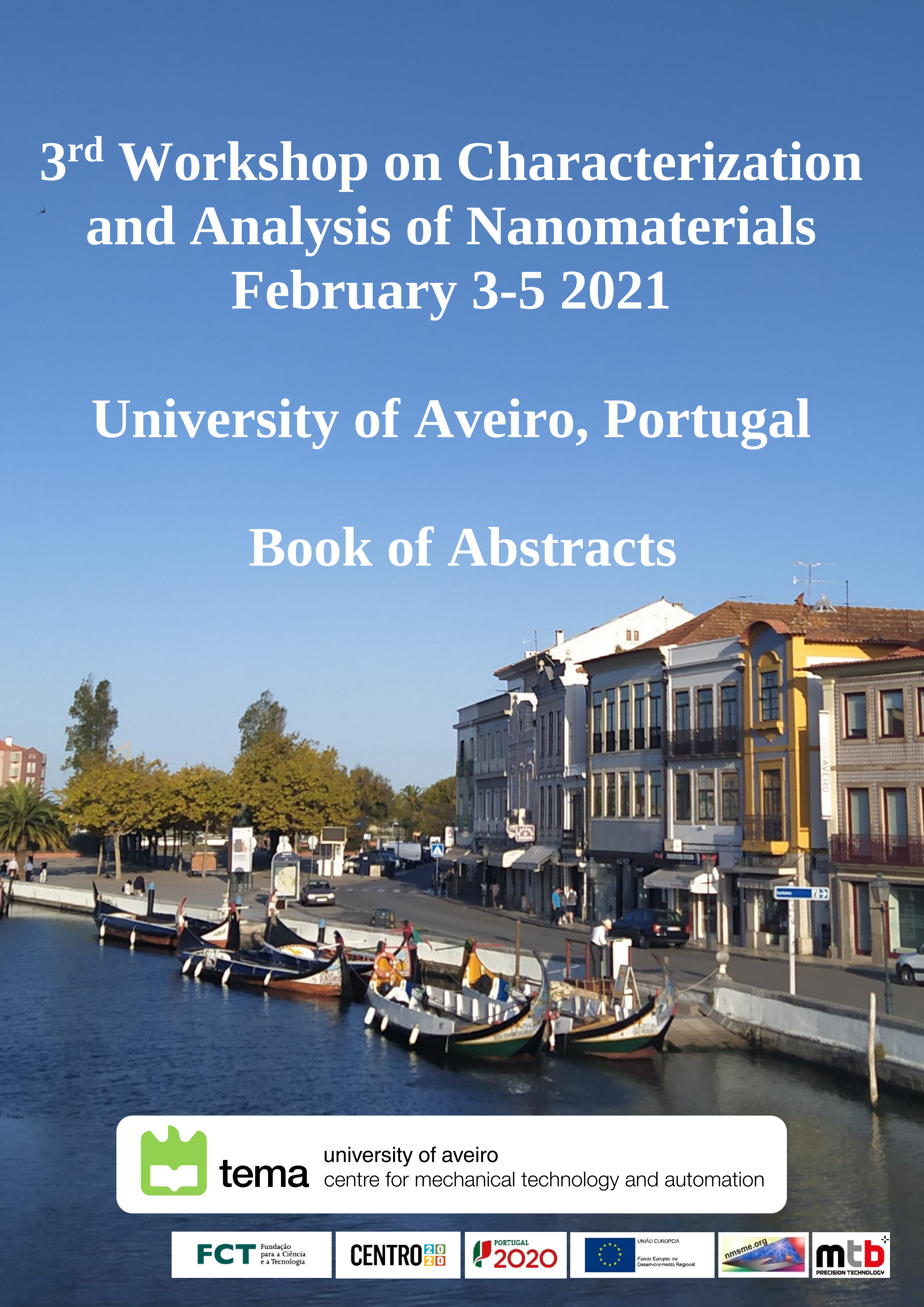
# 3rd Workshop on Characterization and Analysis of Nanomaterials
## February 3-5 2021

## University of Aveiro, Portugal

# Book of Abstracts



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# 3rd Workshop on Characterization and Analysis of Nanomaterials, February 3-5, 2021, University of Aveiro, Portugal
## (3rd WCANM-2021)

**Progress in science depends mainly on the level of experimental technology. Currently, interest in nanomaterials has led to many technological advances and has opened new horizons in understanding nature. Success in these ways was achieved by the development and standardization of methods for determining the characteristics of nanomaterials: X-ray diffraction, electron microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, modelling of nanostructures, etc. A thorough knowledge of these methods is a necessary basis for work in modern science. The major aim of this workshop is to give a detailed description of principles and current state of the art of basic methods for the characterization of nanomaterials.**

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# Work program

## February 3, 2021

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|---|---|
| **3rd Workshop on Characterization and Analysis of Nanomaterials, February 3-5, 2021, University of Aveiro, Portugal (*online*)**<br>**Auditorium 1** | |
| **9:00-9:15** | **WELCOME ADDRESS**<br>**Prof. Dr. António Manuel de Bastos Pereira, Dr. Igor Bdikin** |
| **9:15-10:15** | CHAIR: Prof. Dr. Duncan Paul Fagg<br>**Diffraction methods**<br>**Phase coexistence in Sm-doped $BiFeO_3$ ceramics across structural transitions**<br>**Prof. Dr. Dmitry Karpinsky**<br>*National Research University of Electronic Technology, Moscow, Russia*<br>*Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus* |
| **10:15–10:30** | **Coffee break / Open discussions** |
| **10:30–11:30** | CHAIR: Prof. Dr. Duncan Paul Fagg<br>**The Synergy of Experimental & Computational Studieson the Characterization and Analysis of Nanomaterials**<br>**Prof. Dr. Manuel Melle-Franco**<br>*CICECO, University of Aveiro, 3810-193 Aveiro, Portugal* |
| **11:30–12:00** | **Modeling of the 2D-materials heterostructures based on Ferroelectric polymer PVDF/P(VDF-TrFE) and Transition Metal Dichalcogenides**<br>**Prof. Dr. Vladimir Bystrov**<br>*Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia* |

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| **12:00–12:30** | CHAIR: Prof. Dr. Duncan Paul Fagg<br>**I6. Structural and Impedance Characterization of BCT-CFO Ferrite Composite system**<br>**Prof. Dr. Radheshyam Rai**<br>*School of Basic and Applied Sciences, Department of Physics, Lingayas Vidyappeth, Faridabad, PIN-121002, India* |
| **12:30–13:00** | **O2. Cyclometalated Ir(III) complexes as phosphorescence emitters**<br>**Kahnu Charan Pradhan**<br>*P. G. Department of Chemistry, Utkal University, Bhubaneswar-751004 India* |
| **13:00–14:00** | **Lunch break** |
| **14:00–15:00** | CHAIR: Dr. Gonzalo Guillermo Otero<br>**Atomic Force Microscopy – Forces and Currents in the Nanoscale World**<br>**Prof. Dr. Brian J. Rodriguez**<br>*School of Physics, University College Dublin, Belfield, Dublin 4, Ireland* |
| **15:00–15:20** | **O4. Characterization and evaluation of superabsorbent polymers issued from disposable hygiene products**<br>**Yahya Bachra**<br>*University Hassan II of Casablanca, Faculty of Sciences Ben M'Sick, Department of Chemistry, Laboratory of Biomolecules and Organic Synthesis (BioSynthO), Casablanca, Morocco* |
| **15:20–15:40** | **O5. Fabrication and Characterization of Injectable Chitosan Hydroxyapatite Composite for Bone Tissue Engineering**<br>**Ayoub Grouli**<br>*University Hassan II of Casablanca, Faculty of Sciences Ben M'Sick, Department of Chemistry, Laboratory of Biomolecules and Organic Synthesis (BIOSYNTHO), Casablanca, Morocco* |
| **15:40–16:00** | **O11. Machine learning for molecular modeling: cascade**<br>**Dr. Alla Sapronova**<br>*PetraOS AS, Straume, 5353, Norway* |
| **16:00–16:30** | **Coffee break / Open discussions** |
| **16:30–18:00** | CHAIR: Dr. Gonzalo Guillermo Otero<br>**P1-P11 (posters)** |

## February 4, 2021

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|---|---|
| **3rd Workshop on Characterization and Analysis of Nanomaterials, February 3-5, 2021, University of Aveiro, Portugal (*online*)**<br>**Auditorium 2** | |
| **9:00-9:30** | CHAIR: Prof. Dr. Paula Marques<br>**O7. New starting material hydrogel based on durian rind as the peat water purifier**<br>**Dr. Doddy Irawan**<br>*Department of Mechanical Engineering, Universitas Muhammadiyah Pontianak, Indonesia* |
| **9:30-10:30** | **I1. Growth of Functional Bulk- and Nano-Crystals For Energy Harvesting**<br>**Prof. Dr. Binay Kumar**<br>*Crystal Lab, Department of Physics & Astrophysics, University of Delhi, India* |
| **10:30–10:45** | **Posters/ Coffee break / Open discussions** |
| **10:45–11:45** | CHAIR: Prof. Dr. Paula Marques<br>**X-ray Photoelectron Spectroscopy (XPS)**<br>**Prof. Dr. Jose Angel Martín Gago**<br>*Institute of Material science of Madrid-CSIC,*<br>*Madrid, Spain* |
| **11:45–12:15** | **O8. Formation of the structural fragments in $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se) single crystals**<br>**Dr. A.S. Shkvarin**<br>*M. N. Miheev Institute of Metal Physics, UB of RAS, 620990 Ekaterinburg, Russia* |

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| **12:15–12:45** | **O3. A new method for determining the chirality of peptide nanotubes based on the dipole moments calculations**<br>**Prof. Dr. V. S. Bystrov**<br>*Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, Pushchino, Moscow 142290, Russia* |
| **12:45–13:15** | **O1. Effect of thickness on microstructure of thin chromium films**<br>**Shiva. L. Udachan**<br>*Dept of Physics, Rani Channamma University, Belagavi-591156, Karnataka, India* |
| **13:15–14:00** | **Lunch break** |
| **14:00–15:00** | CHAIR: Dr. Gil Gonçalves<br>**Electron Microscopy**<br>**Observing while it happens: In situ electron microscopy of dynamic processes**<br>**Prof. Dr. Marc Georg Willinger**<br>*Scientific Center for Optical and Electron Microscopy (ScopeM)*<br>*ETH Zürich, Switzerland* |
| **15:00–15:40** | **Techniques for characterization nanomaterials MT Brandão**<br>**João Cascalheira**<br>*MT Brandão Lda* |
| **15:40–16:30** | **I4. Insight into oxide-based memristive devices through the electrical and structural characterization of substoichiometric oxide films**<br>**Dr. Carlos M. M. Rosário**<br>*I3N and Physics Department, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*<br>*Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen University, Sommerfeldstraße 18, 52074 Aachen, Germany* |
| **16:30–16:45** | **Coffee break / Open discussions** |

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| **16:45–17:05** | **O6. Preparation and Characterization of Chitosan-coated Iron Oxide Nanoparticles cross-linked with Dialdehyde Chitosan for Magnetic Drug Delivery System**<br>**Fouad Damiri**<br>*University Hassan II of Casablanca, Faculty of Sciences Ben M'Sick, Department of Chemistry, Laboratory of Biomolecules and Organic Synthesis (BIOSYNTHO), Casablanca, Morocco* |
| **17:05–17:25** | **O9. Local electromechanical properties of valine microcrystals**<br>**Dr. Igor Bdikin**<br>*TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal* |
| **17:25–17:45** | **O10. The influence of albumin on biomimetic formation of calcium phosphates / $TiO_2$ nanowires composites**<br>**Ina Erceg**<br>*Ruđer Bošković Institute, Zagreb, Croatia* |
| **17:45–18:15** | **I7. Chemically modified additive phases in Ti/$TiO_2$ additives incorporated hydrogen storage system $MgH_2$**<br>**Dr. D. Pukazhselvan**<br>*Nanoengineering Research Group, TEMA, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* |
| **18:15–18:30** | **Final discussions and comments** |

* Lectures on basic characterization methods are highlighted in green.

