VIRTUAL ABSTRACTS BOOK – INVITED PAPERS

I.1. Statistical Method for Studying Near and Far Electromagnetic Fields of a 2D Array of Spherical Particles

V. Loiko*, A. Miskevich, N. Loiko

Institute of Physics, National Academy of Sciences of Belarus, Minsk, Belarus
E-mail: loiko@ifanbel.bas-net.by

A semi-analytical method for studying the near and far electromagnetic fields of a two-dimensional array of nano- and microparticles is considered. It takes into account multiple scattering of waves within the quasi-crystalline approximation where a pair correlation function is used to describe the arrangement of particles in an ensemble [1,2]. Formulas are presented that describe (i) the characteristics of far fields, (ii) ensemble-averaged and (iii) the ensemble- and surface-averaged energy densities of electric and magnetic fields on the surface of particles in a light-absorbing medium. They allow finding parameters for getting the desirable far- and near-field characteristics in arrays with long-range and short-range order.

The results of calculations of the near-field enhancement at wavelengths of plasmon resonance of nanoparticles and lattice-induced resonance for the array of silver particles at normal incidence of a plane wave are presented. It is shown that the spectral positions of the maxima of the energy densities of the electric and magnetic fields on the particle surface coincide with the position of the maximum of the lattice-induced resonance absorption, which is observed for the far field. Spectral dependences of the surface-averaged energy densities of the electric and magnetic fields of highly ordered and partially ordered structures composed of nanoparticles have small differences, whereas for structures composed of particles the size of a wavelength, the differences are significant.

The results are of interest for designing 2D arrays when solving problems of optimizing scattering, absorption and emission of light. They can be useful for various applications, in particular for SERS, photocatalysis and photovoltaics.

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I.2. Apatitic Materials for Increasing the Quality of Life

Irina Fierascu[1,2], Radu Claudiu Fierascu[1,3]*, Anda Maria Baroi[1,2], Roxana Ioana Matei (Brazdis)[1,3],Toma Fistos[1,3], Irina Elena Chican[1], Ioana Silvia Hosu[1], Lia Mara Diţu[1,4]
[1] National Institute for Research & Development in Chemistry and Petrochemistry - ICECHIM Bucharest, Romania
[2] University of Agronomic Sciences and Veterinary Medicine of Bucharest, Romania
[3] National University of Science and Technology POLITEHNICA Bucharest, Romania
[4] University of Bucharest, Romania
email: fierascu.radu@icechim.ro

Apatitic materials, particularly hydroxyapatite (HA), have garnered significant attention in recent years for their applications in different important aspects of our daily life, including, but not limited to biomedicine, energy storage, or environmental sustainability.
The present work explores the potential of apatitic materials in two main areas: (1) water purification technologies [1-4], respectively (2) cultural heritage protection [5]. Our own results obtained in these areas, regarding tailoring the properties of apatites to enhance their performance, as well as some practical applications are briefly presented in improving human health and overall quality of life.
Overall, this body of work highlights the versatility of apatitic materials and their promising role in enhancing human well-being. The findings underscore the potential of these materials to not only solve critical technological challenges but also to contribute significantly to the quality of life on a global scale.

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*) Author for Correspondence: Radu Claudiu Fierascu, fierascu.radu@icechim.ro

I.3. Mixtures of Ionic Liquids – Structure, Organisation and Properties

Naomi Elstone[a], Paul D. Lane[b], Joshua Lai[a], Karina Shimizu[c], Bruno Demé[d], Matthew L. Costen[b], Kenneth G. McKendrick[b], Jose N. Canongia Lopes[c], John M. Slattery[a] and **Duncan W. Bruce**[*a]

[a] Department of Chemistry, University of York, Heslington, YORK YO10 5DD, UK;

[b] Institute of Chemical Sciences, School of Engineering and Physical Sciences, Heriot Watt University, Edinburgh EH14 4AS, UK;

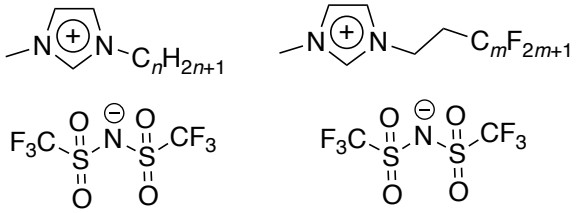
[c] Centro de Química Estrutural, Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049 001 Lisboa, Portugal;

[d] Institut Laue-Langevin, 38000 Grenoble, France.

