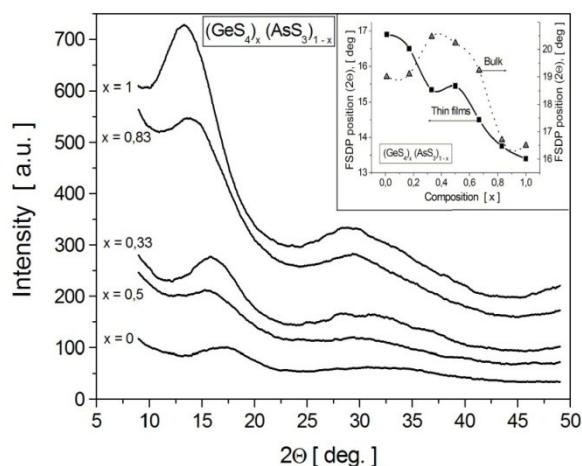


Figure 1. X-ray diffraction patterns of glassy $(\text{GeS}_4)_x(\text{AsS}_3)_{1-x}$ thin films. Inset shows the FSDP position versus films composition in comparison with initial bulk glasses [1]

Besides, the peak positions and the widths of the FSDP depend on film composition. Note that, the composition of the films is similar to the one of initial bulk ChG, as determined by EDX. Inset of Fig.1 illustrates the FSDP position vs. glass composition for both the studied thin films and respective bulk materials. It can be observed an evident difference between the effect of composition on FSDP position in thin films and bulk glasses, although some similarities remain. The careful analysis of FSDP features in thin films with respect to bulk glasses give evidence that by growing the film from vapor phase the disordered network becomes a molecular like structure.

This work was supported by National Agency for Research and Development of Moldova, project PS 20.80009.5007.21; Romanian Ministry of Foreign Affairs and Agence universitaire de la Francophonie (Eugen Ionescu research and mobility grant at NIMP); and Romanian Ministry of Research and Innovation, Core Program 2019–2022 (contract No. 21 N/08.02.2019).

References:

[1] D. Tsiulyanu, S.A. Kozyukhin, M. Ciobanu, Journal of Non-Crystalline Solids 575 (2022) 121207.

Interfacial polarization effect analysis of hybrid recycled cotton fibers reinforced unsaturated polyester composites

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Dielectric measurements were performed on hybrid recycled cotton fibers reinforced unsaturated composites in the frequency range 0.1 Hz - 1 MHz and the temperature range 0 °C - 150 °C. Hybrid recycled cotton fibers are composed of white yarns/indigo denim fabrics in the relative volume fraction 1:1. This dielectric study has revealed the presence of two dielectric relaxations for higher temperatures associated with the interfacial polarization effect and α relaxation. Analysis of the interfacial polarization effects according to Havriliak-Negami model has shown better reinforcement/matrix adhesion for higher weight fraction and for lower mechanical consolidation by the needle punching of the reinforcement. Such result may be attributed to the lower hydrophilic character of the composite according to this dielectric study. However, a thorough investigation should be accomplished by either FTIR or DSC techniques.

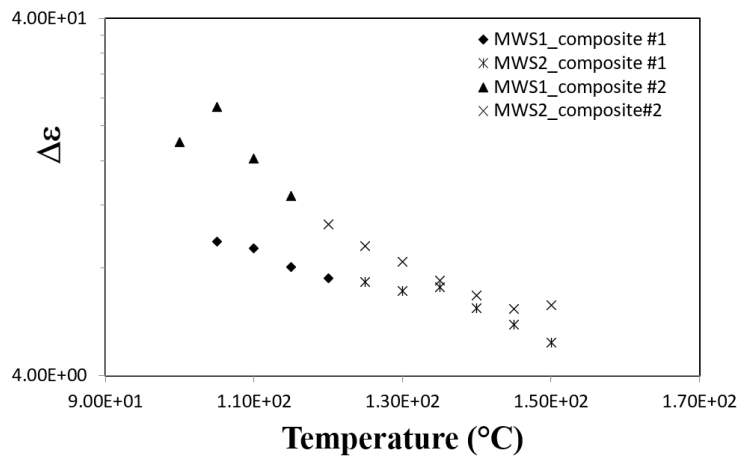


Figure 1. Temperature dependence of interfacial polarization effect strength

Synthesis, characterization and dielectric properties of $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$

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In the present work we have summarized some experimental results about synthesis and investigation of dielectric properties of $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$ prepared by Pechini method and sintered at appropriate temperature, allowing formation of ceramic material. Structural and morphological studies of the as prepared and sintered sample are performed by X-ray powder diffraction, infrared spectroscopy and scanning electron microscopy.

The results obtained show that applying of Pechini method allows pure barium strontium titanate with specified molar ratio to be obtained at relatively low temperature (about 800 °C) than the accepted as a standard for conventional synthesis (about 1200 °C). It is established that the phase composition after sample sintering at 1400 °C differs significantly from the predetermined stoichiometry.

The dielectric properties of the ceramic sample after sintering at 1400 °C are investigated by the method of impedance spectroscopy at different temperatures and frequencies. The obtained impedance spectra are simulated using an appropriate equivalent circuit in order to get information on the bulk resistance and capacitance of the sample. Measurements of the capacitance at fixed frequency are carried out and the dielectric constants at different temperatures were determined.

The authors appreciate the financial support of the Bulgarian National Science Fund under contract KP-06-H28/1.

Effect of surface treatment on the dynamics of relaxation processes in confinement

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Broadband dielectric spectroscopy (BDS) is an outstanding method of studying molecular and collective relaxation processes in various liquid crystalline phases embedded in geometric constraints or doped with various types of nanoparticles with magnetic, semiconductor, metallic or insulators properties [1,2]. BDS enables the study of the effects occurring at the interface of the liquid crystal phase with the pore surface of the porous matrix and the surface of nanoparticles dispersed in the liquid crystal. The dynamics of surface effects influences such macroscopic dielectric parameters as permittivity, dielectric losses, etc. In this context, the surface condition of the pores and nanoparticles plays an important role in modifying the dielectric properties of composite materials, leading to changes in electro-optical properties, electrical conductivity, memory effects, etc.

Previous research has shown that the modification of the pore surface in the Anopore membrane with the use of appropriate surfactants leads to a change in the order of nematics molecules from planar to homeotropic and, consequently, to the possibility of observing molecular processes related to the rotation of the molecule around the short axis (delta process) and reorientation around the direction of the director (librational process) [3].

Doping the nematic or ferroelectric phase of the liquid crystal with the nanoparticles of hydrophilic or hydrophobic aerosil nanoparticles leads to effects related to the distribution of random defects in the structure of the liquid crystal and depends on the surface treatment of the nanoparticles and their concentration [4].

The study investigated the influence of different types of surfactants on the dynamics of relaxation processes for the well-known ferroelectric liquid crystal DOBAMBC embedded in Anopore membrane [5,6]. Depending on the structure of surfactants, the dynamics of the collective processes, especially the Goldstone mode, is modified.

References:

- [1] H. Ayeb, T. Missaoui, A. Mouhli, F. Jomni, T. Soltani, *Phase Transitions* 94 (2021) 37.
- [2] Neeraj, K.K. Raina, *Phase Transitions* 83 (2010) 615.
- [3] S.A. Rózański, G.P. Sinha, J. Thoen, *Liq. Cryst.* 33 (2006) 833.
- [4] S.A. Rózański, *Ferroelectrics* 495 (2016) 53.
- [5] S.A. Rózański, *Physica Status Solidi* 79 (1983) 309.
- [6] S.A. Rózański, R. Stannarius, F. Kremer, S. Diele, *Liq. Cryst.* 28 (2001) 1071.

Ferroelectric and pyroelectric characterization of promising perovskite ceramics

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Perovskite ferroelectrics with morphotropic phase boundary (MPB) [Pb(Zr,Ti)O₃, Pb(Mg,Nb)O₃, etc. display larger piezoelectric properties leading to a nearly vanishing polarization anisotropy facilitating easier polarization rotation between $\langle 001 \rangle_T$ and $\langle 111 \rangle_R$ states by external stress or electric fields [1]. One of the lead-free alternatives that has attracted a tremendous attention for environmental-friendly applications recently is the (Ba,Ca)TiO₃-Ba(Zr,Ti)O₃ (BCZT) at the MPB [1-3]. Investigation of the pyroelectricity of these materials has been of great interest in detecting infrared radiation and thermal imaging systems since this technology does not need expensive cooling systems.