** Presentations of companies produce equipment for characterization materials are highlighted in yellow.

# Poster session

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| **P1** | **Temperature dependent phonon behavior in nanocrystalline $Tm_2O_3$: Fano interference and Phonon anharmonicity**<br>Neha Bura, Ankit Bhoriya, Deepa Yadav, Jasveer Singh, Nita Dilawar Sharma<br>*Pressure, Vacuum & Ultrasonic Metrology section, Physico-Mechanical Metrology Division, National Physical Laboratory, New Delhi-110012, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India* |
| **P2** | **Assessment of adsorption in nano composites of multiwalled carbon nanotubes and polyvinyl chloride, polyethylene, foam polystyrene**<br>A. P. Onanko, D. V. Charnyi, Y. A. Onanko, O. P. Dmytrenko, M.P. Kulish, T. M. Pinchuk-Rugal, O. L. Pavlenko, S. A. Shevchuk, T. O. Busko, P. P. Ilyin<br>*Kyiv national university, Kyiv, Ukraine* |
| **P3** | **Morphology and composition of nanoinclusions in $Fe_{0.25}Ni_{0.25}TiSe_2$**<br>Postnikov M.S., Shkvarin A.S., Merentsov A.I., Patrakov E.I., Titov A.N., Betz-Guttner E., Gregoratti L., Amati M., Zeller P.<br>*M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia; IOM-CNR, Laboratorio TASC, S.S. 14-km 163.5, Basovizza, Trieste, Italy; Elettra – Sincrotrone Trieste S.C.p.A., Trieste, Italy* |
| **P4** | **Temperature-dependent Raman study and Magnetic measurement of the Rare Earth Manganite synthesized by solid-state reaction method**<br>Ankit Bhoriya, Neha Bura, Deepa Yadav, Jasveer Singh, H.K. Singh, Nita Dilawar Sharma<br>*Pressure, Vacuum & Ultrasonic Metrology section, Physico-Mechanical Metrology Division, CSIR-National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi-110012, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India* |
| **P5** | **Modification in the physical properties of Gamma irradiated <011> Oriented TGS single crystals**<br>V.C. Bharath Sabarish, A. Durairajan, M.P. Graça, M.A. Valente, S. Gokulraj, G. Ramesh Kumar<br>*University College of Engineering Arni-Thatchur- Anna University, Chennai -632 326, India; Department of Physics, University of Aviero Portugal; Department of Physics, C. Kandasamy Naidu College, Chennai 600102, India* |
| **P6** | **Synthesis and characterization of $BiFeO_3$ –Graphene and $BiFeO_3$ –MWCNT Nanocomposites**<br>C.Anandaraj, R. Venkatapathy, V.C. Bharath Sabarish, P. Kalaivani, A. Durairajan, M.P. Graça, M.A. Valente, S. Gokul Raj, G. Ramesh Kumar<br>*University College of Engineering Arni-Thatchur- Anna University, Chennai -632 326, India; Department of chemistry/Arunai College of Engineering Thiruvannamalai, Tamilnadu, 606603, India; 3I3N-Aveiro-Department of Physics / University of Aveiro, Portugal; Department of Physics /C. Kandaswami Naidu College for Men Chennai, Tamilnadu, 600102, India* |

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| **P7** | **Modification of Structural, Optical and Morphological Characteristics of Bismuth Ferrite Thin Films using Swift Heavy Ion Irradiation (SHI)**<br>Venkatapathy Ramasamy, Durairajan Arulmozhi, Manuel Pedro Fernandes Graca, Manuel Almeida Valente, Gokulraj Srinivasan, Ramesh Kumar Gubendiran<br>*Department of Physics / University College of Engineering Arni, Anna University, India; I3N-Aveiro-Department of Physics / University of Aveiro, Portugal; Department of Physics / C. Kandasamy Naidu College for Men Chennai. India* |
| **P8** | **Photocatalytic degradation of synthetic microfibers**<br>Patrick Seleš, Tina Radošević, Damjan Vengust, Mateja Podlogar<br>*Jožef Stefan Institute, Slovenia; Jožef Stefan International Postgraduate School, Slovenia; Faculty of Chemistry and Chemical Technology, University of Ljubljana, Slovenia* |
| **P9** | **An Efficient Crystal-layer Arrangement of Spinel $NiFe_2O_4$/reduced graphene oxide for Enhancing Oxygen Evolution Reaction Performance**<br>Pratik V. Shinde, Chandra Sekhar Rout, Manoj Kumar Singh<br>*Centre for Nano and Material Sciences (CNMS), Jain University, Jakkasandra, Ramanagaram, Bengaluru - 562112, Karnataka, India; Department of Physics - School of Engineering and Technology (SOET), Central University of Haryana (CUH), Mahendergarh - 123031, Haryana, India* |
| **P10** | **Cell adhesion to Ti and Mg based materials**<br>A. Bystrova, Yu. Dekhtyar, J. Schmidt, H. Sorokins, A. Rapoport, G. Khroustalyova<br>*Riga Technical University, Kalku Street 1, LV-1658, Riga, Latvia; Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia; INNOVENT e. V. technology development, Prüssingstraße 27B, 07745 Jena, Germany; University of Latvia, Raina bulvaris 19, LV-1586, Riga, Latvia* |
| **P11** | **Synthesis and characterization of ZnO nanoparticles by wet chemical co-precipitation**<br>Mohammed Hussain Alnajar, Nidhi Sinha and Binay Kumar<br>*Crystal Lab, Department of Physics & Astrophysics, University of Delhi, Delhi 110007, India; Department of Electronics, SGTB Khalsa College, University of Delhi, Delhi 110007, India* |

# Centre for Mechanical Technology Automation (TEMA), Department of Mechanical Engineering, University of Aveiro

In a world of constant change, the capacity of adjustment is essential. The Centre for Mechanical Technology and Automation (TEMA) is highly aware of this factor and fully comprehends the relevance of the R&D conducted in the research unit and its impact on society (academic, industrial/business and civil) and is experiencing a crucial transition period of structural adaptation to ensure the continued pursuit of scientific excellence with a contextualized translation in(to) innovation, competitiveness and citizenship of the community. This transition aims to ensure the essence of TEMA and to capitalize the background of expertise of its members that is enriched by the diversity of scientific fields, distributed in six main areas of knowledge: applied mechanics; applied energy; biomechanics; modelling & simulation; nanoengineering and transportation technologies.

Based on its Human Capital and Capacities, the Centre for Mechanical Technology and Automation (TEMA) embraces a mission aiming to contribute to a sustainable industry, with specially focus on the surrounding SMEs, and to the wellbeing of society. This is pursued by the development of excellence, cutting-edge and high impact research and innovation in engineering and technology, a mission made possible by the Researchers that compose TEMA, together with a responsible and effective fulfillment of the strategic mobilizing projects.

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Prof. Dr. António Manuel de Bastos Pereira
Director of TEMA - Centre for Mechanical Technology and Automation

# Plenary lectures

# Modeling of the 2D-materials heterostructures based on Ferroelectric polymer PVDF/P(VDF-TrFE) and Transition Metal Dichalcogenides

**V. S. Bystrov**[1,*], E.V. Paramonova[1], A.V. Sapronova[1,2], A. V. Bystrova[1,3], Hong Shen[4], Xiangjian Meng[4], Jianlu Wang[4], L.A. Avakyan[5]

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[5]*Southern Federal University, Department of Physics, 344090 Rostov-on-Don, Russia*

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Transition metal dichalcogenides (TMDCs), such as $MoS_2$, $MoSe_2$, $MoTe_2$, $WS_2$, etc., are layered materials with strong in-plane bonding and weak out-of-plane interactions enabling exfoliation into two-dimensional layers of single unit cell thickness [1].

Recent advances in nanoscale materials characterization and device fabrication have opened up new opportunities for two-dimensional (2D) layers and 2D-materials of thin TMDCs in nanoelectronics and optoelectronics. TMDCs monolayers are very promising for many applications, especially in the fields of in optics as emitters and detectors, in electronics as transistors. All these TMDCs have sizable bandgaps that change from indirect to direct in single monolayers, allowing applications such as transistors, photodetectors and similar electro-optical devices [2]. It is first of all due that their monolayers have a direct band gap $E_g$, which is strongly depending from external applied electric fields.

The great opportunity to create such an electric field, is proposed approach to use the field induced by polarization of the ferroelectric polymers such as PVDF and P(VDF-TrFE) [2, 3]. These polymers can exist in the ferroelectric phase and are capable of create significant polarization in very thin layers, up to 5 Å [4]. Such polymers are named as two-dimensional ferroelectrics (2D-ferroelectircs) [5, 6]. By combining these polymer ferroelectric layers and thin TMDCs monolayers, hybrid nanostructures can be created, that are convenient for design of new photodetectors with controlled properties. The prominent properties of this hybrid structure arise and benefit namely from the ferroelectric-polarization-induced ultra-high electric field of the PVDF or P(VDF-TrFE), that impact on TMDCs layers and control the band gap $E_g$.

In this work, we simulate, as a first example, such a hybrid structure based on PVDF and $MoS_2$ layers and study their features and properties [7]. For calculating $MoS_2$, the methods of density functional theory (DFT) are used, implemented in the VASP program. Semi-empirical quantum-chemical methods (PM3, ZINDO/1) based on the HyperChem software package are used to model and study both individual layers of the hybrid structure and the features of their joint interaction. The results obtained convincingly show a strong influence on the width of the $MoS_2$ bandgap $E_g$ from the side of the PVDF layers, creating polarization $P$ and an electric field $\boldsymbol{E}$, which affects $MoS_2$ layers. In addition, the dependence of the band gap $E_g$ under the action of electric field $\boldsymbol{E}$ from the distance between the layers PVDF and $MoS_2$ has been established.

Similarly other possible “TMDCs+PVDF” models with various TMDCs components ($MoSe_2$, $MoTe_2$, $WS_2$) [8, 9] are proposed, considered and analysed. The variations of the parameters for these different models are tested and studied to determine and adjust some suitable models of these hybrid nanostructures. Additionally are investigated different models for TMDCs monolayers configuration and influence of these changes on the final affected heterostructures results. The data obtained are analysed in comparison with other known computed and experimental data. The perspective proposals for development and applications of these hybrid heterostructures are discussed and reviewed. Authors thankful to Russian Foundation for Basic Researches grant # 20-51-53014_a. Prof. Xiang-Jian Meng expresses his gratitude to National Natural Science Foundation of China (NNSFC) for grant # 61574151, Prof. Hong Shen for grant # 62011530043.

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# Atomic Force Microscopy – Forces and Currents in the Nanoscale World

**Brian J. Rodriguez** *

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To realize the potential of nanoscience and nanotechnology requires the ability to image, manipulate, and control matter on the nanoscale. Atomic force microscopy (AFM) techniques allow access to the nanoscale world through structural, functional, and chemical imaging and manipulation on nanometer scales. Beyond imaging surface topography, AFM has found an extremely broad range of applications for probing magnetic, electronic, mechanical, and electromechanical properties. In this presentation, a general overview of AFM and techniques used for characterization of nano/functional materials will be provided. Special attention will be devoted to the development and implementation of voltage-modulated AFM techniques such as piezoresponse force microscopy, and recent work from our group will be highlighted. Specifically, the AFM tip loading-force dependent evolution of strain effects in ferroelectric bismuth ferrite thin films, from structural phase changes and mechanically-enhanced switching currents at low forces (< 1 µN) to nanomechanical machining at higher forces (> 10 µN), will be presented. In this work, switching behavior and switching currents are found to be affected by force, with coercive fields decreasing with increasing loading force. Notably, switching-relateed currents increase with applied force and may enable polarization state determination in ferroelectric memory applications. Through a systematic investigation of a range of AFM parameters, including force, we demonstrate that AFM-based machining is an effective tool for rapid and precise modification of local regions of the film, as well as for the fabrication of several different nanostructures, including nanocapacitor arrays with individually addressable ferroelectric elements. AFM-based machining of ferroelectric nanostructures offers advantages in select cases over established techniques, such as bottom-up approaches and focused ion beam milling, where low damage and low-cost modification of already-fabricated thin films are required.