Ionic liquids (ILs) are commonly, if inaccurately, defined as salts that are molten below 100 °C. Perhaps the greatest number are based on cations of *N*-alkylated heterocycles with a variety of different anions, such that the combination of the two engenders a low melting point. While they have a very wide range of actual and putative uses being attractive *inter alia* for their vanishingly low volatility and seemingly infinite tunability, preparing a unique IL for each application is an unsustainable approach.

However, by mixing ILs in varying proportions it is possible to prepare libraries of liquids simply and efficiently from a much smaller number of pure, component ILs, so tuning bulk and surface structures, and a range of other physical properties, facilitating the search for ILs suitable for a range of applications. A major challenge, however, is that the design rules linking liquid structure and properties to composition are not well understood in ILs.

We began by studying IL mixtures containing cations with different alkyl chain lengths and a common anion ($[C_nMIM][Tf_2N]$ – opposite) using techniques such as reactive-atom scattering/laser-induced fluorescence (RAS-LIF), small-angle X-ray (SAXS) and neutron (SANS) scattering, viscometry and surface tension, complemented by atomistic molecular dynamics simulations. The results showed that the physical properties, interface and nanostructure of the mixtures could be tuned as a function of both chain length and composition although interestingly, the majority of properties do not vary as a simple linear function of composition.



ILs used in this work.

More recently, we have turned our attentions to mixtures prepared from components where one bears a hydrocarbon chain and the other a fluorocarbon chain ($[C_nMIM]_{1-x}[C_{m+2}MIM\text{-}F_{2m+1}]_x[Tf_2N]$ – above). There are fundamental questions that arise from such a study deriving from what can be poor-to-non-existent miscibility between longer-chain hydrocarbons and fluorocarbons and then how they relate to surface and bulk structure. These are of interest in this work as one aim is the deployment of these IL mixtures as solvents for catalysis.

The presentation will discuss the structure and properties of the various mixtures, determined using the range of techniques indicated above, as a function of both the chemical nature of the components and their chain lengths, with an emphasis on both surface and bulk organisation. In addition, the role of electrostatic charge in the (im)miscibility of hydrocarbon/fluorocarbon mixtures will be explored.

Indicative References

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I.4. Optical applications of Liquid Crystals

P.L. Almeida[1*]

[1] ISEL - Polytechnic University of Lisbon, Mechanical Engineering Department
Rua Conselheiro Emídio Navarro, 1, 1959-007 Lisboa, Portugal
[*] Email: pedro.almeida@isel.pt

Since the identification of liquid crystalline (LC) materials in 1888, the optical properties of LC materials have attracted much interest. These fascinating materials are capable of reconciling the mechanical properties of flowing liquids with the optical properties of some solid crystals, being optically anisotropic. Interest in LC materials increased dramatically following their successful application in information displays in the 1960s. As a consequence of this increased interest on the part of industry, there was a large increase in research into LC materials intended for electro-optical applications, which allowed the development and exponential growth of much of the technology currently available.

This fundamental and applied research has focused not only on the application of liquid crystals in information displays, but also on other types of applications, based on the optical properties of liquid crystals and their ability to respond to external stimuli. In recent decades, liquid crystals have emerged as an important new class of materials capable of being used as chemical, electrical, mechanical and optical actuators and sensors, used to produce a wide variety of displays and other applications such as privacy windows and sensors due to anisotropic nature and adaptability [1].