The present investigation is aimed at the pyroelectric investigation of various potential lead-based and lead-free piezoelectric oxides to understand the effect of structurally induced strain on pyroelectric figures of merit. We synthesized high-density ceramics of Pb(Zr,Ti)O₃, Pb(Mg,Nb)O₃, PbTiO₃, and BCZT by conventional ceramic processing. Detailed ferroelectric properties, were studied as a function of temperature, electric field, and frequency. From the pyroelectric measurements carried out using the charge integration method, pyroelectric figures of merit like pyroelectric coefficient and detectivity were computed. The results are correlated based on the composition and lattice strain.

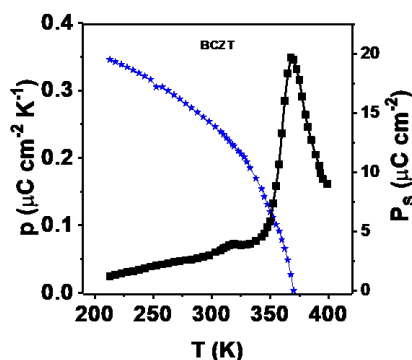


Figure 1. Temperature dependent pyroelectric coefficient and spontaneous polation of BCZT ceramic

This work is supported by the DRDO, New Delhi through a project.

References:

- [1] W. Liu, X. Ren, Phys. Rev. Lett. 103 (2009) 257602.
- [2] A.B. Haugen, J.S. Forrester, D. Damjanovic, B. Li, K.J. Bowman, J.L. Jones, J. Appl. Physics 113 (2013) 014103.
- [3] E.V. Ramana, A. Mahajan, M.P.F. Graça, S.K. Mendiratta, J.M. Monteiro, M.A. Valente, Mater. Res. Bull. 48 (2013) 4395.

Numerical simulation of coffee grounds pyrolysis for biofuels production

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Renewable energy sources represent one of the best strategies available to reduce environmental problems and the use of fossil fuels [1-2]. Among the most promising renewable energies to limit the increase of greenhouse effect is biomass, where it can be converted into useful products (biofuels) through the thermochemical conversion. An important recycling chain can be formed through bio energy production and energy conversion from wastes [3]. Among the advanced biomass conversion technologies, thermochemical processes offer considerable potential and must be optimized. Pyrolysis is a very promising solution for the production of high-quality bio-oils and chemicals with high energy. residence time, process temperature, flow rate, and biomass type strongly affect bio-fuels yield. In this study, the effect of temperature and residence time on bio-fuels yield during coffee grounds pyrolysis was investigated using Super Pro Designer simulator. The results obtained from the different simulation tests show that the maximum bio-oil yield (34%) was achieved at a temperature of 550 °C and a residence time of 0.5 s. However, a temperature of 700 °C and a residence time of 12 s are the optimal conditions to maximize the yield of syngas with a production of 23%. The maximal Biochar production (43%) was achieved at a temperature of 400 °C and a residence time of 0.5 s. These exploitations have shown that the energy content of coffee grounds can be exploited by pyrolysis or gasification in order to obtain important end products that can be exploited as fuels.

References:

- [1] IEA (2000), World Energy Outlook 2000, IEA, Paris <https://www.iea.org/reports/world-energy-outlook-2000>
- [2] Communication from the Commission, & Communication from the Commission, Energy for the future: renewable sources of energy-White Paper for a Community strategy and action plan, COM 97 (1997) 599.
- [3] Md. Alhaz Uddin, S.Y.A. Siddiki, S.F. Ahmed, Z.I. Rony, M.A.K. Chowdhury, M. Mofijur, Energies 14 (2021) 7654.

Hysteresis of surface plasmon polariton effective index induced by liquid crystal reorientation

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We present a theoretical study of the effect of the orientational instability of a nematic liquid crystal (NLC) on the value of the effective refractive index of a surface plasmon polariton. A plane-parallel NLC cell with an initial homeotropic orientation of the director is considered. The cell is placed in a constant electric field parallel to its substrates (Figure 1a). The external electric field can lead to a change in the orientation of the director in the NLC cell. One of the polymer substrates of the cell is in contact with a thin layer of metal, so that a surface plasmon polariton can propagate at the interface “NLC” - “polymer film” - “metal”. Surface plasmon oscillations are very sensitive to the dielectric properties of the medium, therefore, by changing the electric field strength, it is possible to control the propagation properties of the surface plasmon polariton, in particular, its effective refractive index. The equilibrium distributions of the director in the NLC cell were found by minimization of the free energy functional taking into account different elastic constants and the finite energy of the NLC anchoring with the substrates. Analytical expressions for the propagation parameters of the surface plasmon polariton in the structure “NLC” - “polymer film” - “metal” were obtained by applying the adapted perturbation theory [1].

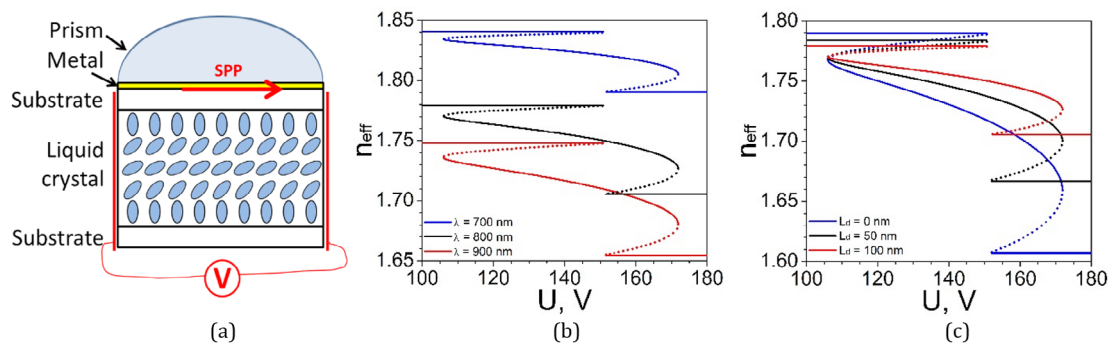


Figure 1. Geometry of the NLC cell (a). Dependence of the effective refractive index of the surface plasmon polariton on the applied voltage at different wavelengths (b) and at different thicknesses of the polymer film (c)

It was established that the change in the effective refractive index of the surface plasmon polariton can be accompanied by hysteresis. Analytical expressions for the parameters and conditions for the existence of hysteresis were obtained, and it was established that the latter depend significantly on the values of the cell parameters: when the coupling energy increases and when the dielectric permittivity ratio $\epsilon_a/\epsilon_{||}$ decreases, the width of the hysteresis decreases. The value of the effective refractive index increases with an increase in the energy of the director’s anchoring with the substrate and with a decrease in the values of the wavelength and the applied voltage (Figure 1b, c). The range of possible values of the effective index of the surface polariton expands as the thickness of the polymer film decreases and the wavelength increases.

References:

[1] K. Daly, S. Abbott, G. D’Alessandro, D. Smith, M. Kaczmarek. J. Opt. Soc. Am. B. 28 (2011) 1874.

Nanocomposite molecular films based on nanocrystalline cellulose and liquid crystals

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Functional and smart materials are materials possessing adaptive capabilities to external stimuli. They can adopt or be controlled by the external stimulus or conditions, which gives new possibilities to create materials with targeted and specific properties. Functional materials are often multi-component substances that display new effects and properties that differ from individual components' properties.

In this work, the investigation of the preparation procedures and molecular stability of Langmuir films based on cellulose nanocrystals (CNC) and liquid crystals (LC) are presented. The main goal of the work is to obtain and analyze thin layers made of liquid crystals stabilized with polymers. Understanding the phenomena occurring at the molecular level in these systems will allow to control factors that significantly impact their macroscopic properties. Choosing also, as one of the components, a natural biodegradable polymer also has an ecological aspect. The liquid crystal/polymer systems were characterized in terms of the selection of components, their concentrations, and exposure time using a polarizing microscope, optical spectroscopy, and other auxiliary methods.

References:

- [1] N. Bielejewska, R. Hertmanowski, *Journal of Molecular Liquids* 323 (2021) 115065.
- [2] N. Bielejewska, R. Hertmanowski, *Colloids and Surfaces B: Biointerfaces* 187 (2020) 110634.