# Observing while it happens: *In situ* electron microscopy of dynamic processes

**Marc Willinger** *

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Modern analytical transmission electron microscopes are capable of delivering picometer resolved information about the geometric arrangement of atoms. It is possible to simultaneously obtain quantitative information about the elemental composition of a material and even to measure the local electronic structure or electric and magnetic fields. One of the side-effects of using strongly interacting electrons for the imaging process is the requirement of a good vacuum near the sample and throughout the optical system. Obtaining detailed information about the state of an isolated material in vacuum is not sufficient if we are interested in processes such as material growth- and decomposition, corrosion or (electro)catalysis. With the availability of MEMS- (micro electro mechanic systems) technology based TEM holders for *in situ* experiments, it is now possible to study the response of a material to a physical or chemical stimuli and study gas-phase, temperature and electrochemically induced processes. Since atomic motions can be fast and the temporal resolution of conventional microscopes is limited and furthermore, processes are often related to collective dynamics of many atomic species, a combination of high-resolution imaging with context embedded observation at lower magnification is required.

In my presentation I will show how the combination of *in situ* scanning and transmission electron microscopy enables a multi-scale approach for the study of functional materials in their relevant state. Examples range from CVD growth of 2D materials [1] to corrosion processes and catalysed surface reactions (see Figure1) [2]. It will be shown how *in situ* microscopy reveals the beauty of complex dynamics in systems that are operated far from thermodynamic equilibrium. The field is still relatively new and with the development of more sensitive and faster detectors as well as further improvement of tools for *in situ* electron microscopy, we are looking towards an exciting expansion of our possibilities to study complex processes related to atomistic dynamics.

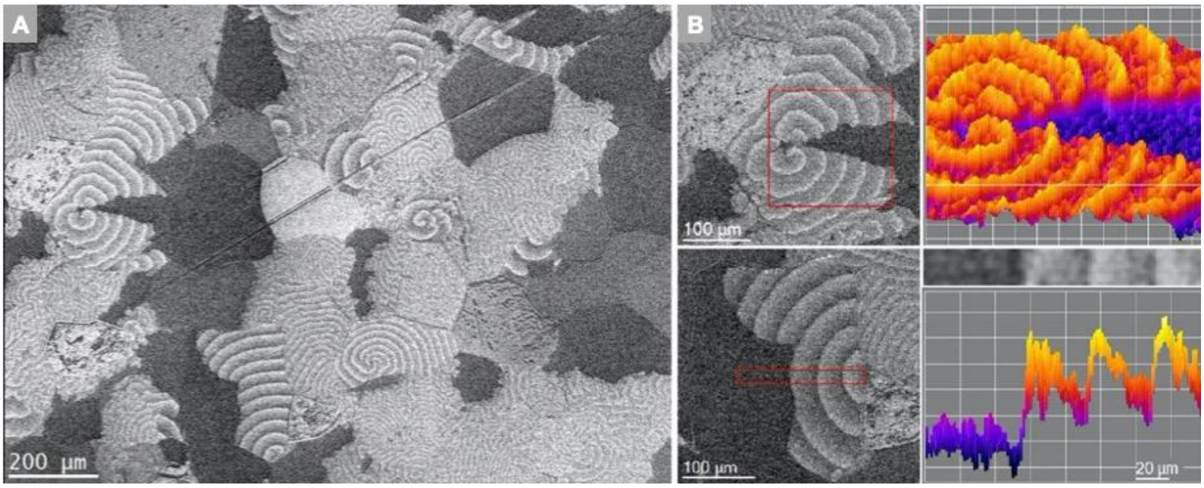

**Figure 1:** **A** shows an overview image recorded during $NO_2$ hydrogenation on Pt at T = 172 °C; $p_{NO2}$:$p_{H2}$ ≈ 1:10; $p_{tot} = 3.6 \times 10^{-2}$ Pa. Propagating chemical waves give rise to beautiful dissipative structures. **B** shows the variation in contrast between subsequent light-off events and 3D plots of the secondary electron intensity.

**References:**

Z.-J. Wang *et al.*, *ACS Nano*, **2015**, 9, 1506–1519, Z.-J. Wang *et al.*, *Nature Communications*, **2016**, 7:13256, Z.-J. Wang *et al.*, *Adv. Mater. Interfaces*, **2018**, 1800255, M. Huang *et al.* Nature Nanotechnology, **2020**, doi:10.1038/s41565-019-0622-8

C. Barroo, Z.-J. Wang, R. Schlögl, M.-G. Willinger, *Nature Catalysis*, ***2019***, doi:10.1038/s41929-019-0395-3

# The Synergy of Experimental & Computational Studies on the Characterization and Analysis of Nanomaterials

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Computer modelling has become a key feature to understand and predict existing and new materials. From our extensive experience applying and developing computational models, we will illustrate through examples how computer models yield key information on diverse nanotechnology problems such as magnetic graphenes [1], covalent organic frameworks, [2] large bottom-up aromatic molecules [3] and inorganic nanoparticles [4].

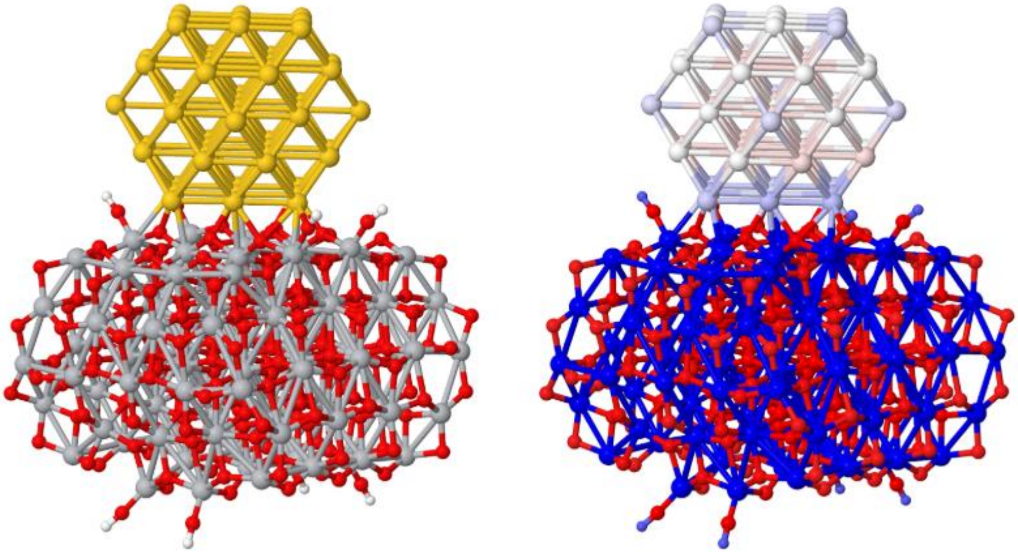

**Figure 1.** Structure (left) of a gold nanoparticle adsorbed on a titania nanoparticle and charge transfer (right) in water.

[1] *Bow in Awe to the New Nanographene.* **Nature Nanotechnology** 15, 2020, 8–9.
[2] *A Wavy Two-Dimensional Covalent Organic Framework from Core-Twisted Polycyclic Aromatic Hydrocarbons.* **Journal of the American Chemical Society** 141, 2019, 1403–10.
[3] *Revisiting Kekulene: Synthesis and Single-Molecule Imaging.* **Journal of the American Chemical Society** 141, 2019, 15488–93.
[4] *Enhanced Photocatalytic Activity of Au/TiO2 Nanoparticles against Ciprofloxacin*. **Catalysts**, 10, 2020, 234.

# X-ray Photoelectron Spectroscopy (XPS)

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In this talk, fundaments and perspectives of XPS will be given. Special emphasis will be made in discussing the unique capabilities emerging from the use of synchrotron radiation facilities. The talk will be illustrated with examples in the field of nanoscience and nanotechnology. Some variants of this technique, as diffraction, imaging or near ambient-pressure XPS will be discussed.

# Invited speakers

# I1. Growth of Functional Bulk- and Nano-Crystals For Energy Harvesting

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Pressure, temperature, doping, etc. can change the ferroelectricity, pyroelectricity, piezoelectricity, ferromagnetism properties of a functional material and hence transducer, sensor, actuator can be developed. In the present talk our recent results in respect of lead based and lead free perovskite like PMN-PT and BNKT bulk crystals and nanocrystals will be presented along with recent developments in piezoelectric versatile ZnO [1-5].

Various binary, ternary and quaternary systems based on PMN-PT were synthesized and extremely high values of piezoelectric coefficient (>1380 pC/N), pyroelectric coefficient (>2000 $\mu Cm^{-2}$ °$C^{-1}$) and remnant polarization (upto 60 μC/cm2) were. Single crystals of 1-2 cm size were grown by high temperature flux method. Nano-crystallites of these high performing crystals were obtained by ball milling. It has been shown that the ferro-/pyro-/piezelectric properties of these nanocrystals are better than the nanoparticles obtained from polycrystalline power of these materials. In the third category, doped ZnO nanoparticles were synthesized by low temperature chemical reaction which exhibited excellent piezoelectricity.

These nanocrystals were used to prepare organic binder based thick tapes. The performance of these tapes as a pressure sensor and energy harvester were studied under varying pressure and frequency of applied force. It was shown that these nanogenerators can perform without any degradation upto several thousands of impulses. It has been further shown that the use of bulk single crystals in place of nanoparticles can provide much higher energy output.

1. “True-remanent, resistive-leakage and mechanical studies of flux grown 0.64PMN-0.36PT single crystals” Binay et al. Arabian J. of Chemistry 13 (2020) 2596–2610
2. “$Y^{3+}$ doped 0.64PMN-0.36PT ceramic for energy scavenging applications: Excellent piezo-/ferro-response with the investigations of true-remanent polarization and resistive leakage” Binay et al. J. of Alloys and Compounds 790 (2019) 274– 287
3. “Lead Free Relaxor Ferroelectric $Na_{0.47}K_{0.47}Li_{0.06}Nb_{0.94}Sb_{0.06}O_3$ Crystals for Opto-Electronic Applications”Binay et al. Crystal Growth and Design 15 (2015) 1852-1860
4. “Tb-doped ZnO:PDMS based flexible nanogenerator with enhanced piezoelectric output performance by optimizing nanofiller concentration” Binay et al. Ceramics International 46 (2020) 24120–24128
5. “A review on piezo-/ferro-electric properties of morphologically diverse ZnO nanostructures” Binay et al. J. of Alloys and Compounds 816 (2020) 152491

# I2. Phase coexistence in Sm-doped $BiFeO_3$ ceramics across structural transitions

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The work describes an evolution of the crystal structure occurring under increase in the dopant concentration in Sm-doped $BiFeO_3$ compounds prepared by sol-gel technique. In particular, the structural phase transitions from the polar rhombohedral to the anti-polar orthorhombic followed by the non-polar orthorhombic phase driven by the dopant content in the compounds $Bi_{1-x}Sm_xFeO_3$ ($0.08 \leq x \leq 0.2$) are studied using both local scale and microscopic measurement techniques, viz. X-ray diffraction, transmission and scanning electron microscopies, EDS experiments and piezoresponse force microscopy.

Increase in samarium concentration leads to the structural transition from the polar active rhombohedral phase (space group *R3c*) to the non-polar orthorhombic phase (s.g. *Pbnm*) via a formation of metastable anti-polar orthorhombic phase (s.g. *Pbam*). The morphotropic phase boundary region determined from the diffraction results is characterized by two concentration ranges having coexistent polar rhombohedral and anti-polar orthorhombic phases ($0.12 < x < 0.15$) and the anti-polar and non-polar orthorhombic phases ($0.15 < x < 0.18$) (Fig.1).

Analysis of the SEM data allowed to determine a decrease in the average grain size of the crystallites from ~ 0.5 μm for the compounds with $x \leq 0.14$ down to ~ 0.4 μm for the compounds with $0.18 \leq x \leq 0.20$. A decrease in the average grain size is associated with an increase in the amount of oxygen vacancies which in turn slows down growth of crystallites. The EDS results testify that the element content corresponds to the designed chemical formulas for the appropriate compounds, while a careful analysis of the EDS data has allowed to clarify a certain difference in the elements distribution as a function of the dopant content while it does not affect main conclusions.

TEM measurements have revealed that the morphotropic phase boundary region estimated by diffraction experiments is characterized by a wider concentration range, viz. $0.08 \leq x \leq 0.20$. The results of the PFM measurements have demonstrated a notable reduction in the average domain size as well as a decrease of the crystallites size with the dopant content which confirms the results of the SEM and XRD measurements. Polar active regions can be identified on the PFM images (Fig. 2) as areas with bright and dark contrasts with the amplitude of the piezoresponse signal larger than 5 pm. The change of the piezoresponse sign reveals differently distributed polarization inside the crystallites. It should be noted that the PFM contrast images obtained for the compound with x = 0.08 are characterized by a presence of the regions with close-to-zero PFM signal (below 2 pm) showing the presence of the non-polar or anti-polar phase inclusions.