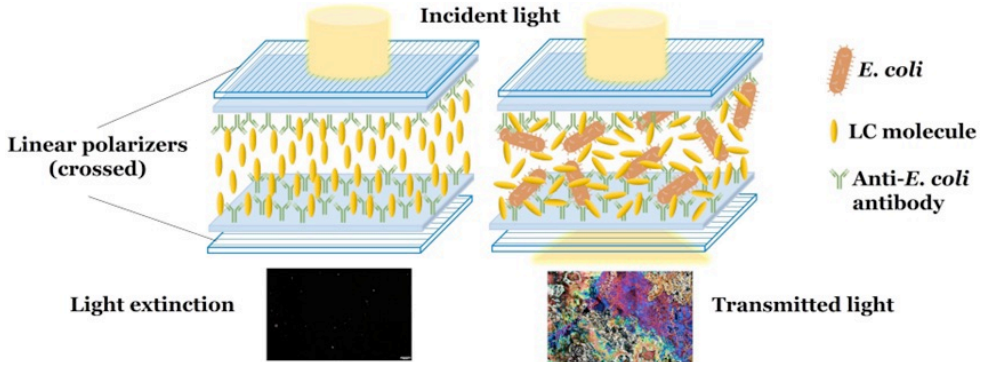

Figure 1. Working principle of a liquid crystal based *E.coli* bacteria sensor.

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I.5. Thiourea-Based Liquid Crystals: Metallomesogens, Gel Formation, and Luminescence

V. Cîrcu[1*], M. Iliş[1], D. Mănăilă-Maximean[2], M. Micutz[1]

[1] University of Bucharest, Bucharest, Romania
Email: viorel.circu@chimie.unibuc.ro
[2]University Politehnica of Bucharest, Bucharest, Romania

Thiourea represents an interesting scaffold used to create new compounds with a wide range of applications, including biology, catalysis, nanotechnology, materials science. While N-H groups can be exploited in designing various H-bonding receptors, the C=S thione group is instrumental in coordination chemistry as it can bind to various metals. When supported by the C=O carbonyl group of an adjacent acyl fragment, the coordination abilities of the N-acylthioureas are enormous, leading to very stable metal complexes. But, despite the exceptional coordination capacities, thiourea-based ligands are not commonly used to create liquid crystals (LCs) or metal complexes with liquid crystalline behavior (metallomesogens). This is due to the limitations imposed by the molecular structure of the resulting complexes. This work will present an investigation of the effect of using ligands containing sulfur (benzoylthiourea-type derivatives—BTU) on the mesomorphic behavior of palladium(II), platinum(II), and copper(I) complexes. The organic ligands may be either simple or functionalized with different types and numbers of mesogenic groups. These products exhibit a combination of liquid crystalline properties and metal-dependant highly intriguing emissive properties. While the BTU organic derivatives can produce physical LC gels with E7, some palladium(II) complexes can display both gel and lyotropic phases in alcohol solvents. Various structural parameters can be adjusted to produce lamellar liquid crystal phases or columnar phases, which are assigned according to commonly used techniques: differential scanning calorimetry (DSC), polarized optical microscopy (POM), and X-ray diffraction (XRD).

*) Author for Correspondence: viore.circu@chimie.uibuc.ro

I.6. Use of Nanofluids in Flat Plate Collectors

C. Stanciu[1*], and D. Stanciu[1]

[1] National University of Science and Technology POLITEHNICA
Bucharest, Romania
Email: camelia.stanciu@upb.ro

Nowadays efforts are made to develop more efficient techniques for enhancing energy conversion and improving operation of such systems. In this context, a special attention is directed towards the use of nanofluids in all possible type of applications – solar collectors to convert solar radiation into thermal energy, refrigeration, heat pumps, air conditioning systems, etc. A base fluid is used in which a certain volume fraction of nanoparticles are mixed in order to improve thermal properties and thus the final desired result.

The proposed paper provides a simple mathematical modelling,, as well as numerical and graphical results for several days operation of a flat plate collector in which a nanofluid is used. Sensitivity studies with respect to volume fraction of different nanoparticles are included.