Li⁺ and W⁺ ion irradiation induced changes on the electrical properties of BaSnO₃ ceramics

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In the present work, Barium stannate ceramics (BaSnO₃) was synthesized using the high-temperature mixed-oxide technique. This technique consists of both calcination and sintering. The precursor's barium carbonate (BaCO₃) and strontium oxide (SnO₂) were calcinated at 800 °C for 6 hours and sintered at 1400 °C for 4 hours and made into pellets. They were irradiated with Lithium (Li⁺) and Tungsten (W⁺) ion of 50 MeV energy at a fluence of 1×10¹² ions/cm². XRD reveals the crystalline nature of the prepared BaSnO₃ ceramics. The samples were electrode using air drying silver paste on both sides to analyse the electrical properties. The dielectric spectroscopy for the prepared BaSnO₃ ceramics and ion irradiated BaSnO₃ ceramics were recorded from room temperature to 400 °C in a frequency range of 1 kHz to 2 MHz for every 5 degrees. The dielectric constant of the BaSnO₃ ceramics was determined. A. C. conduction mechanism of the ceramics was recorded and the activation energy of the sample before and after ion irradiation was calculated using the Arrhenius plot. The morphology of both prepared and irradiated ceramics was analysed using SEM images.

References:

- [1] S. Chahib, D. Fasquelle, G. Leroy, Materials Science in Semiconductor Processing 137 (2022) 106220.
- [2] R. Köferstein, L. Jäger, M. Zenkner, T. Müller, S.G. Ebbinghaus, Journal of the European Ceramic Society 30 (2010) 1419.
- [3] P. Rajasekaran, M. Arivanandhan, N. Sato, Y. Kumaki, T. Mori, Y. Hayakawa, K. Hayakawa, Y. Kubota, R. Jayavel, M. Shimomura, Journal of Alloys and Compounds 894 (2022) 162335.

Electron scattering by magnetic quantum dot in the topological insulator

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We study the effect of electron scattering by magnetic regions in topological insulators characterized by spin-momentum locking. As calculation method we used perturbation theory and partial wave summation approaches to analyze the role of system parameters in different scattering regimes. We demonstrate that the specific features of spin-momentum locking lead to strong differences in the scattering cross-section compared to the conventional spin-independent scattering of electrons in semiconductors. The features include, e.g., the scattering anisotropy and the unusual energy dependence of the scattering cross-section. These results can be used to understand the kinetic effects in topological insulators with magnetic disorder and for design of the magnetization patterns to control the coupled spin and charge density dynamics.

We make a step in the direction of understanding the ability to manipulate and design coupled charge-spin density transport by engineering magnetic structures on the surface of topological insulator. To do so we consider scattering of electron by a circular quantum dot with a uniform magnetization. By qualitative, semiquantitative, and numerical analysis of the scattering we demonstrate the main features of the scattering process determined by the spin-momentum locking and discuss its difference from the conventional scattering problem in quantum physics.

Moreover, we studied qualitatively (by considering the wavepacket motion and by using Born approximation) and quantitatively (by phase scattering theory, both analytically and numerically) electron scattering from a nanoscale magnetic quantum dot on the surface of topological insulator. We demonstrated that the scattering is asymmetric with respect to the scattering angle. We also calculated the total cross-section and its asymmetry factor. These results can be useful for the design of spintronic devices on topological insulators with magnetized quantum dots.

Electric and structural properties of ZnO-based surge arrester ceramics

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Surge arresters are devices used to protect units of equipment connected to power transmission and distribution systems against electrical transients resulting from lightnings or high voltage system's faults switching. This is usually achieved with varistors, non-linear devices whose resistance is highly dependent on voltage. An active element in varistors is ZnO-based ceramic with admixture of Bi₂O₃ and Sb₂O₃ oxides.

Our paper reports on the study of the basic parameters of low-voltage (applied in low-voltage distribution systems) surge arresters from four various commercial manufacturers. A batch of 10 varistors from each manufacturer was randomly selected for the tests, for which basic electrical parameters were determined, i.e. leakage current and reference voltage before and after the discharge current of 8 μs / 20 μs duration. Additionally one sample of each varistor batch was aged applying 50 consecutive lightning strikes. The tests of the surge arresters confirmed large dispersion of crucial parameters and exceeding the declared value of the threshold voltage due to the poor quality of product of one manufacturer, while the tests of the arresters from three other manufacturers did not clearly indicate the best product.

The results of electric parameters measurements were consistent with material studies performed by X-ray powder diffraction (pXRD) and energy dispersive X-ray spectroscopy (EDS). The latter results confirmed significant differences in the chemical composition and microstructure of varistors from different manufacturers, which could affect their electrical properties. Also, the effect of exposure to multiple current strokes or exceeding the critical load could be observed as gradual internal changes in the ZnO-based ceramic of the varistor.

The proposed research methodology can therefore be the basis for forecasting the stability of arrester parameters in operating conditions.

Impact of bismuth iodide (BiI₃) interfacial layer on perovskite solar cell based MAPbI₃

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Perovskites have gained popularity as an absorber layer in thin film solar cells during the last decade, because to their inexpensive cost and improved conversion efficiency [1]. In this study, solar cell capacitance simulator (SCAPS) was utilized to investigate of bismuth iodide (BiI₃) on the performance of a solar device. According to our results, the addition of a thin layer of BiI₃ at the interface between the Perovskite active layer and the HTL effectively improves hole extraction by defect passivation (i.e., decreases charge recombination and ion migration), which in turn improves device performance in comparison to a typical reference architecture. As top cell active layer, based on alternative porous silicon, the PSi anti-reflection coating (ARC) layers [2] and transparent conducting oxide (TCO) layer [3]. Our findings reveal that the structure with TCO is more efficient where the optimum configuration is (TCO/CuO/BiI₃/MAPbI₃/ZnO) with power conversion efficiency of 17.61% of efficiency, Fill Factor (FF) of 81.20%, open circuit voltage (Voc) of 16.7996 V and, Short circuit current (Jsc) of 1.2906 mA·cm⁻².

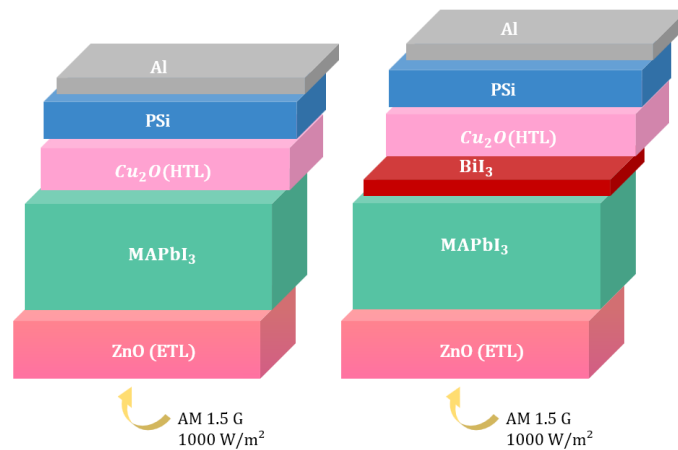


Figure 1. Schematic of the device structure of perovskite solar cell

References:

- [1] Q. Lin, A. Armin, R.C.R. Nagiri, P.L. Burn, P. Meredith, Nature Photonics 9 (2015) 106.
- [2] Khaldun A. Salman, Khalid Omar, Z. Hassan, Superlattices 50 (2011) 647.
- [3] S. Srivastava, P. Lohia, D.K. Dwivedi, International Conference on Electrical and Electronics Engineering (ICE3) (2020) 612.

Starch-based protonic conductors

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Searching for new organic-based and environment-friendly materials is one of the most interesting topics in the field of solid-state ionics. One of the proposed group of materials are compounds based on cellulose, which has wide application potential, from sensors to medicine [1,2]. Moreover, cellulose was also investigated as an electrolyte to use in fuel cells [4,5]. Such electrolytes should combine high electrical conductivity with good mechanical properties. Unfortunately, the cellulose-based conductors although often possess pretty high protonic conductivity (4×10^{-1} S/m at 160 °C) [6], have one major weakness, which is thermal instability, caused by the water built into the structure of the cellulose backbone.