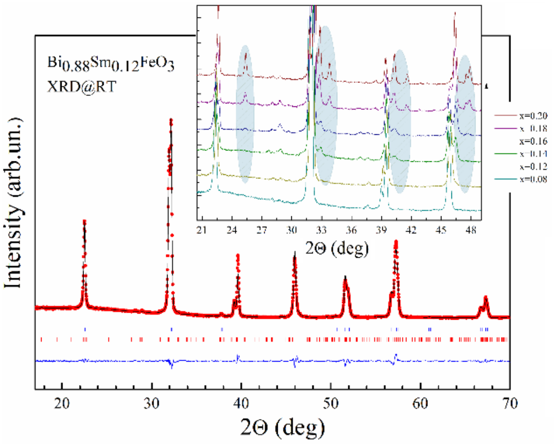

Fig. 1. Room-temperature XRD pattern obtained for the compound $Bi_{0.88}Sm_{0.12}FeO_3$. The inset shows concentration-driven evolution of the diffraction peaks.

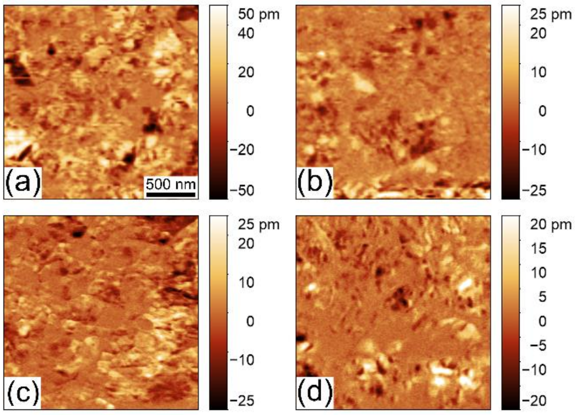

Fig. 2. PFM images of $Bi_{1-x}Sm_xFeO_3$ compounds with x = 8% (a), 12% (b), 18% (c), 20% (d).

Taking into account the XRD, PFM and TEM data one can conclude about the presence of the nanoscale fraction of the anti-polar orthorhombic phase in the compound with x = 0.08 while the compound is characterized by single phase structural state assuming the X-ray diffraction data solely. Notable difference with the results of microscopic measurements is justified by the presence of the polar active and the non-polar regions in the compounds having single phase non-polar orthorhombic ($x > 0.18$) and the polar rhombohedral structural state ($x < 0.12$) respectively as determined by the diffraction measurements.

## References

[1] D. V. Karpinsky, A. Pakalniškis, G. Niaura et al., Ceram. Int., 47, 5399 (2020).
[2] D. V. Karpinsky, I.O. Troyanchuk, M. Tovar et al., J. Alloys Compd., 555, 101 (2013).

# I3. Insight into oxide-based memristive devices through the electrical and structural characterization of substoichiometric oxide films

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As key enablers of a new electronics paradigm for energy-efficient neuromorphic computing, memristive devices such as redox-based resistive random-access memory (ReRAM) have been the focus of much research and development. $Ta_2O_5$ is one of the most popular ReRAM materials, and $Ta_2O_5$-based ReRAM rely on the nonvolatile change of the resistance via the modulation of the oxygen content in conductive filaments. However, the filaments' structure and exact composition are currently under intense debate, with the two current models considering filaments composed of oxygen vacancies and those containing metallic Ta. In this work we provide insight into the filament's structure and composition by means of a detailed electrical and structural characterization of substoichiometric $TaO_x$ thin films, grown to try and match the material of the filaments. A comparison with conduction filaments in $Ta_2O_5$-based ReRAM devices has proven very useful.

Structural analysis of the $TaO_x$ films through X-ray diffraction and electron microscopy reveals the presence of Ta clusters inside the films. Importantly, there have been independent observations of metallic Ta in the filaments [1,2]. Moreover, the $TaO_x$ films with $x \sim 1$ show the same transport mechanism as metallic Ta films, for most of the measured temperature range from 2 K to 300 K, which is associated with conduction in disordered metals. Beyond the transport mechanisms, both cases share a carrier concentration on the order of $10^{22}$ $cm^{-3}$ and a positive magnetoresistance at $T < 30$ K. It is concluded that the transport in the $TaO_x$ films with $x \sim 1$ is dominated by a percolation chain of Ta clusters embedded in an insulating $Ta_2O_5$ matrix. On the other hand, the conductive filaments in $Ta_2O_5$ ReRAM devices exhibit the same transport mechanisms observed for the $TaO_x$ and Ta thin films [3]. Accordingly, the electrical transport in the conductive filaments inside $Ta_2O_5$-based ReRAM devices is found to be determined by percolation through Ta clusters [4].

[1] M.K. Yang et al., *Sci. Rep.* **5**, 14053 (2015).
[2] Y. Ma et al., *ACS Appl. Mater. Inter.* 10, 23187 (2018).
[3] C.M.M. Rosário et al., *Appl. Phys. Lett.* **112**, 213504 (2018).
[4] C.M.M. Rosário et al., *Nanoscale* **11**, 16978 (2019).

# I4. Janus-layers in $TiS_2$ – $TiSe_2$ solid solution

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Layered dichalcogenides of transition metals are represented as a sequence of two-dimensional structural fragments X-T-X, where X = S, Se or Te, and T is a transition metal of IV, V or VI groups. Structural fragments are separated by a wide van der Waals gap. In fact, these materials have no volume and consist of only one surface. In solid solutions based on systems of this kind, theorists have long expected an increase in the effects of segregation. With the substitution along the chalcogen sublattice, it is expected that segregation should lead to the formation of the so-called Janus layers, consisting of a sequence of monatomic layers X1-T-X2, where X1 and X2 are chalcogenes of different types.

We found the formation of S-Ti-Se Janus layers in the single crystals $TiS_2$ - $TiSe_2$ solid solution. For this, a set of methods was used, such as HREM, Fermi surface mapping, ARPES with non-resonant and resonant Ti2p-3d and S2p-3d excitation, the method of electromotive force of electrochemical cells relative to a metal not included in the sample under study, etc. ...

It was found that the Janus layers are in coherent connection with the rest of the lattice and thermodynamically they can be considered as a chemical component of a solid solution. It was found that the characteristic size of the coherent Janus layer is ~ 100 nm. The concentration boundaries of the stability of the Janus layers are determined. The presence of Janus layers explains the anomalously high diffusion mobility in the stability region of the Janus layers and the weak effect of substitution along the chalcogen sublattice on the stability of the CDW state in $TiSe_2$.

# I5. Powder X-ray diffraction characterization of nanoscale structural and magnetic states for double manganites of rare earth elements

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Double manganites $R\mathrm{BaMn_2O_6}$ with ordered alternate stacking of $R\mathrm{MnO_3}$/$\mathrm{BaMnO_3}$ layers where $R$ is rare earth element attracts a special interest due to presence of two magnetic phase transitions close to room temperature; that makes them perspective magnetocaloric and magnetoresistive materials. These materials as well as ordinary manganites $R\mathrm{MnO_3}$ have complicated phase diagram with a number of magnetic, electrical and structural phase transitions. Moreover magnetic, electrical and structural states have mutual influence as magnetic, charge and lattice excitations are strongly coupled. Using X-ray powder diffraction we demonstrate that applied magnetic field may change not only a magnetic state from paramagnetic to ferromagnetic but also the lengths of Mn-O bonds and so, the crystal structure. As magnetic states in manganites of rare earth elements is often inhomogeneous with strong ferromagnetic or ferromagnetic fluctuations into antiferromagnetic matrix so applied magnetic field may change a ratio of volume fractions of nanoscale magnetic domains. It is possible to detect magnetic state of the materials using powder X-ray diffraction because the thermal expansion coefficients demonstrate a jump at II order phase transitions at Curie or Néel temperatures.

As an example for $\mathrm{PrBaMn_2O_6}$ double manganite we revealed the origin of structural phase transition accompanied by the elongation of the a-axis and the contraction of the c-axis. Our findings suggest that the structural phase transition is caused by splitting of $e_g$-doublet states due to orbital ordering at metal-insulator phase transition.

The work was performed via the RFBR project No 19-29-12013 with use of the equipment of Collective Use Center “Ural-M”.

# I6. Structural and Impedance Characterization of BCT-CFO Ferrite Composite system

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This paper focuses mainly on the dielectric and electrical characterization of a synthesized BCT-CFO ferrite composite. $(Ba_{0.85}Ca_{0.15}TiO_3)_{1-x}$-$(CoFe_2O_4)_x$ ( where x = 0.10, 0.20, 0.30 and 0.40) (BCT-CFO) ferrite composites were prepared thru high-temperature solid-state reaction technique. X-ray diffraction study confirmed a double-phase (Ferroelectric/Ferrite phase) compound of perovskite structure with tetragonal/Cubic symmetry. Investigation of the dielectric, electrical properties and impedance study of this ceramic has occurred in the frequency range ($10^2$-$10^6$ Hz) and temperature range (RT - 410˚C). At temperature 35˚C ferro to paraelectric phase transition was observed and the maximum value of dielectric constant ~1000 at 10 kHz for x = 0.10. Nyquist plots were fitted and showed both grain and grain boundary contributes to relaxation. Region-wise conductivity characterization and estimation of activation energy determined from the temperature reliance of ac conductivity. At various temperatures, the frequency dependence AC impedance plots were utilized to characterize the electrical conduction of the sample which demonstrated the negative temperature coefficient of resistance character. Complex impedance and modulus Cole-Cole plots focused on the relaxation phenomenon are poly scatter and non-Debye type in nature. The composite having 40 wt% of CFO exhibited maximum polarization, remnant polarization and coercive field of Ps-5.1 mC/cm2, Pr-1.4 mC/cm2 and Ec-11.6 kV/cm respectively.

# I7. Chemically modified additive phases in Ti/$TiO_2$ additives incorporated hydrogen storage system $MgH_2$

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Owing to its high reversible gravimetric hydrogen density (7.6 wt.%) magnesium hydride is considered as the most suitable material for vehicular applications (target capacity: 5.5 wt.%). However, an important drawback of $MgH_2$ system for commercial applications is its higher dehydrogenation temperature, typically >350 °C (target temperature: 85 °C). Our recent research works prove that the hydrogen desorption temperature can be reduced and better performance can be achieved within the temperature range of 200–300 °C by employing $TiO_2$ as additive. We have optimized the experimental conditions required for making bulk amount of $TiO_2$:$MgH_2$ hydrogen storage powder but the catalytic understanding remains elusive. In view of this, the investigations of the current team mainly focused on exploring how $TiO_2$ involves in the catalytic interaction with $MgH_2$ [1,2]. By employing in situ X ray diffraction technique we proved that reduction of titania, resulting to evolution of a monoxide rock salt nanocrystalline phase is the main interaction in a 3 mol.% $TiO_2$ additive mixed $MgH_2$. We also found evidence for the existence of homogeneously distributed Ti in a crystalline rock salt matrix by using a combined analysis of X – ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM) and elemental chemical mapping techniques. Titanium in $Ti^{3+}$ and $Ti^{2+}$ valance states was confirmed by X - ray photoelectron spectroscopy (XPS). Differential scanning calorimetry (DSC) study proves that the reduced Ti oxide phases promote the low temperature dehydrogenation of $MgH_2$. This observation is a clear evidence that the MgO rock salt layer existing in oxide additives loaded $MgH_2$ is not necessarily a barrier layer that blocks the diffusion of hydrogen. On the other hand, after exploring these information we made another test by using oxide free Ti (Ti metal) as additive for $MgH_2$. Our interest is to check when we force our system to an oxygen free Ti based additive environment, how the catalytic activity occurs and how it compares and contrasts with $TiO_2$ loaded $MgH_2$. We observed that a mild mechanical milling leaves Ti chemically unchanged, while formation of stable $TiH_{2-x}$ occurs upon strong mechanical milling. $TiH_{2-x}$ further transforms to $TiH_2$ upon recycling the powder (dehydrogenation and subsequent hydrogenation) and lowers the activation energy of $MgH_2$ to 89.4 kJ/mol.$H_2$ [Ea of as-received $MgH_2$ is 153 kJ/mol.$H_2$]. From these it is clear that the oxidation state of Ti ends up in $Ti^{2+}$ state, regardless of whatever be the initial state of Ti additive. These observations provide us promising new insights, and interestingly it also support the view that lattice strain may be an important factor in the catalysis of additives incorporated hydrogen storage system, $MgH_2$.