*) Author for Correspondence

I.7. Short wave infrared sensitive SiGe nanocrystals with charge storage properties

M.L. Ciurea[1,4,*], M.T.Sultan[2,3] I. Stavarache[1], C. Palade[1], A.M. Lepadatu[1], A.Slav[1], I. Dascalescu[1], O. Cojocaru[1], V.S. Teodorescu1, H.G. Svavarsson[2] T. Stoica[1],

[1]National Institute of Materials Physics, 077125 Magurele, Romania
Email: ciurea@infim.ro
[2]Reykjavik University, Menntavegur 1, 102 Reykjavik, Iceland
Email: muhamads@ru.is
[3]Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland
[4]Academy of Romanian Scientists, 3 Ilfov Str., 050094 Bucharest, Romania

$Si_{1-x}Ge_x$ nanocrystals (NCs) in oxide matrices have been extensively studied due to their promising and attractive properties resulting from bandgap tuning by varying SiGe stoichiometry, NC size and by strain engineering. These properties are very promising for different device applications as optical sensors, light emitting diodes, solar cells and nonvolatile memories (NVMs). For enhancing the device performances, commonly used structures are multilayers (MLs) consisting in a stack of pairs of SiGe/oxide layers. It is shown that MLs enhance the optical properties by NCs surface passivation, and by controlling NCs size and interface with oxide matrix, these being beneficial for optical sensors. In MLs NVMs multiple tunneling processes taking place in ML floating gate (FG) ensure a better control of variable programing and retention behavior device.

In this paper are presented ML structures (preparation & characterization) of SiO_2 *cap /[SiGe with d thickness/*$SiO_2]_N$ where N is repetitions number [1]. They were studied by focusing on both VIS-SWIR sensitivity for optical sensors applications, and on charge storage properties for NVMs.

For using as photosensors, SiGe layer thickness (*d*) and repetitions number (*N*) were varied by keeping the same value for total thickness of all SiGe layers. As resulted, by increasing *N*, the spectral photocurrent intensity grows due to increasing tensile strain. By increasing Ge concentration and reducing NC size, a red-shift in peak position by quantum confinement in SiGe NCs, was observed.

ML NVM is a MOS capacitor as top *contact /* HfO_2 *-gate oxide / (SiGe NCs or SiGe NCs in* HfO_2 *as FG /* HfO_2 *-tunel)*$_n$ *n =1,2..5* is the number of floating gates FG-SiGe NCs and the number of pairs FG NC SiGe / HfO_2 -tunel, respectively. ML NVMs with highest performances are of type 5 FG NC SiGe having memory window of ΔV_{fb} = 6.68 V, 11% capacity decrease after first 10^4 s in the retention curve C-t and 15.3% after 10 years.

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*) Author for Correspondence: ML Ciurea, email: ciurea@infim.ro

I.8. ON ARCHITECTURAL INTEGRATION of COLOURED BUILDING SYSTEMS based on PHOTOVOLTAICS (BIPV).

Laurentiu Fara[1,2]*, Ana Maria Badea[1], Dan Crăciunescu[1], Alexandru Diaconu[1], Silvian Fara[1]

[1]*Department of Physics, Faculty of Applied Sciences, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania*
Email: lfara@renerg.pub.ro
[2]*Academy of Romanian Scientists, 050091 Bucharest, Romania*

Coloured Building Integrated Photovoltaic (BIPV) Systems represent a technically and economically highly efficient technology for use of coloured solar cells within building envelopes to harvest solar energy and produce electrical energy. There are two novelties of this invited lecture.

The first novelty consisted in the discussion of two identified advanced types of solar cells, namely: (1) DSSC (dye sensitized solar cells), and (2) STHSC (Si-based tandem heterojunction metal-oxide solar cells) selected for coloured BIPV systems. The correlation between the energetic and aesthetic aspects of these two types of solar cells was discussed based on numerical modeling [1].

The second novelty was represented by a complex approach on reliability analyze that would investigate the studied coloured BIPV systems using their degradation parameters and long-term stability improvement through the encapsulation method.

The conclusions of this invited article would highlight the architectural integration of coloured BIPV systems based on two advanced SCs, namely STHSCs (see Figure 1) and DSSCs that can be considered as an innovative solution.