To solve the problem of thermal instability, we present the results of studies of new organic composites, based on another organic material – starch. The starch, which acts as a “matrix” of composites, is combined with imidazole, which is responsible for providing good electrical properties. Newly obtained materials were studied using DSC, and TGA techniques to obtain information about thermal properties. Electric properties were studied using the impedance spectroscopy method. The studied materials show good thermal stability and high protonic conductivity ($\sigma_{dc} = 5 \times 10^{-2}$ S/m, see Figure 1).

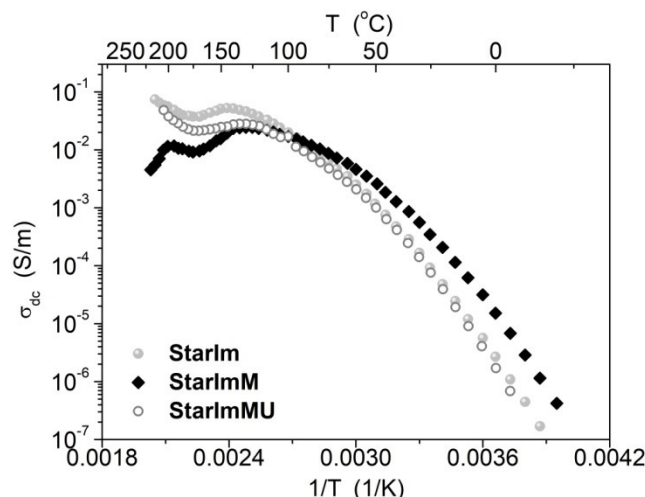


Figure 1. Arrhenius plot of DC conductivity of three starch-imidazole composites

References:

- [1] B.R. Evans, H.M. O'Neill, V.P. Malyvanh, I. Lee, J. Woodward, *Biosensors and Bioelectronics* 18 (2003) 917.
- [2] R.J. Moon, A. Martini, J. Nairn, J. Simonsen, J. Youngblood *Chem. Soc. Rev.* 40 (2011) 3941.
- [3] S. Ummartyotin, H. Manuspiya, *Renewable and Sustainable Energy Reviews* 41 (2015) 402.
- [4] I. Smolarkiewicz, A. Rachocki, K. Pogorzelec-Glaser, R. Pankiewicz, P. Ławniczak, A. Łapiński, M. Jarek, J. Tritt-Goc, *Electrochimica Acta* 155 (2015) 22.
- [5] I. Smolarkiewicz, K. Pogorzelec-Glaser, P. Ławniczak, M. Matczak, R. Pankiewicz, *Cellulose* 28 (2021) 843.
- [6] J. Tritt-Goc, Ł. Lindner, M. Bielejewski, E. Markiewicz, R. Pankiewicz, *Carbohydrate Polymers* 225 (2019) 115196.

An innovative approach to produce black phosphorus from red phosphorus via the addition of small amounts of iron

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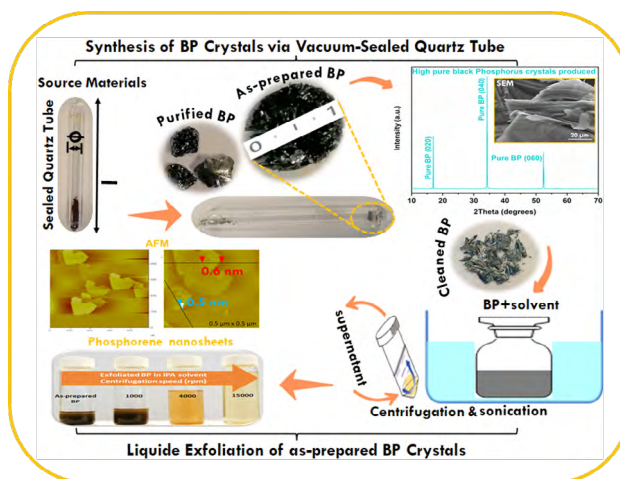
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Black phosphorus, one of the most stable allotropic forms of phosphorus, is a promising material for energy storage and conversion, and has been prepared by the solid state “transport reaction” route under low pressure and at temperatures of 550 °C and 650 °C. Our goal is to prepare large crystals of black phosphorus (more than 1 cm) by a simple, efficient and less expensive innovative method. The synthesis consists in an allotropic transformation of red phosphorus into black phosphorus in a quartz tube, by the addition of small amounts of iron (Fe), tin (Sn) and tin IV iodide (SnI₄). X-ray analysis (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDX) and Raman spectroscopy were used to confirm the quality, crystallinity and chemical purity of the prepared black phosphorus.

Our present method is based on the use of Fe as an additive to facilitate chemical transport, with a considerable improvement in the process over traditional preparation methods such as the method that uses the precious metal gold (Au) as a catalyst in the reaction. Our method used thus allows to obtain black phosphorus with a higher yield and high crystallinity. Therefore, this invention will be an opportunity for scientific researchers to explore other approaches for the preparation of this material for many applications.



Dielectric and magnetic response of $\text{Sr}_{1-x}\text{Nd}_x\text{Fe}_{12}\text{O}_{19}$ ($0 \leq x \leq 0.09$) hexaferrite nanoceramics

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M-type hexaferrites are interesting for applications due to their unusual crystal structure and the ability to be used in a range of ceramics [1]. Ferrimagnetic unit cell with $Z = 2$ contains two electric dipoles switchable in the hexagonal direction. On cooling the structure of single crystals results in quantum paraelectric behavior along the c axis [2,3]. The ferrimagnetic properties of M-hexaferrites are related to Fe^{3+} magnetic dipoles arranged along the c axis in tetrahedral and octahedral coordination with O^{2-} and superexchange $\text{Fe}^{3+}\text{-O}^{2-}\text{-Fe}^{3+}$ interaction. Rare earth doping of the ferrite ceramics has been found to substitute the Sr^{2+} ions and stabilize the hexagonal structure [4,5]. As the magnetic properties are sensitive to the size effect we studied the effect of Nd^{3+} doping on strontium hexaferrite nanoceramics prepared by coprecipitation method [6]. The XRD studies (X'Pert PANalytical, refined by Rietveld method) pointed to a low decrease in the lattice parameters with increasing x and the hexagonal structure was found to exist up to $x = 0.07$. The ferromagnetic structure was found to exist at room temperature for $x \leq 0.07$ with an increase in the coercive field. The dielectric response of neodymium doped samples (0.03, 0.05, and 0.07) was found to exhibit high temperature maxima related to the presence of polar oxygen vacancies created by the valence difference between Sr^{2+} and Nd^{3+} . At low frequencies a considerable decrease in room temperature permittivity is apparent due to poor electric conductivity of the grain boundaries. The electric conductivity of the grain interior was found to increase with increasing frequency at high frequencies.

References:

- [1] R.C. Pullar, Prog. Mater. Sci. 57 (2012) 1191.
- [2] H.B. Cao, Z.Y. Zhao, M. Lee, E.S. Choi, M.A. McGuire, B.C. Sales, H.D. Zhou, J.-Q. Yan, D.G. Mandrus, APL Mat. 3 (2015) 062512.
- [3] S.-P. Shen, Y.-S. Chai, J.-Z. Cong, P.-J. Sun, J. Lu, L.-Q. Yan, S.-G. Wang, Y. Sun, Phys. Rev. B 90 (2014) 180404(R).
- [4] L. Lechevallier, J.M. Le Breton, A. Morel, P. Tenaud, J. Magn. Mater. 316 (2007) e109.
- [5] L. Lechevallier, J.M. Le Breton, A. Morel, P. Tenaud, J. Phys. Condens. Matter 20 (2008) 175203.
- [6] A. Hilczer, K. Pasińska, E. Markiewicz, A. Pietraszko, B. Andrzejewski, Acta Phys. Pol. 133 (2018) 669.

Comparative study of AgGaSe₂ and AgGaTe₂ chalcopyrite-based solar cells

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This paper presents a comparative study of chalcopyrite based solar cells using two different buffer layers such as AgGaSe₂ and AgGaTe₂ [1,2]. Simulation is an interesting tool for studying the behavior of every component of a solar cell device as well as for analyzing the performance of the full device.