**References:**

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# Oral presentations

# O1. Effect of thickness on microstructure of thin chromium films

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Physical properties of thin films are often governed by the environment present during the film formation, the substrate orientation with respect to the evaporating source, nature of depositing material, microstructure and film thickness. Therefore this paper reports the effect of thickness on microstructure of thin chromium films. The experimental techniques of preparation of chromium films is by thermal evaporation in vacuum. Fabrication of thin chromium films was done in the thickness range (10-80) nm on cleaned glass substrates, at a rate of 0.5 nm/s under a pressure of $10^{-6}$ Torr at room temperature of $22^0$C . After this, the films were taken out of the vacuum chamber for structural, topographical and morphological analysis using Transmission Electron Microscope(TEM), Atomic Force Microscope (AFM), Scanning Electron Microscope (SEM) and Energy Dispersive Spectroscopy (EDS) studies. It is observed that in the initial stages of growth, island structures were noticed. As the thickness increases, the islands grow vertically in the columnar fashion and the smoothness increases. It has been confirmed that the material under investigation is chromium as evidenced by EDS peaks.

# O2. Cyclometalated Ir(III) complexes as phosphorescence emitters

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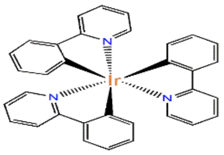
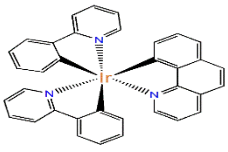
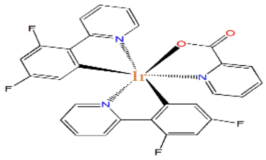
Cyclometalated Ir(III) complexes are phosphorescence emitters. They are used in organic light emitting diodes (OLEDs), bioimaging probes, oxygen sensors, anticancer agents, photoredox catalysts, pH sensors, and so on because of their remarkable optoelectronic properties.
Iridium complexes can be categorized as **$IrL_3$, $IrL_2L'$** and **$IrL_2A$** where L and L′ are different cyclo metallating ligands, ‘A’ is an ancillary ligand that binds to Ir(III) via two hetero atoms



**$IrL_3$**

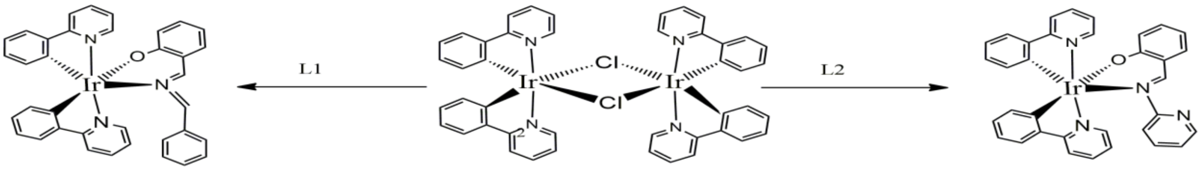


**$IrL_2L'$**



**$IrL_2A$**

The Phenyl Pyridine and related derivatives have attracted interest as precursors to highly fluorescent metal complexes of possible value as organic light emitting diodes(OLEDs). The proposed studies on iridium complexes, therefore designed with heteroleptic iridium complexes composed of phenyl pyridine, substituted phenyl pyridine and ancillary ligands and thus obtained iridium complexes expected to act as phosphors. Each combination of ligands would give rise to HOMO-LUMO separation which would reflect in luminescence behaviour of new complexes[1].



**$[Ir(ppy)_2L1]$** **$[Ir(ppy)_4Cl]_2$** **$[Ir(ppy)_2L2]$**

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# O3. A new method for determining the chirality of peptide nanotubes based on the dipole moments calculations

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A new method for describing the helical biomolecular structures of various levels of hierarchical organization in peptide nanotubes (PNT) of the different chirality and calculating the PNT's chirality sign are developed and proposed. This method is based on the dipole moments calculations for PNT's amino acids. Peptides are convenient building blocks for creation of various molecular structures and bio-mimetic nanomaterials. For such nanostructures chirality ("L" – left or "D" - right) play important role due to the various PNT properties with different chirality, that are manifested in many nanotechnological and biomedical applications. It is known that each amino acid (and their dipeptides) have their dipole moments. The method makes it possible to characterize the chirality sign and to quantify it's value for PNT □-helices, based on the dipole moments of the amino acids forming the nanotube. When self-organizing them into PNT, the dipole moments of individual amino acids and dipeptides are oriented sequentially along a common curved line, which has the shape of a helix and forms a cylindrical helix of the nanotube. Particular, for the L-FF dipeptides ("L" chirality), the individual vectors of these dipoles are aligned along the line of the right screw (right helix), signed as right chirality "D" (Fig. 1). Accordingly, for D-FF - a left "L"-helix is formed [1, 2].

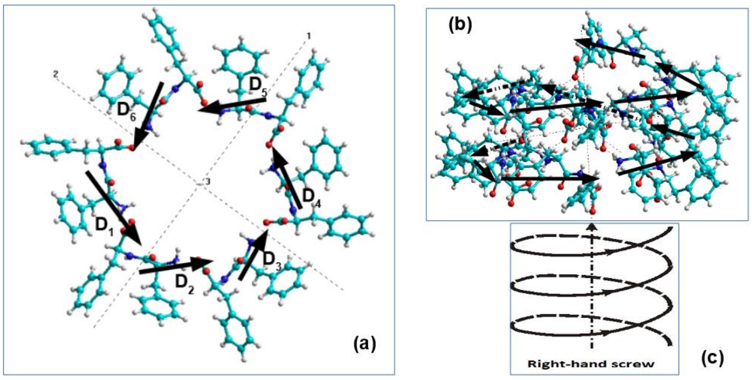

**Figure 1.** Arrangement of individual dipoles Di in the structure of the right (D) nanotube based on L-FF: a) view perpendicular to the Z-axis; b) part of the right helix D for L-FF of 2 turns; c) right screw.

To evaluate and calculate the index and sign of chirality, it is proposed to use a *mixed (or vector-scalar) product* of three successive vectors of dipole moments **$D_i$**. This approach is similar to the method developed in [3] for calculating the sign of chirality based on the vectors constructed between each two adjacent anchor points of the position of a-carbon atoms *Ca* in adjacent amino acids of polypeptide chain. This work provides the calculation the sign of chirality for diphenylalanine (FF) PNT based on dipeptides of different initial chiralities (L-FF and D-FF).

Using the approach similar [3], and applying it to the vectors of dipole moments of the individual dipeptides $\boldsymbol{D_{t,i}}$ ($D_{t,i} = \sqrt{D_{x,i}^2 + D_{y,i}^2 + D_{z,i}^2}$, where $D_{t,i}$ is the total dipole moment of the *i*-th dipeptide vector in the helix structure of the PNT, $D_{x,i}$, $D_{y,i}$, $D_{z,i}$ are the components of the *i*-th vector $D_{t,i}$ in Cartesian coordinates), we can write down the chirality index of the spiral structure $c_{total}$ ; for the normalized chirality $c_{norm}$:

$$c_{total} = \sum_{i=1}^{n-2}\left(\left[D_{t,i}, D_{t,i+1}\right], D_{t,i+2}\right), \quad c_{norm} = \frac{c_{totaL}}{\left(D_{t,i}^{av}\right)^3} \qquad (1)$$

For the cases of nanotubes of different initial chiralities, studied in [1, 2], we obtain, respectively, the following calculated values of the chirality index/sign in Table 1.

**Table 1.** Chirality Index and Sign for PNT with different initial dipeptide chirality L-FF and D-FF, computed using various methods

| Initial dipeptide chirality | Calculated method (using HyperChem) | Chiral index $\boldsymbol{c_{norm}}$ (normalized) | Chiral sign | Chirality type of PNT |
|---|---|---|---|---|
| **L- FF** | Amber | **= +1.19047** | **«+», > 0** | **D** |
| | PM3 RHF | **= +1.36575** | **«+», > 0** | **D** |
| **D- FF** | PM3 RHF | **= -1.23908** | **«-», < 0** | **L** |
| | Amber after PM3 | **= -1.15905** | **«-», < 0** | **L** |

Thus, here we have shown that the calculation of the sign of chirality PNT according to the proposed method (algorithm) based on the components of the dipole moments Dx, i, Dy, i, Dz, i corresponding to individual dipeptides L-FF and D-FF, leads to the correct resulting sign the chirality of the entire nanotube, which is opposite to the chirality of the original dipeptides. That is, for L-FF the nanotube has a chirality sign $c > 0$, which corresponds to the right screw D of the entire nanotube, while for the initial D-FF dipeptides, the chirality sign is $c < 0$, which corresponds to the left screw L of the entire nanotube. The result obtained is in full agreement with the law of the change in the sign of chirality of structures with the complication of their hierarchy organization level. Authors thankful to Russian Foundation for Basic Researches grants ## 19-01-00519_a & 20-51-53014_a.

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# O4. Characterization and evaluation of superabsorbent polymers issued from disposable hygiene products

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Superabsorbent polymers (SAPs) are materials that can absorb and retain large volumes of water and aqueous solutions. They are therefore suitable for a variety of useful applications in agriculture, medicine, and industry in general. However, their greatest application is as a liquid-absorbent material in disposable diapers. Disposable diapers and incontinence protection for the personal care market are improving rapidly. Nowadays, this market is experiencing great growth in regions where the birth rate is very high, such as developing countries that place superabsorbent material among the materials in daily demand on the market [1].

The superabsorbent material for the absorbent core contains, for the most part, a polyacrylate-based material [2]. In this approach, representative samples of the best-selling diapers were taken to be characterized and to evaluate their liquid absorption. The characterization and evaluation of SAP samples were performed by fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), X-ray diffraction (XRD), free swelling capacity (FSC), centrifuge retention capacity (CRC), absorption under load (AUL), absorption rate (AR), particle size distribution (PSD), determination of pH and moisture content (MC). The polyacrylate-based structure of the SAP samples has been confirmed by FTIR, TGA, SEM, and XRD analysis, subsequently, by the comparative study, the most suitable superabsorbent material performances in saline solution were for FSC 47 g/g, CRC 35.26 g/g, and AUL 0.3psi 27.4 g/g. Finally, it's has been deduced that some diapers have a reasonable selling price, while others have a higher price in relation to quality. As well as, SAPs were ranked in order of performance based on the results of this study.

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# O5. Fabrication and Characterization of Injectable Chitosan Hydroxyapatite Composite for Bone Tissue Engineering

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Injectable hydrogels have emerged as promising biomaterials for tissue engineering applications [1]. The aim of this work was to fabricate an injectable porous scaffold material hydroxyapatite (HAp)/ chitosan composite hydrogel and investigate its potent application in bone tissue engineering [2]. However, the hydroxyapatite was successfully synthesized from eggshells waste and confirmed by various chemical’s techniques [3].

Hydroxyapatite was successfully synthesized using eggshell waste as a raw material. Eggshell waste and orthophosphoric acid were co-precipitated for 2 h at an ambient temperature. The pH of the solution was adjusted to 10 using ammonium hydroxide. Then, 10–30 wt% of hydroxyapatite was loaded into the chitosan film. Furthermore, the hydroxyapatite (HAp)/chitosan (CS) composite has been confirmed by scanning electron microscopy (SEM), thermogravimetric analysis (TGA), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and the swelling behavior of the composite was observed in phosphate buffer saline solution.

Finally, the hydroxyapatite (HAp)/chitosan (CS) composite presented good excellent properties as a tissue engineering material.