Solar cell capacitance simulator (SCAPS)-1D has been the tool used for numerical simulation of such devices. The photovoltaic structure design based on chalcopyrite (AgGaSe₂ or AgGaTe₂) absorber with buffer layer as CdTe is presented in Figure 1. Influences of thickness of absorber and buffer and absorber and dopant concentration on the performance of photovoltaic solar cells are studied. Comparable efficiencies of 17.52% and 23.76% for PV devices made of CdTe/AgGaSe₂ and CdTe/AgGaTe₂, respectively, under AM1.5 illumination are observed.

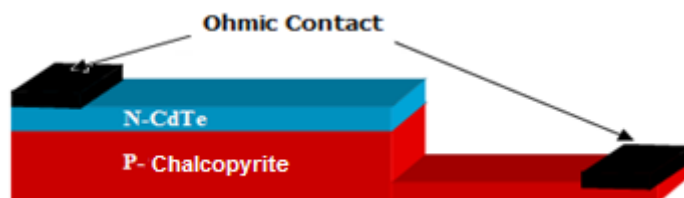


Figure 1. Schematic structure of the simulation solar cell

References:

- [1] W. Wu, K. Wu, Z. Ma, R. Sa, Chemical Physics Letters 537 (2012) 62.
- [2] J.K. Larsen, O. Donzel-Gargand, K.V. Sopiha, J. Keller, K. Lindgren, C. Platzer-Björkman, M. Edoff, ACS Applied Energy Materials 4 (2021) 1805.

Low temperature dielectric, magnetic and spectral behaviour of pure and Mn doped multiferroic BiFeO₃ nano ceramics

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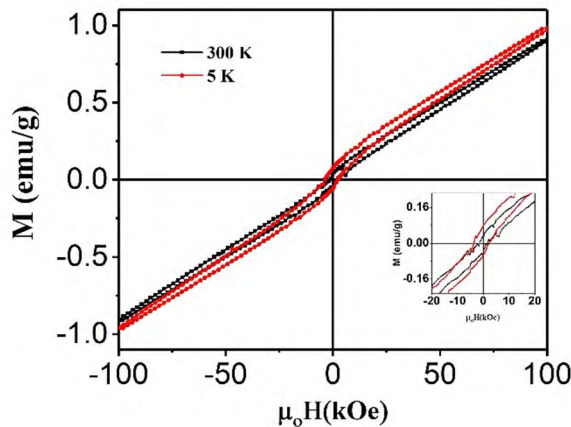
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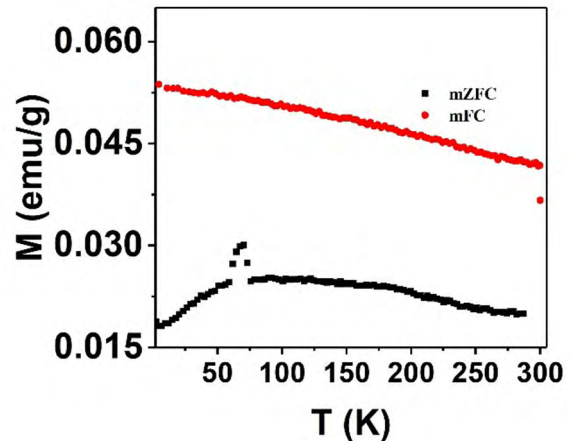
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Bismuth ferrite (BFO) nano powders and manganese doped BFO have been synthesized from sol-gel route. The single phase nature of powders was ascertained through powder XRD, followed by Rietvelt refinement. Raman scattering signals obtained for BFO from 50 K to 600 K suggest the possible phonon modes of rhombohedral unit cell. Dipole interaction at the low temperature regime from 100 to 400 K has been studied. The magnetic character of the powders has also been assessed through VSM analysis. The obtained results have been consolidated and would be discussed in detail.



M Vs H



M Vs T

References:

- [1] X. Yu, X. An, Solid State Commun. 149 (2009) 711.
- [2] K. Prashanthi, M. Gupta, Y.Y. Tsui, T. Thundat, Appl. Phys. A 110 (2013) 903.
- [3] S.K. Singh, K. Maruyama, H. Ishiwara, Applied Physics Letters 91 (2007) 112913.

Modelling and simulation of the optical properties of zinc oxide thin films targeting the optimal configuration (ZnO/Substrate)

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Zinc oxide (ZnO) present one of the most important materials in a wide variety of optoelectronic systems with large and varied applications [1]. It is a popular II-VI semiconductor material for devices with possible applications such as: piezoelectric transducers, transparent electronics in solar cells, gas sensors, saw devices. According to several research [2], Zinc oxide is the most promising in optoelectronic applications, especially in the UV region. The understanding of the optical properties of Zinc oxide thin layers on different substrates is also needed to determine the optimal configuration (ZnO/substrate) for best performance. In this work, we start our simulation by executing a Matlab code in order to study the Sellmeier equation. The light transmission behavior of ZnO/BK7 and ZnO/Quartz is examined. the variation of ZnO film thickness and the different parameters of the Sellmeier model were studied. This approach help us to identify the optimal configuration (ZnO thin film/substrate) for transparent thin layers used in optoelectronic applications. the results obtained by the different simulations show that the refractive index and extinction coefficient decreases with increase in the wavelength . Therefore the optimal structure for transparent thin films used in optoelectronic apps is (ZnO/quartz) with small thicknesses (in the range of 10 nm) because of its high transmission percentage achieved (94%).

References:

- [1] M. Willander, O. Nur, Q.X. Zhao, L.L. Yang, M. Lorenz, B.Q. Cao, D.L.S. Dang, Nanotechnology 20 (2009) 332001.
- [2] X.W. Sun, H.S. Kwok, Journal of Applied Physics 86 (1999) 408.

Dielectric properties of strontium-substituted barium titanate glass-ceramics

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Glass-ceramics of the compositions (23.1-y) Na₂O/17.1 BaO/6 SrO/23 TiO₂/y Al₂O₃/7.6 B₂O₃/17.4 SiO₂/5.8 Fe₂O₃ with y = 0 or 3 (in mol%) are synthesized using the traditional glass melt-quenching technique. The obtained materials are thermally treated above the glass transition temperature. Their phase composition and microstructure are analyzed. X-ray diffraction shows that the as quenched materials contain Ba_{1-x}Sr_xTiO₃ while a small amount of Ba-fresnoite is additionally indicated after thermal treatments. The microstructure, crystal morphology and elemental composition of the prepared samples are analyzed by scanning electron microscopy combined with energy dispersive X-ray spectroscopy. The dielectric properties of the obtained materials are investigated by impedance spectroscopy as a function of the frequency (10 to 10⁶ Hz) and the temperature (-170 to 300 °C). All samples are electrical insulators in the investigated temperature range. The samples treated for 100 h at 550 °C show the highest dielectric constant.

Funding acknowledgment The authors express their gratitude to the Bulgarian National Science Fund, contract KP-06-N28/1 for the financial support.

Stress dependent photovoltaic effect in the ferroelectric $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_x\text{Ti}_{1-x}]\text{O}_3$ crystal

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The Shockley–Queisser limit determines the maximum possible photovoltaic (PV) efficiency at 33.7 percent for single-junction semiconductor-based solar cells. This limitation however does not apply to ferroelectric (FE) photovoltaic materials where each unit cell can act as a PV junction. However to advance the ferroelectric PV cells to market competitive level the better understanding of physical mechanisms behind the photovoltaic response (the bulk PV effect [1-3]) in ferroelectrics is essential. Such a study however prefers samples in a single crystal form to sort out any possible extrinsic contributions occurring in thin films [4] and ceramics [5]. In this work the lead magnesium niobate lead titanate (PMN-PT) family FE crystals with the general formula of $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_x\text{Ti}_{1-x}]\text{O}_3$ can serve as an inexpensive model compound for PV properties investigation.

The $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.68}\text{Ti}_{0.32}]\text{O}_3$ ferroelectric crystals of (001) orientation were supplied by Crystal-Gmbh (Germany) in a shape of rectangle with the edges along [010] and [100] directions. The silver paste electrodes were deposited perpendicular to [010]. The ferroelectric hysteresis loops were obtained at room temperature using the external electric field at ultralow frequency to prevent electrical damage. The samples were illuminated using a 365 nm light emission diode produced by Thorlabs Inc. The ferroelectric loops, time-current and time-voltage measurements were performed with Keithley electrometer. The light intensity dependence of the PV response was measured at remnant FE states obtained for subcoercive and overcoercive regions. A significant influence of the ferroelectric poling state on the PV properties under UV light which can be explained in terms of ability of internal electric field to separate light generated photocarriers. The PV response was found to depend on the sign of the FE poling being larger for positive electric fields.