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# O6. Preparation and Characterization of Chitosan-coated Iron Oxide Nanoparticles cross-linked with Dialdehyde Chitosan for Magnetic Drug Delivery System

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Recently, chitosan (CS) was given much attention as a functional biopolymer for designing various hydrogels for industrial, environmental and biomedical applications, but their biomedical use is limited due to the toxicity of the crosslinker agents[1]. To overcome this inconvenience, we developed an auto cross-linked material based on a chitosan backbone that carries an amino and aldehyde moieties[2]. This new drug delivery system (DDS) was designed by using oxidized chitosan (OCS) that crosslinks chitosan (CS). In the first part, a simple, rapid, low-cost and eco-friendly green method was introduced to synthesize magnetite nanoparticles ($Fe_3O_4$-NPs) successfully. These nanoparticles $Fe_3O_4$ have received a great deal of attention in the biomedical field. Especially in a targeted drug delivery system, drug-loaded $Fe_3O_4$-NPs can accumulate at the tumor site by the aid of an external magnetic field and increase the effectiveness of drug release to the tumor site. In the second part, we have incorporated the $Fe_3O_4$-NPs into chitosan/oxidized chitosan solution because of their unique magnetic properties, outstanding magnetism, biocompatibility, lower toxicity, biodegradability, and other features. Three drugs (5-Fluorouracil (5-FU), Caffeine and Ascorbic acid) were embedded into the magnetite solution that became quickly a hydrogel.

The successful production of the hydrogels and ferrogels was confirmed by (FT-IR), (TGA), (SEM), (VSM) analysis at room temperature. Finally, results showed that our hydrogels and ferrogels may be technologically used as devices for drug delivery in a controllable manner[2].

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# O7. New starting material hydrogel based on durian rind as the peat water purifier

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The clean water crisis is still a problem that cannot be resolved worldwide, including in Indonesia. Indonesia is a maritime country where 2/3 of its territory is water. It has unlimited water sources that can be used as clean water and one of the biggest water source its the peat water. However, unfortunately, we can't use peat water as a source of clean water because of the high concentrations of natural organic compounds and Fe, making the colour of peat water brown and have a terrible smell. One of the ways to reduce high concentrations of organic compounds and Fe is the absorption techniques. In this study, researchers made hydrogel utilizing Durian Rind waste. Durian rind contains high cellulose, which has the potential as a hydrogel starting material. Durian rind has the advantage of being an adsorbent because it can absorb organic compounds and Fe; it can also be an effective anti-bacterial. This research is an experimental study. The results showed that hydrogel based on Durian rind could be used as a peat water purifier. The results of FTIR analysis show that cellulose-based on durian rind has been successfully produced. The hydrogel that we made was able to expand (swelling ratio) of 857%. It means that the hydrogel is hydrophilic and capable of absorbing $Fe^{2+}$ ions that pollute peat water. The measurement results of the degree of cross-linkage showed that the hydrogel strength was 98.23%. The AAS analysis also shows that the hydrogel could absorb $Fe^{2+}$ ions 25%. Thus, with hydrogel, it can be a great solution as a peat water purifier.

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# O8. Formation of the structural fragments in $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se) single crystals

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One of the promising areas of practical use of Layered transition metal dichalcogenides (LTMDs) is a spintronics. Solid solutions $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se) are suitable for this purpose, which was shown both by theoretical and experimental studies. However, there is no information in literature about the electronic structure according to the angle-resolved photoemission (ARPES) studies. We assumed that the difficulties are concerned with the formation of the structural fragments inside the $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se) single crystals. The current study is aimed to prove the existence of the structural fragments inside the $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se) single crystals as well as to study the morphology of their surface. The study by Scanning PhotoElectron Microscopy method were performed on single crystal samples. The SPEM experimental results clearly indicate the presence of the structural fragments in the single crystals of $Cr_xTi_{1-x}Ch_2$ (Ch = S, Se). These fragments differ in the chemical composition and chemical bonding.

The formation of the $TiSe_2$-based and $CrSe_2$-based structural fragments in the $Cr_{0.78}Ti_{0.36}Se_2$ single crystal was confirmed experimentally using SPEM technique. This morphology may be responsible for the blurring of the preliminary obtained ARPES images of this crystal. The fragments are also formed in $Cr_{0.34}Ti_{0.66}S_2$, however they differ not in the chemical bonding of chalcogen, like in $Cr_{0.78}Ti_{0.36}Se_2$, but in the concentration of superstoichiometric Ti.

# O9. Local electromechanical properties of valine microcrystals

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Piezoelectricity is the ability of noncentrosymmetric crystals to produce mechanical stress/strain under electric field or charge under mechanical stress. This property has long been used in acoustic transducers, sensors/actuators, piezomotors, nanorobots, energy harvesters, piezoMEMS. Now a research activity on nanoscale materials shifts from inorganic substances to polymers and biology objects. Recently, novel organic and bio-organic materials have been found to be ferroelectric at room temperature [1]. Currently, it is becoming increasingly obvious that develop new methods for investigation of biological microstructures is extremely necessary. So, in case of virus infections (Pandemia COVID-19) one of main problem is rapid diagnosis in resource-limited settings, which are especially relevant for all global health problems of the modern world. The advent of Atomic Force Microscopy (AFM) provides a potent tool for investigating the structures and properties of biological samples at the micro/nanoscale under near-physiological conditions, which promotes the studies of single-cell behaviours from one side and high resolution single organic molecules from another side. AFM has achieved great success in single-cell observation, single DNA molecules, proteins, organic microstructures and manipulation for biomedical applications, demonstrating the excellent capabilities of AFM in addressing biological issues at the single-macromolecular level with unprecedented spatiotemporal resolution. We shown the applicability of piezoresponse force microscopy (PFM) for studying a broad range of polar materials at the nanoscale for biological / organic complex materials: organic polymers [2], organic nano tubes [3], organic fibers [4], organic composite films [5], organic single crystals [6].

Here we show AFM and PFM investigations of valine microcrystals of different lengths, thicknesses, and orientations has been observed stemming from the simple evaporation method used (Fig.1).

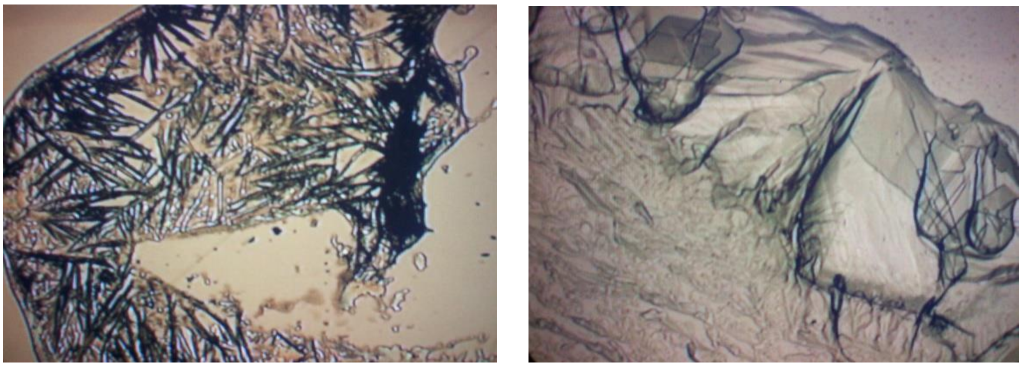
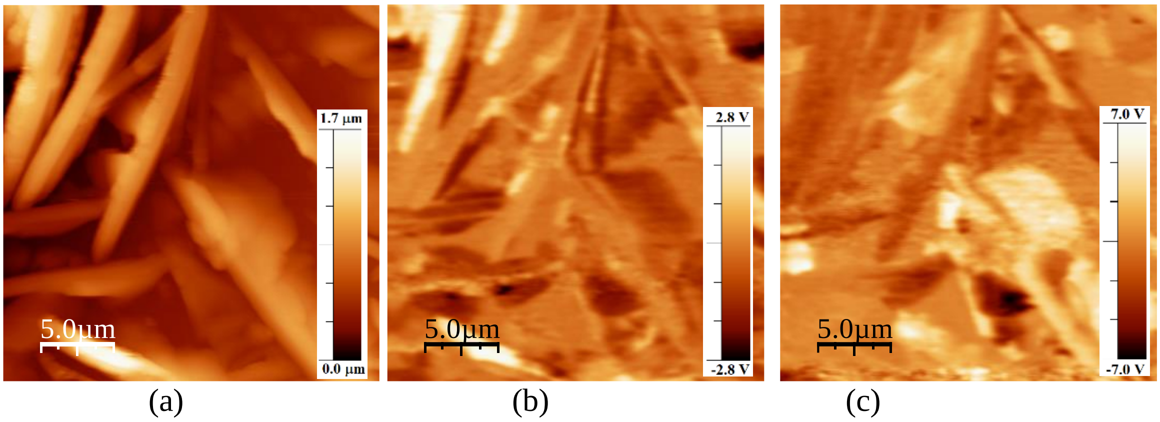


**Fig.1.** Representative optical images (from 0.1 and 1.0 mg ml$^{-1}$ valine solution) of valine microcrystals.



(a) (b) (c)

**Fig.2.** (a) Topography image of a valine micro crystals (0.1 mg ml$^{-1}$ concentration). PFM image: (b) out-of-plane PFM, and (c) in-plane PFM.

Figure 2 shows typical topography and piezoresponse images (OOP and IP) of valine microcrystals. The obtained values of polarization and piezoelectric coefficients are very high in comparison with many piezoelectric materials (Table 1).

**Table 1.** Piezoelectric coefficient several piezoelectric materials.

| | FF tubes | $LiNbO_3$ | PVDF | ZnO | PZT | Valine |
|---|---|---|---|---|---|---|
| $d_{15}$ | 40 pm/V | 74 pm/V | -31 pm/V | -13.9 pm/V | 170 pm/V | 88 pm/V |
| $d_{33}$ | 11 pm/V | 16 pm/V | -38 pm/V | 10.6 pm/V | 160 pm/V | 219 pm/V |

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# O10. The influence of albumin on biomimetic formation of calcium phosphates / $TiO_2$ nanowires composites

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Composite materials based on calcium phosphates (CaPs) and $TiO_2$ nanomaterials have recently attracted attention as new and innovative implant materials for bone regeneration.[1] In addition, they can be prepared by the biomimetic method, considered to be a green synthesis route. *In vivo*, implant performance is affected by surface adsorption of soluble proteins from blood and interstitial fluids. Among them, albumin is the most abundant. However, its role in the formation of CaPs on titanium implants is still not clarified.

In order to fill this void, the influence of albumin on biomimetic formation CaPs on $TiO_2$ nanowires (TiNW) has been investigated. The TiNWs were prepared using a hydrothermal method. CaPs/TiNW composites were prepared by precipitating CaPs in the presence of TiNW. Precipitation systems were prepared by fast mixing of equal volumes of $CaCl_2$ and $Na_2HPO_4$ solutions in the double-walled glass vessel. TiNW and/or BSA were added in $Na_2HPO_4$ solution. The progress of the reaction was followed by monitoring the changes of pH in the precipitation systems. Formed precipitates were filtered after 60 minutes of reaction time and characterized by Fourier – transform infrared spectroscopy, Raman spectroscopy, X-ray powder diffraction, scanning electron microscopy and transmission electron microscopy.

It was shown that TiNWs act as promotors while BSA acts as an inhibitor of CaP formation. None of the additives influenced the composition and the morphology of the formed precipitate. The obtained results point to a biomimetic preparation route of multifunctional CaP based biominerals.

**Acknowledgment:** This work has been fully supported by Croatian Science Foundation under the project HRZZ- IP-2018-01-1493.

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# O11. Machine learning for molecular modeling: cascade

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The application of Machine Learning (ML) methods in computational chemistry promises to overcome the pitfalls of traditional computational methods like the demand on time and hardware [1]. ML methods can predict material properties by constructing atomic force fields (FFs) from the learned relation between chemical structure and potential energy. When a sufficient amount of reference data is used for training, the accuracy of ML-based FFs is close to the accuracy of ab initio methods [2,3].

The time required to construct ML-based FFs is much smaller when compared to the classical approach. The bottleneck here is a training process: for every new configuration, one has to obtain a new training dataset and re-train the ML model [4]. The requirement to fully re-train the ML model sets the limit on the number of configurations that a single ML model can learn, because this would require to deal with ever-increasing training dataset. To overcome this limitation, we propose to apply an incremental learning paradigm that supports continuous new (and only new) data insertion to extend the existing model's knowledge.

We propose a workflow that utilizes an incremental learning ensemble strategy. This strategy incorporates semi-unsupervised learning processes that take place whenever new data emerge and adjust what has been learned according to the new examples. The workflow is designed to allow a new information injection from a molecular modeling database or locally stored topology files. The cascade of Extreme Learning Machines is used for sequential learning. The prototype software is released in the Python programming language.

The test run of the prototype software demonstrates that the proposed incremental learning approach can be used for ML-based FF construction for large multi-molecular complexes. Semi-unsupervised continuous knowledge extension ensures that the model learns as more data became available and the accuracy of the ML FFs increases with time.