The influence of stress on the PV properties and electric bias field will also be presented along with theoretical investigations of the local atomic environment, electronic structure calculations and Born effective charges analyses. For first-principles calculations, a $2 \times 2 \times 2$ supercell with 40 atoms is used to study the local structures of $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.75}\text{Ti}_{0.25}]\text{O}_3$. Periodic DFT calculations were carried out using the plane-wave pseudopotential method as implemented in the CASTEP code. Exchange and correlation were approximated using the GGA PBE functional. The plane-wave cut-off energy was 800 eV. Brillouin zone sampling of electronic states was performed on a $4 \times 4 \times 4$ Monkhorst-Pack grid. The equilibrium crystal structures were obtained via geometry optimization in the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization scheme after which the residual forces were converged to zero within $0.005 \text{ eV \AA}^{-1}$. The structure of PMN-PT corresponds to $A(\text{B}'\text{B}'')\text{O}_3$ in which B-site is shared by Mg, Nb and Ti. It is established that the relative displacements of Pb atom and the atoms in the B-site from the high-symmetry positions are the dominating factor for the macroscopic properties such as polarization in PMN-PT solid solutions. The Pb^{2+} 6s lone-pair electrons bring about a large Pb displacement and a significant Pb contribution to the overall polarization [6]. Analysis of the local structure shows, that Pb moves toward the Mg-Nb face and avoid the Ti-Nb face. It is found that in the crystal under hydrostatic compression the magnitude of Pb and B-site cations displacements is reduced. As result the structure became more centrosymmetric, which leads to the decrease of the polarization and should decrease the PV effect, as confirmed experimentally.

This work was supported by the Ministry of Education and Science of Ukraine and by the Franco-Ukrainian Dnipro (PHC) program № 46789RH.

References:

- [1] K.T. Butler, J.M. Frost, A. Walsh, Energy Environ. Sci. 8 (2015) 838.
- [2] C. Paillard, X. Bai, I.C. Infante, M. Guennou, G. Geneste, M. Alexe, J. Kreisel, B. Dkhil, Adv. Mater. 28 (2016) 5153.
- [3] S.Y. Yang, J. Seidel, S.J. Byrnes, P. Shafer, C.-H. Yang, M.D. Rossell, P. Yu, Y.-H. Chu, J.F. Scott, J.W. Ager III, L.W. Martin, R. Ramesh, Nat. Nano. 5 (2010) 143.
- [4] M.L. Calzada, R. Jiménez, A. González, J. García-López, D. Leinen, E. Rodríguez-Castellón, Chem. Mater. 17 (2005) 1441.
- [5] K. Takagi, S. Kikuchi, J.-F. Li, H. Okamura, R. Watanabe, A. Kawasaki, J. Am. Ceram. Soc. 87 (2004) 1477.
- [6] H. Tan, H. Takenaka, C. Xu, W. Duan, I. Grinberg, A.M. Rappe, Phys. Rev. B 97 (2018) 174101.

Structural, phonon and dielectric properties calculations based on DFT and modern theory of polarization

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Dielectric properties are crucial to understand many functional materials, predict their behavior and eventually optimize their performances under intrinsic and/or extrinsic effects. Until now, many approaches were developed and explored to investigate more or less deeply the appropriate properties. One of the most appealing, accurate and exciting approach is first principle simulations based on Density Functional Theory (DFT), especially after the appearance of the modern theory of polarization and the easiness of access to powerful computational resources. In our present work, we will benefit from the available theoretical and technical enhancements to establish structural optimization and thermal stability of the promising lead free ferroelectric material SnTiO_3 , followed by systematic focus on dielectric properties using berry phase and Wannier centers formalisms. The methods and results will be examined and discussed by comparison to the prototypical ferroelectric material PbTiO_3 .

Study of the parameters of influence on the critical conditions of the flashover

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The flashover insulators of high voltage overhead lines are the evolution of an electric discharge along its polluted surfaces until the short-circuiting of the high voltage to ground. It interrupts the distribution of electrical energy, often causing load shedding of the line supported by the disturbing insulator. To overcome this phenomenon and protect the power transmission network from this type of problem, which is the main cause of frequent outages, it is imperative to study the favorable conditions, which govern the evolution of the discharge. Many works, both theoretical and experimental, have been carried out in this field, the aim of which is to find the critical conditions and the circumvention criteria.

This work focuses on the influence of electrical and geometric quantities likely to determine the critical conditions for flashover a polluted insulator. The study will be done on a new laboratory model called a diamond model, similar to a real insulator. To check the validity of this model and determine the critical conditions, we measured the critical voltage and current, for different values of electrolytic resistivity and different thicknesses. The results obtained allowed us to conclude that the critical voltage essentially depends on the resistivity at any position and whatever the depth of the layer polluting.

References:

- [1] Z. Aydogmus, M. Cebeci, IEEE Trans. Dielectr. Electr. Insul. 11 (2004) 577.
- [2] S. Flazi "Etude du contournement électrique des isolateurs H.T. pollués. Critère d'élongation de la décharge et dynamique du phénomène", thèse de doctorat Es-science, Université Paul Sabatier, Toulouse 1987.
- [3] S.A. Bessedik, H. Hadi, "Particle swarm optimization technique for the estimation of arc parameters for pollution flashover", 9ème Conférence Nationale sur la Haute Tension, CNHT'2013, Univ. laghouat. Avril 2013
- [4] F.A. Hamza Slamet, "Contribution à l'étude du modèle développé d'un isolateur pollué", Mémoire de magister, Université USTO, Algérie 2012.
- [5] M.F. Bouchelga, R. Boudissa, S. Kornhuber, K.D. Haim, "Effet du rayon de courbure des électrodes sur l'évolution des décharges électriques parallèles sur une isolation polluée sous tension continue positive", 11 ème CNHT, 2019, 29-30 avril 2019 Oran, Algérie
- [6] M. Slama, "Experimental Characterization and Mathematical Modelling of Surface Flashover of Solid Insulator in Air", the 19th International Symposium on High Voltage Engineering, Pilsen, Czech Republic, August, 23-28, 2015.

Theoretical modeling of structural, electronic and optical properties of tin dioxide

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Tin dioxide (SnO_2), which is an oxide material that crystallizes in the rutile structure, is one of the most important materials in semiconductor industries. It is a wide band gap n-type transparent semiconductor: $E_g = 3.59$ eV [1]; it can therefore be used for many applications such as photo-detectors, gas sensors, solar cells, etc. This material can also be found in the orthorhombic structure.

The structural, electronic and optical properties of tetragonal SnO_2 single crystals were investigated by considering the local density approximation (LDA) based on the density functional technique (DFT) as implemented in Quantum Espresso. The optimized lattice parameters, $a = 4.7519$ Å and $c = 3.2353$ Å, are in good agreement with the experimental data, $a = 4.737$ Å and $c = 3.185$ Å [2]. In LDA approximation, the calculated value of the energy gap was found to be $E_g = 1.81$ eV. This value presents a very significant deviation from the measured value which is 3.59 eV. By introducing the Hubbard correction, through the LDA+U approximation, the new calculated value was found to be $E_g = 3.25$ eV, which is in good agreement with the experimental data.

For the optical properties of tetragonal SnO_2 single crystals, we calculated the refractive indices as a function of the energy of incident photons for light polarized perpendicular and parallel to the c-direction. The respective values of the infinite wavelength ordinary and extraordinary refractive indices were found to be $n_o = 2.67$ and $n_e = 2.61$.

References:

- [1] K. Reimann, M. Steube, Solid State Communications 105 (1998) 649.
- [2] W.H. Baur, Acta Crystallographica 9 (1956) 515.

Study of samarium doped ceria prepared by ionic gelation method and solid state reaction synthesis

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In the present work two series of Sm – doped cerium oxides $Ce_{1-x}Sm_xO_{2-x/2}$ were prepared by ionic gelation (IG) method and solid state reaction (SSR) route. The nanopowders obtained were used to study the effect of dopant concentration on the structure and thermal properties of the final materials.