Authors thankful to Russian Foundation for Basic Researches grant # 20-51-53014_a.

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# Poster presentations

# P1. Temperature dependent phonon behavior in nanocrystalline $Tm_2O_3$: Fano interference and Phonon anharmonicity

**Neha Bura** [1, 2, *], Ankit Bhoriya[1, 2], Deepa Yadav [1, 2], Jasveer Singh [1],
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We report the temperature dependent variation in the vibrational properties of nano-crystalline thulium sesquioxide ($Tm_2O_3$) in the temperature range of 80-440 K. The structural characterizations revealed the nanocrystalline nature of the cubic phase of the sample. The phonon modes in the Raman spectra of the sample were found to exhibit red shift with an increase in the sample temperature. The most prominent $F_g$+$A_g$ mode was observed at 383 $cm^{-1}$ at ambient temperature, and its line shape was found to be asymmetric in nature. Detailed analysis revealed that the asymmetricity was caused by constructive Fano interference. This asymmetric Raman mode was fitted with the Briet Wigner Fano (BWF) line shape [1]. The asymmetry parameter, q was calculated and the variation of this q with the temperature was found to follow a bell-shaped curve. Similar results have been reported by Banerjee et al in the case of SrTiO3 and $Ca_xSr_{1-x}TiO_3$ [2]. The anharmonic constants for the sample were calculated in the given temperature range up to 440 K. The temperature dependency of the phonon frequency revealed a 3-5 times greater magnitude of explicit anharmonicity as compared to that of implicit anharmonicity, with the dominance of the three-phonon process as determined by the linewidth variation of the $F_g$+$A_g$ mode with varying temperature.

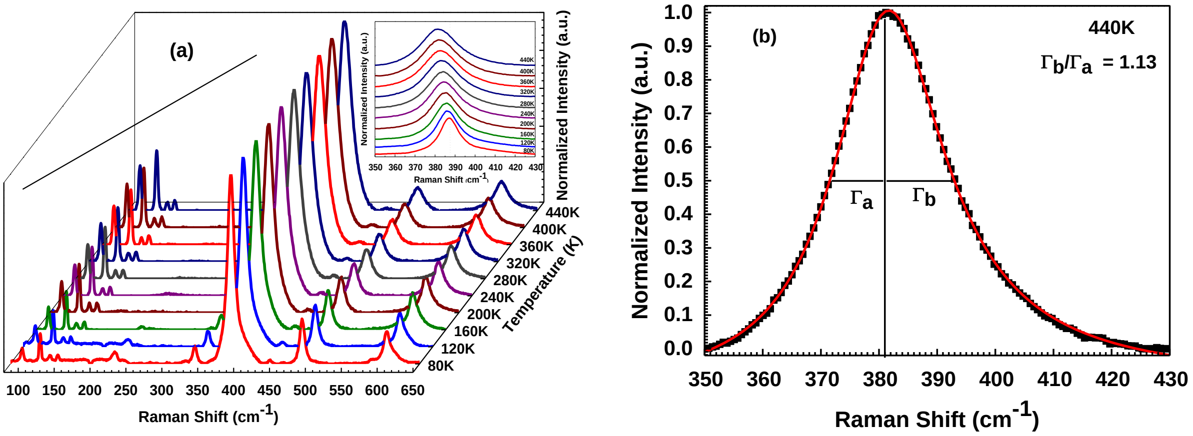

Figure 1: (a) Variation of the phonon modes with the varying sample temperature. The inset shows red shift in the $F_g$+$A_g$ phonon mode with the temperature. (b) The fitting of asymmetric $F_g$+$A_g$ mode using BWF line shape at 440K. The values of $\Gamma_a$ and $\Gamma_b$ are 13.21 and 11.69 $cm^{-1}$ respectively.

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# P2. Assessment of adsorption in nano composites of multiwalled carbon nanotubes and polyvinyl chloride, polyethylene, foam polystyrene

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T. M. Pinchuk-Rugal, O. L. Pavlenko, S. A. Shevchuk, T. O. Busko, P. P. Ilyin

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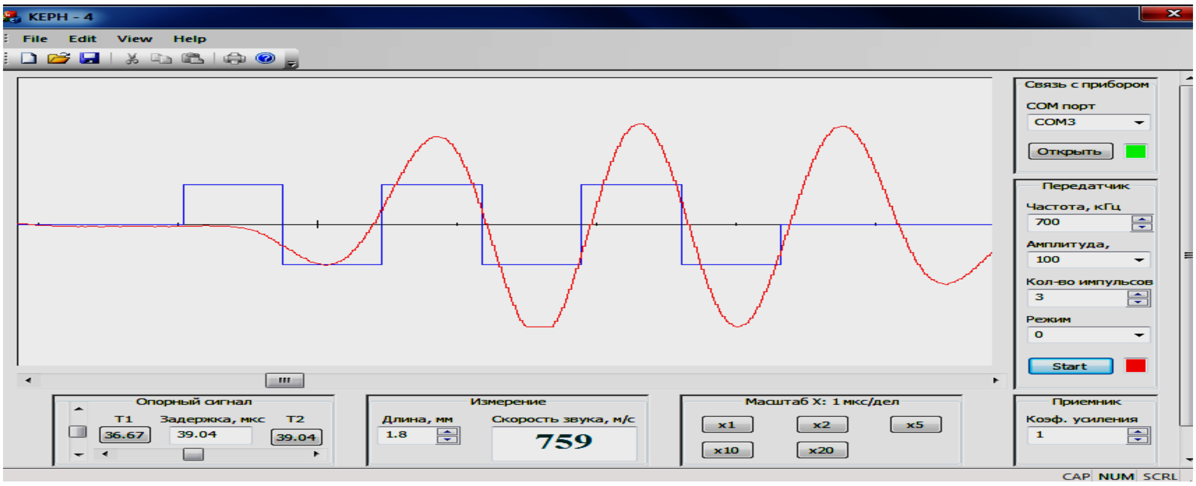
With the purpose of determination of temperature position of relaxation of the shear modulus $\Delta G/G_o$ simultaneously with the internal friction measuring temperature dependence of $G = \rho V_{\perp}^2$ [1] in figure 1 was measured.



Связь с прибором
COM порт: COM3
Передатчик
Частота, кГц: 700
Амплитуда,: 100
Кол-во импульсов: 3
Режим: 0
Приемник
Коэф. усиления: 1
Опорный сигнал
T1: 36.67
Задержка, мкс: 39.04
T2: 39.04
Измерение
Длина, мм: 1.8
Скорость звука, м/с: 759
Масштаб X: 1 мкс/дел

***Figure 1.*** *The data plot illustration of the quasitransverse elastic waves velocity* $V_{\perp} = 759$ *m/s in nano composite of low-density high pressure polyethylene* $(C_2H_4)n$ *+ 3% MWCNT + 0,5% dye DBSQ by impulse-phase ultrasonic method at frequency* $f_{\perp} = 0,7$ *MHz*

## Conclusions

1. The annealing of the structure defects in nano composites bends out of shape the type of internal friction temperature spectrum $Q^{-1}(T)$.

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# P3. Morphology and composition of nanoinclusions in $Fe_{0.25}Ni_{0.25}TiSe_2$

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The current work is aimed to study the interaction between $Fe_{0.25}TiSe_2$ and $Ni_{0.25}TiSe_2$ during the $Fe_xNi_yTiSe_2$ single crystal grows using the gas transport reaction method.

Single crystals of $Fe_{0.25}Ni_{0.25}TiSe_2$ were grown from a mixture of mono-intercalated powders of $Fe_{0.25}TiSe_2$ and $Ni_{0.25}TiSe_2$ using gas transport reactions method with iodine as a carrier gas.

During the study, it was found that hexagonal inclusions $(Ni,Fe)_4Se_5$, coherently related with this crystal, are formed on the surface of the main crystal.

However, along with hexagonal inclusions $(Fe,Ni)_4Se_5$, rodlike formations (whiskers) are also observed lying on the surface of the main crystal. The shape of these crystals is similar to that of $Ti_3Se_4$ crystals, which have a monoclinic structure. The formation of whiskers, presumably $Ti_3Se_4$, is possible when the free energies of $Ti_3Se_4$ and $(Fe,Ni)_4Se_5$ coincide at the crystal growth temperature.

Scanning photoelectron microscopy data show that the crystal surface in contrast to nickel and selenium looks almost the same, while in contrast to titanium it is inverted. This indicates the formation of individual NiSe fragments on the surface of the matrix substrate. Nano-ARPES of inclusions $(Fe,Ni)_4Se_5$ showed that the spectrum of electrons in inclusions is determined by the crystal field of the crystal-substrate, although the concentration of electrons does not coincide with the concentration in the substrate.

Thus, we can conclude that the formation of $(Fe,Ni)_4Se_5$ crystals is associated with the capture of selenium and, consequently, the depletion of the starting material with selenium, which causes the formation of $Ti_3Se_4$ whiskers.

# P4. Temperature-dependent Raman study and Magnetic measurement of the Rare Earth Manganite synthesized by solid-state reaction method

**Ankit Bhoriya**[1,2,*], Neha Bura[1,2], Deepa Yadav [1,2], Jasveer Singh [1], H.K. Singh[2,3],
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We report the correlation between the magnetic, vibrational, and structural properties of rare earth manganite, $Nd_xSr_{1-x}MnO_3$. These rare-earth perovskites exhibit multiple electronic orderings such as charge ordering, magnetic ordering, and orbital ordering.[1] Sr doped $NdMnO_3$ shows great diversity in magneto-electrical phases as a function of the dopant. For the present study, $Nd_{0.4}Sr_{0.6}MnO_3$ and $Nd_{0.5}Sr_{0.5}MnO_3$ were synthesized by the solid-state reaction method. X-ray diffraction and X-ray photoelectron spectroscopy were employed for the structural phase and compositional analysis, respectively. Raman spectroscopy were used for electronic characterization. $Nd_{0.4}Sr_{0.6}MnO_3$ and $Nd_{0.5}Sr_{0.5}MnO_3$ were found to have the orthorhombic phase (*Pbnm*) and possess similar crystallite size ≈ 81 nm and ≈ 78 nm, respectively. The existence of the desired ratio of trivalent and tetravalent Mn was confirmed from the XPS measurements. The magnetization studies unraveled three transitions corresponding to spin-glass (SG), charge ordering (CO), and ferromagnetic (FM) ordering in the temperature range from 20 to 300 K, as shown in figure 1(a). [2]. Further, the temperature-dependent Raman studies in the range 80-440 K were carried out as shown in figure 1(b), to study the temperature-dependent phonon behaviour, which revealed a direct correlation between the temperature-dependent Raman data and the CO and FM transitions. Our results show a distinct correlation between the magnetic and charge ordering and the electronic vibrations.

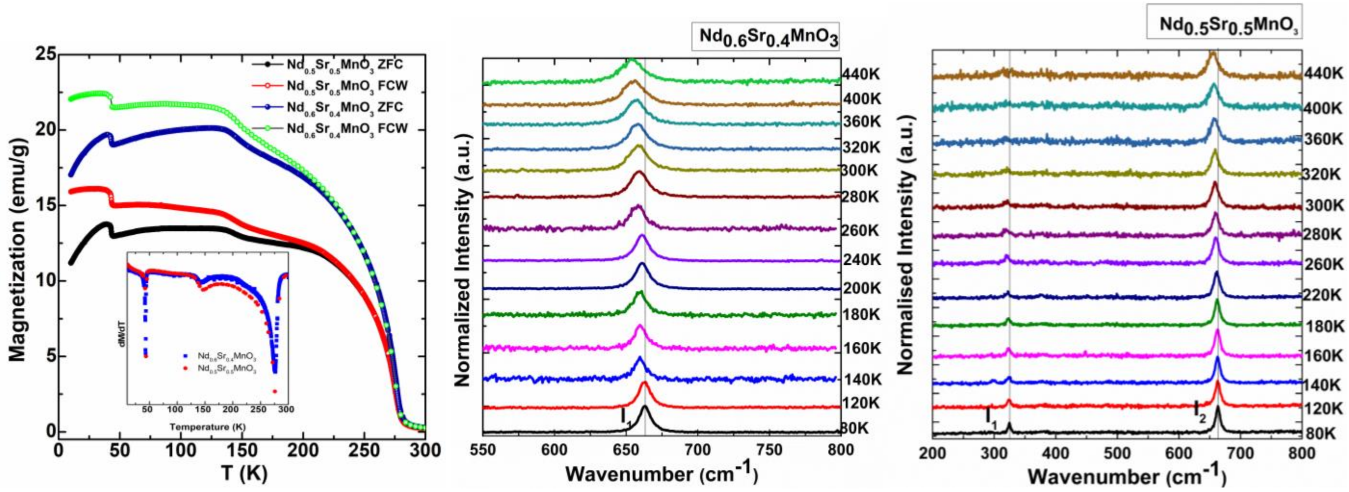

Figure 1(a): Variation of Magnetization with temperature for $Nd_{0.4}Sr_{0.6}MnO_3$ and $Nd_{0.5}Sr_{0.5}MnO_3$ with derivative plot in the inset (b) Raman profile at various temperatures.