The IG samples were synthesized after gelling of ionic solutions of sodium alginate and metal ($Ce(NO_3)_3 \cdot H_2O$, $Gd(NO_3)_3 \cdot H_2O$) nitrates and following thermal treatment of the gel. The SSG samples preparation includes preliminary high-energy milling of the initial oxides (cerium and samarium) and subsequent heating of the resulting homogeneous mixture. The synthesis was carried out at a low heating rate and holding at 1300 °C for 4 hours.

The powder samples were morphologically and structurally characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and infrared spectroscopy (IR). Their thermal behavior was analyzed by differential scanning calorimetry (DSC), and the presence of Ce^{3+} ions was verified by X-ray photoelectron spectroscopy (XPS). The results obtained show that applying of ionic gelation method allows $Ce_{1-x}Sm_xO_{2-x/2}$ with different molar ratios (Ce/Sm) to be obtained at relatively low temperature (about 500 °C) than the conventional solid state reaction synthesis (about 1300 °C).

The authors appreciate the financial support of the Bulgarian National Science Fund under contract КП 06-H59/13. The study has been carried out using facilities of ESHER funded by the Ministry of Education and Science, Contract No. Д01-160/2018.

YOUNG SESSION

Grain size effects on dielectric properties of yttrium doped BaTiO₃ ceramics

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Due to the wide range of applications of ceramics, interest in investigating all the parameters that influence the properties of these materials has constantly been on the increase. In the past fifty years, various studies were conducted on the effects of grain size on the properties of different ceramics. In the present study, a brief report of the effect of grain size on the electrical properties of the yttrium doped BaTiO₃-based ceramics (x = 0 and 2%). As the range of electrical properties of this type of ceramics is quite extensive, this paper focuses on basic issues such as dielectric properties. Barium titanate (BaTiO₃) doped yttrium ceramics with various grain sizes were prepared by a conventional sintering method at 1250 °C and 1300 °C. These structures tetragonality was identified using powder X-ray diffraction. BaTiO₃ has a uniform grain size when the sintering step was at 1250 °C, but the doped sample consists of a different shape and size with homogeneous morphology and dense microstructure, as observed by scanning electron microscopy. The permittivity and the dielectric losses of the ceramics as a function of frequency and temperature are investigated. The dielectric constant dependences on temperature and frequency showed an increase in permittivity as the grain sizes increased. Besides, The degree of relaxation (γ) decrease from 1.49 to 1.06 when the grain size of BT increase, but for BYT 2%, γ increase from 1.27 to 1.31.

Effect of organic additive on the electrodeposition of a copper deposit: electrochemical and corrosion resistance study

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Organic and inorganic additives are frequently used in copper electroplating procedures to increase coating qualities such as brightness, reduce roughness, thickness, hardness, and corrosion resistance [1]. The effects of additives on copper electrodeposition from aqueous solution have been studied extensively.

In this study, an investigation was done on the influence of organic additive on the electrodeposition behavior of a copper deposit. The effect of an organic additive, AN, on electrodeposited copper was investigated at various concentrations. Leveling, grain refining and brightening agent effects have been identified for AN use. Properly selected concentrations of the organic additive AN added in the electroplating bath partially converged the adsorbed additive and optimized the leveling effects. In addition, the morphology of the copper deposits obtained in the absence and in the presence of organic compounds was studied by scanning electron microscopy (SEM), also techniques of linear polarization resistance and electrochemical impedance were used in order to check the additive effect on the corrosion of the deposit [2,3]. The results revealed that the AN additive increased the strength of the deposit, as well as an improvement in the degree of roughness and crystallite size upon addition of AN, whereas it was concluded that in the presence of AN additive the polarization resistance (R_p) increase attesting a good corrosion resistance.

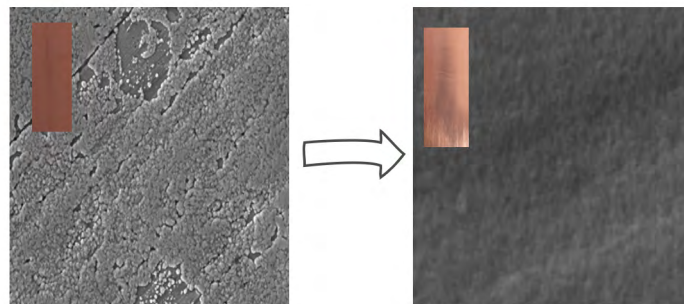


Figure 1. SEM micrographs of the copper electrochemical deposition without and with additive

References:

- [1] C. Lin, J. Hu, J. Zhang, P. Yang, X. Kong, G. Han, Q. Li, M. An, *Surfaces and Interfaces* 22 (2021) 100804.
- [2] R.A. Belakhmima, N. Errahmany, M. Ebn Touhami, H. Larhzil, R. Touir, *Journal of the Association of Arab Universities for Basic and Applied Sciences* 24 (2017) 46.
- [3] M.Y. Zaki, K. Nouneh, M. Ebn Touhami, R.A. Belakhmima, A.C. Galca, L. Pintilie, M. Taibi, *Optical Materials* 83 (2018) 252.

Valorization of three apatitic calcium phosphates (PTCa, HA and OCPa) as steel corrosion inhibitors in NaCl 3%: Characterization and comparison

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Cost, environmental safety and inhibiting efficiency are the main factors for choosing a corrosion inhibitor. In fact, the majority of inhibitors (organic and mineral) present very high anti-corrosive properties towards the surrounding environment [1]. On the other hand, they cause remarkable damage to the material in contact with the environment because of their toxicity.

In this regard, apatitic calcium phosphates have attractive properties such as biodegradability, non-toxicity and ease of processing with high purity. They are biomaterials used most often in the biomedical field as bone implant materials, which makes them a focus of interest for researchers to apply as corrosion inhibitors of materials [2].

The objective of our study is to evaluate the anticorrosive power of the three apatitic phosphate (PTCa, HA and OCPa) on steel in 3% NaCl. The three phosphates prepared by double decomposition [3] are first characterized by chemical analysis (CA) and by Fourier Transform Infrared (FTIR) adsorption spectroscopy. Then, they were tested by electrochemical techniques such as Electrochemical Impedance Spectroscopy (EIS) and Stationary Polarization (PDP). The results obtained revealed that the addition of the studied inhibitors leads to a decrease of the kinetics of the steel corrosion processes. This dwindle depends on the concentration, the temperature and the immersion time. Moreover, the inhibitory efficiency is about 87% at 200 ppm, 91% at 100 ppm and 92.5% at 50 ppm respectively for PTCa, HA and OCPa. the steel surface morphology was studied by SEM/EDX in the presence of the three inhibitors and some thermodynamic parameters were then calculated and discussed.

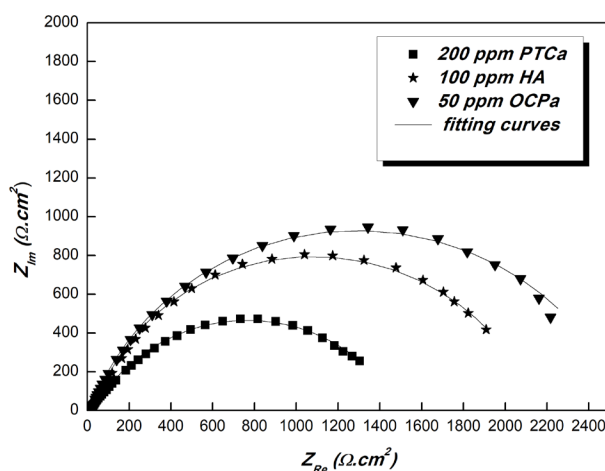


Figure 1. The impedance diagrams for the steel in the Nyquist plane in the presence of the optimum concentration of the three inhibitors in NaCl 3%

References:

- [1] S. Sahoo, S. Nayak, D. Sahoo, M. Mallik, Materials Today: Proceedings 18 (2019) 2642.
- [2] N. Ferraa, M. Ouakki M. Cherkaoui, M.B. Ziatni, Journal of Bio- and Tribo-Corrosion 8 (2022) 23.
- [3] J.C. Heughebaert, G. Montel, Bull. Soc. Chim. F 8-9 (1970) 2923.

Electrical conductivity study of epoxy polymer loaded with reduced Graphene Oxide particles

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In this study, we analyze the electrical properties of reduced Graphene Oxide (rGO) mixed into epoxy resin polymer, Diglycidyl Ether of Bisphenol A (DGEBA) [1]. In order to understand the electrical conduction mechanism of the samples, DC electrical conductivity measurements of the samples were carried out in the temperature range of 240 - 400 K. The experimental results fit well with Mott's model of three-dimensional variable range hopping conduction [2-3]. The values of Mott's temperature, density of states at the Fermi energy, average hopping distance and barrier height for the composites were calculated and presented.

References:

- [1] Y. Nioua, S. El Bouazzaoui, B.M.G. Melo, P.R. Presas, M.P.F. Graca, M.E. Achour, L.C. Costa, C. Brosseau, J. Mater. Sci. 52 (2017) 13790.
- [2] Z.H. Wang, C. Li, E.M. Scherr, A.G. MacDiarmid, A.J. Epstein, Phys. Rev. Lett. 66 (1991) 1745.
- [3] A.J. Epstein, H. Rommelman, R. Bigelow, H.W. Gibson, D.M. Hoffmann, B.D. Tanner, Phys. Rev. Lett. 50 (1983) 1866.

Novel schiff base complexes and natural dye as sensitizers in dye sensitized solar cells

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The use of extracted natural compounds as dye sensitizers is a promising option for the fabrication of low-cost solar cells. The latter devices transform solar energy directly into electricity. In the present study, Aloe Latex Solid (ALS), that is a yellow orange solid compound extracted from the Aloe Vera leaves, was deposited on a TiO₂ thin film (TiO₂/ALS) for the construction of two different configurations of solar cells. The UHPLC-DAD-ESI-MS analysis, UV-Vis and FTIR spectroscopic studies were performed for the prepared dye sensitizer. In fact, the performance of the TiO₂/ALS composite was investigated in a heterojunction dye sensitized solar cell (HJ-DSSC) and a liquid electrolyte-based dye sensitized solar cell (LE-DSSC) to identify the architecture with highest efficiency of sunlight conversion. The obtained results showed encouraging photovoltaic performances with an open circuit voltage (Voc) varying from 0.13 up to 0.30 V, and fill factors (FF) less than 40%. Interesting solar conversion efficiencies were obtained for both architectures with a maximum value of about 1.17% corresponding to the LE-DSSC configuration.

Imidazole-loaded KIT-6 mesoporous materials with high proton conductivity

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The search for clean and high-power energy seems to be one of the most important topics all over the world [1]. For this reason, in recent years there has been a growing interest in energy conversion devices including fuel cells, especially proton exchange membrane fuel cells (PEMFC). Thanks to their small size, safety and high energy density, PEMFCs find application in portable electronics and vehicles [1,2].

The most commonly used electrolyte in PEMFCs is Nafion whose operation depends on the presence of water. As one of the most important challenges is to increase the PEMFC working temperature above 100 °C without accompanying a decrease in proton conductivity, many research groups have been working on obtaining highly conductive materials working in anhydrous conditions. In this regard, the use of porous materials e.g. MOFs, COFs, zeolites and OMS is becoming more and more popular [1-5].

Our present work focuses on the synthesis and characterization of anhydrous proton-conducting materials constituting mesoporous KIT-6 molecular sieves loaded with imidazole molecules. Firstly KIT-6 materials varying in Si/Al ratio were synthesized and some of them were modified by two methods: ion exchange with cerium species or anchoring of sulfonic acid groups by means of reaction with 3-mercaptopropyltrimethoxysilane (MPTMS) and subsequent oxidation with H₂O₂. The resulting porous matrices were characterized by PXRD, N₂ sorption, FTIR and then impregnated with imidazole to obtain sieve-molecular composites. The proton conductivity of composites was investigated by impedance spectroscopy. All tested materials show high proton conductivity in a wide range of temperatures (20 - 120 °C) increasing with an increase in temperature and imidazole loading.

References:

- [1] S.-S. Liu, Q.-Q. Liu, S.-Z. Huang, C. Zhang, X.-Y. Dong, S.-Q. Zang, *Coord. Chem. Rev.* 451 (2022) 214241.
- [2] F. Xiang, S. Chen, S. Zheng, Y. Yang, J. Huang, Q. Lin, L. Wang, S. Xiang, Z. Zhang, *ACS Appl. Mater. Interfaces* 13 (2021) 41363.
- [3] M. Furtmair, J. Timm, R. Marschall, *Microporous Mesoporous Mater.* 312 (2021) 110745.
- [4] A. Jankowska, A. Zalewska, A. Skalska, A. Ostrowski, S. Kowalak, *Chem. Commun.* 53 (2017) 2475.
- [5] A. Jankowska, A. Ostrowski, S. Kowalak, *Microporous Mesoporous Mater.* 298 (2020) 110059.

Study of physicochemical properties of new composite films formed by cellulose derivatives with imidazole

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In many laboratories around the world, research is conducted to find materials that could be used in hydrogen fuel cells. One of the essential elements of hydrogen fuel cells is the membrane that separates the two electrodes and acts as an electrolyte. For technological reasons, it is necessary that the electrolyte has a and is stable in the temperature range in which the cell operates.

The investigated composites were made of cellulose derivative and imidazole. The mass concentration of imidazole in the samples was 0, 10, 15, 20, 30, 40, and 50%. The electrical conductivity value increases with increasing imidazole concentration in the sample. It proves that imidazole molecules are involved in the proton diffusion process.

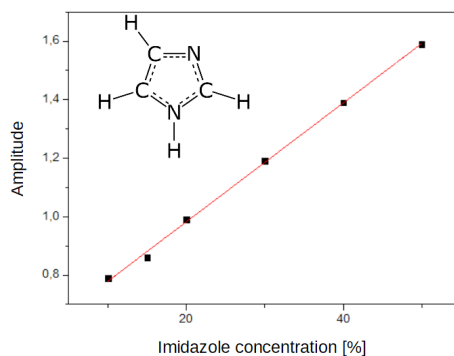


Figure 1. Dependence of amplitude on imidazole concentration

In the temperature range between 40 and 60 °C, an anomaly was observed, which is visible for samples with higher percentages of imidazole. To answer questions about the nature of temperature-induced changes in the proton conducting material under study, vibrational and electronic spectroscopy methods were used.

In order to study the electronic structure of the samples, the absorption and emission spectra were recorded with the use of excitations in the spectral range from 220 to 320 nm. The vibrational structure of proton conductors has been investigated using various measurement techniques: Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) and Attenuated Total Reflection (ATR).

Thermo-optical analysis (TOA), thermogravimetry (TG), and differential scanning calorimetry (DSC) were used to study the thermal properties of the new proton conductors. It was observed that the decomposition temperature of the tested films decreases with increasing imidazole content.

Analysis of the ionic liquid trapped in carbon matrices using FTIR, Raman and dielectric spectroscopy

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We report the results of spectral analysis of the ionic liquid 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide (EMIM TFSI) and 1-Ethyl-3-methylimidazolium bis(fluorosulfonyl)imide (EMIM FSI) restricted inside activated carbon (AC) which is form by graphite microcrystals with the void volume of diameter of 0.9 to 4 nm.

Experiments were conducted using Dielectric Spectroscopy, Raman spectroscopy and Fourier-transform infrared spectroscopy (FTIR). Based on results of the experiment we have calculated relaxation time of the ionic liquid and EMIM TFSI inside the carbon nanopores. The decrease of the melting temperature of the EMIM TFSI confined in nanopores had been observed. Spectral analysis of FTIR shows the shifts of the peaks of selected bonds of the ionic liquid molecule trapped in the pores of the activated carbon in relation to the bulk liquid. We observed that the degree of shift of the spectrum peaks depends on the size of the pores and specific bond of molecule.

Additionally, the analysis of the contact angles of the ionic liquid inside the carbon matrices was performed.

We would like to thank National Scientific Centre for the financial support under the grant of UMO-2016/22/ST4/00092.

References:

- [1] N. Shimodaira, A. Masui, Journal of Applied Physics 92 (2002) 902.
- [2] N.R. Dhumal, K. Noack, J. Kiefer, H.J. Kim, The Journal of Physical Chemistry A 118 (2014) 2547.

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Ministry of Education and Science
Republic of Poland

**Conference Seventh International Symposium on Dielectric Materials
and Applications ISyDMA'7 - a task financed from funds of the
Minister of Education and Science for the „Doskonała Nauka” programme.**