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# P5. Modification in the physical properties of Gamma irradiated <011> Oriented TGS single crystals

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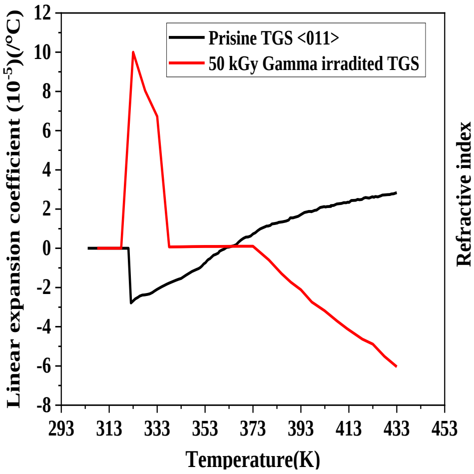
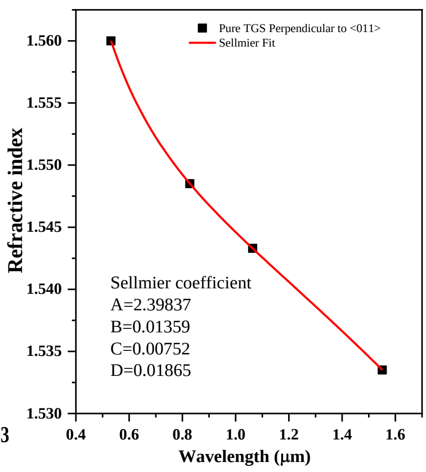
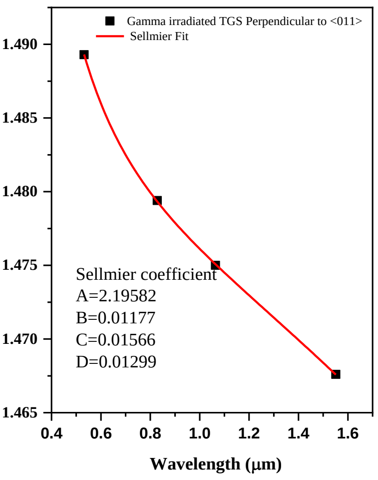
Transparent single crystals of ferroelectric Triglycine sulphate (TGS) has been successfully grown along <011> orientation for the first time from Sanakaranayan Ramasamy (SR) method. The grown crystal was subjected to gamma irradiation with a dosage of 50 kGy. Gamma induced changes in the crystal has been investigated using the tools like Low temperature Raman, “ac” conductivity and piezoelectric measurements. The change in thermos mechanical response and refractive index of the material were also studied. The overall obtained results have been discussed in detail.







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# P6. Synthesis and characterization of BiFeO$_3$ –Graphene and BiFeO$_3$ – MWCNT Nanocomposites

**C.Anandaraj**[1,*], R. Venkatapathy[1], V.C. Bharath Sabarish[1], P. Kalaivani[2], A. Durairajan[3], M.P. Graça[3], M.A. Valente[3], S. Gokul Raj[4], G. Ramesh Kumar [1*]

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Nanocomposites of MWCNT and Graphene with BiFeO$_3$ (BFO) have been synthesised from sol-gel technique. The composite nature of as prepared powder was characterized using powder XRD, FTIR and Raman analysis. UV-Vis-NIR absorption spectrum of BFO-Graphene indicates the change in energy band gap of BiFeO$_3$ due to graphene inclusion. However, MWCNT based BFO did not yield favourable results for determining its ‘$E_g$’ values. Dielectric and “ac” conductivity BFO-Graphene witnessed higher ‘$\varepsilon_r$’ values and it provides a fair due for its use in super capacitor applications. C-V measurements on these composites confirm the presence of increased pseudo capacitance of composites over the pristine BFO samples.

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[2] A.Datta, S.Chakraborty, S.Mukherjee, Int. J. Appl. Ceramic Technology, 1-11(2017) synthesis of carbon nanotube (CNT)-BiFeO$_3$ and CNT-Bi$_2$Fe$_4$O$_9$ nanocomposites and its enhances photocatalytic properties.

# P7. Modification of Structural, Optical and Morphological Characteristics of Bismuth Ferrite Thin Films using Swift Heavy Ion Irradiation (SHI)

**Venkatapathy Ramasamy**[1, *], Durairajan Arulmozhi[2],
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Polycrystalline Bismuth Ferrite [$BiFeO_3$-BFO] thin films with a thickness of 180 nm were deposited on indium tin oxide [ITO] coated glass substrates using pulsed laser deposition technique. The grown films were irradiated with an energy of 100 MeV $Ni^{7+}$ ions at various ion fluences viz., $1x10^{11}$, $1x10^{12}$ and $1x10^{13}$ ions/$cm^2$. Modification of structural, optical and morphological properties of the BFO thin films upon ion irradiation were analyzed using glancing incidence angle X-Ray Diffraction [GIXRD], UV-Vis NIR Spectroscopy, Photoluminescence, Raman Spectroscopy and Field Emission Scanning Electron Microscopy [FESEM]. GIXRD pattern confirmed the rhombohedral unit cell structure of BFO indexed with hexagonal phase, belonging to the space group R3c. FESEM results reveals that the pristine BFO films consists of agglomerated grains with diffused grain boundaries. Upon irradiation, the agglomeration of the grains considerably reduced and becomes sharper. The other interesting results would be discussed in the paper presentation.

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# P8. Photocatalytic degradation of synthetic microfibers

**Patrick Seleš**[1,2,*], Tina Radošević[1], Damjan Vengust[1], Mateja Podlogar [1,3]

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Research over the last few decades has shown that microplastics have reached critical levels in the environment [1]. They diversely enter the ecosystem and with them, they bring toxic chemicals such as dyes. The most frequent source of microplastic fibers are households, especially their waste water, from where the most problematic pollutants enter natural water system and even ground water. With this study we will present an attempt to degrade microplastic fibers released from washing machines, with the non toxic photocatalytic approach.

Fibers of the most common synthetic textile, polyamide (PA), polypropylene (PP) and polyethylene terephthalate (PET) were exposed to a photocatalytic process. They were dispersed in suspension of ZnO powder, which was prepared by hydrolysis method using zinc acetate, lithium hydroxide and absolute ethanol [2]. Synthesized nanopowder was characterized using X-ray diffraction analysis (XRD) and transmission electron microscopy (TEM). Photocatalytic experiments were performed in an incubator under visible light irradiation for 48 hours. Fibers were dried and the degradation rate was analyzed. The morphology of the fiber's surface was compared before and after photocatalytic experiments using scanning electron microscope (SEM) and Raman spectroscopy. After photodegradation SEM analysis reveals that the surfaces of the fibers were modified. Further Raman analyses confirmed those changes which enabled a correlation between those two methods. For future work we expect that the kinetics of the degradation process will be increased with proper doping of nano ZnO.

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# P9. An Efficient Crystal-layer Arrangement of Spinel $NiFe_2O_4$/reduced graphene oxide for Enhancing Oxygen Evolution Reaction Performance

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The global energy demand has been swelling rapidly and the depletion of traditional energy resources, as well as their severe impact on global warming, air pollution, and high carbon dioxide emissions, ring a bell for mankind's civilization to generate clean and sustainable energy sources. In recent years, hydrogen has attracted significant attention as a clean, efficient, and durable energy carrier source [1]. Toward this end, one of the most attractive and competitive technology to generate hydrogen is the electrocatalytic water-splitting. As well known, electrocatalytic water splitting involves two independent half-reactions, hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) [2]. In comparison to the HER, OER is commonly considered as a major bottleneck to achieving highly efficient water-splitting. To date, advanced electrocatalysts for the OER are ruthenium-iridium based compounds [1-2]. However, the intrinsic characteristics such as extreme scarcity, stability, high cost of these catalysts, greatly hindered their large-scale applications.

The slant of blending graphene with transition metal oxides and their derivatives is considered one of the highly appealing paths for the energy conversion process. In this perspective, specifically, our investigations focused on the controllable growth of spinel $NiFe_2O_4$ nanostructures on layered graphene oxide by a facile solvothermal method [3]. The effect of different Ni wt.% (0%, 2%, 4%, and 6%) on the morphology of hybrid as well as on electrochemical performance was studied. The optimized $NiFe_2O_4$/rGO hybrids exhibit much enhanced OER performance and deliver a current density of 10 $mA/cm^2$ at an overpotential of only 302 mV with a small Tafel slope of 63 mV/dec. These results imply that it is possible to fabricate even more advanced, highly stable, robust, non-noble metal-based OER electrocatalysts by optimizing the compositional and structural assets.

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# P10. Cell adhesion to Ti and Mg based materials

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The aim of the study was to identify the ability of materials based on titanium and magnesium to adhere cells for biomedical applications.

The six groups of samples were investigated: $TiAl_6V_4$; $TiAl_6V_4$ CaP-coated; MgCa; MgCa CaP-coated; MgCa Ga-doped CaP-coated; and MgCa Zn-doped CaP-coated. The Saccharomyces cerevisiae yeast cell immobilization was provided during the experiments. The UV irradiation was used for the changing of the surface electrical charge value. The method of photoelectron emission spectroscopy was used for measurements of the surface electric charge value.

| Type of material | The area covered with immobilized cells of the surface of unirradiated samples, % | The area covered with immobilized cells of the surface of irradiated for 1-hour samples, % |
|---|---|---|
| $TiAl_6V_4$ | 5.24 | 6.83 |
| $TiAl_6V_4$ coated with CaP | 6.53 | 3.20 |
| MgCa | 13.11 | 29.15 |
| MgCa coated with CaP | 7.18 | 9.62 |
| MgCa coated with CaP+Ga | 4.45 | 3.23 |
| MgCa coated with CaP+Zn | 6.96 | 3.09 |

Samples MgCa irradiated with UV radiation for 1 hour have the largest area covered with cells. Therefore, this material needs further in-depth study for biomedical applications.

The study was carried out as part of the COFUND-ERANET-RUS-PLUS-68 / 08/01/2018 project.

# P11. Synthesis and characterization of ZnO nanoparticles by wet chemical co-precipitation

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Zinc oxide (ZnO) has a growing scientifical and technological importance due to its piezoelectric, semiconducting, optical and dielectric properties. Moreover, ZnO possesses other distinguished characteristics, such as bio compatibility, non-toxicity and there exists a diversity in its external size and shape with simple structure. With reduction in size, novel electrical, mechanical, chemical and optical properties are introduced. Though no switchable polarization as well as no dielectric phase transition has ever been observed for un-doped ZnO crystal as a result of firmly formed tetrahedron by strong covalent bonding, evidence of ferroelectricity of undoped ZnO nanorods has been provided by polarization−electric field (P vs E) hysteresis loops. In the present work, Pure ZnO nanoparticles were synthesized using wet chemical precipitation. Powder X-ray diffraction, FT-IR and Raman spectra were used to confirm that prepared ZnO structures were single phase wurtzite type. FESEM technique were used to probe the morphology of as-synthesized ZnO sample. Energy Dispersive X-ray (EDX) spectroscopy was used to investigate the presence of the chemical compositions Zn and O in the ZnO nanostructure. The optical band gap of the ZnO nanoparticles estimated from UV-VIS absorption spectra is calculated. The photoluminescence properties of the unadulterated ZnO nanoparticles were studied. Interestingly, dielectric phase transition was found at 170 °C in pure ZnO nanoparticles. The results obtained were analysed and interpreted.

# Company presentations

# Techniques for characterization nanomaterials from MT Brandão

**João Cascalheira**

*MT Brandão Lda.*

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# Notes

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