Figure 1. The BIPV systems based on STHSC with reflective layers and a 4 step-laser scribing for several colors

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*) Author for Correspondence: Laurentiu Fara

I.9. Research on Comparison and Simulations of Various Thin-Film Solar Cell Types

A. Drăgulinescu[1*]

[1] Electronic Technology and Reliability Department, 'Politehnica' Univ. of Bucharest, 1-3 Iuliu Maniu Blvd., Bucharest, Romania, RO-060032
Email: dragulinescu@yahoo.com

This paper has the goal to present our research on some of the main types of thin-film solar cells. Due to their very promising properties and performance, we designed and simulated nine different structures of perovskite solar cells (seven of them having as active layer only perovskite, whereas the eighth contained both perovskite and silicon, and the ninth a combination of perovskite with CIGS). For comparison purposes, we also analyzed two structures of organic solar cells and three other solar cell types (one a-Si, one CIGS and one GaInP/InGaAs/Ge) structures. We compared the best performance of the different types of cells that we simulated, together with the results for other recent structures that were proposed in literature.

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*) Author for Correspondence

I.10. Infrared spectroscopy supports the molecular dynamics obtained for oxide nanopowders by dielectric spectroscopy

L. Frunza[1*], I. Zgura[1], C.P. Ganea[1], and D Manaila-Maximean[2]

[1] National Institute of Materials Physics, 405A Atomistilor Street, 077125 Magurele, Romania
Email: lfrunza@infim.ro, irina.zgura@infim.ro
[2] University Politehnica of Bucharest, Department of Physics, 313 Spl. Independentei, 060042 Bucharest; Academy of Romanian Scientists, 3 Ilfov str., 050044 Bucharest, Romania
Email: doina.manaila@upb.ro

This contribution makes an overview of our works concerning characterisation of oxide nanopowders which are nowaday materials widely used in industrial applicaions and in fundamental research as well.

We have accordingly studied aerosils, molecular sieves, tin oxide, mixed oxides, some of them having semiconductor properties. These materials were used as pristine substances or as composites when have been mixed with different organics (such as liquid crystals). In the latter case we can speak about confinement in one, two or three dimensions, confinement which introduce special interactions.
Investigatioms by dielectric spectroscopy of molecules into a constrained geometry as function of frequency and of temperature have shown a relaxation process which is slower than those belonging to the bulk molecules. In addition, it was observed that the temperature dependence of the relaxation time does not change at the phase transition temperatures corresponding to the bulk material See for example one of the latest papers [1].
On the other hand it is known that the interaction of IR radiation has been widely investigated for inorganic and organic materials. Thus the specific molecular vibrations of the sample constituents can be observed, providing qualitative and quantitative information. In this work Fourier-transform infrared methods are employed to measure spectra in the condensed phase: we refer mostly to the mid infrared region (4000–400 cm^{-1}). This region of the spectrum is particularly sensitive to the detailed structural and environmental properties of complex hydrogen-bonded species as it was found in our case.
So, we have employed novel complementary measurements and theoretical techniques to explore the low frequency intramolecular dynamics of model molecules with constrained structures.
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*) Author for Correspondence:

I.11. Electrochemical Engineering of Semiconductor Porous Templates and Nanowire Arrays: Control of the Shape and Growth Direction

Eduard V. Monaico[1]

[1]National Center for Materials Study and Testing, Technical University of Moldova, Bd. Stefan cel Mare 168, Chisinau, Republic of Moldova
Email: eduard.monaico@cnstm.utm.md

Nowadays electrochemical methods present a viable alternative, offering a more accessible and flexible approach to design and fabricate semiconductor nanostructures. This work will cover the development of semiconductor porous structures through electrochemical etching of semiconductor substrates [1]. It will highlight how the combination of the photolithography and electrochemical etching, using photoresist masks and subsequent anodization, enables the possibilities to control the pore growth direction [2,3]. This approach facilitates the creation of porous domains with different shapes, offering enhanced control over material properties and broader application possibilities.
It will be discussed the transition from porous structures to networks of semiconductor nanowires obtained through electrochemical etching, possessing higher quality compared to those grown by other techniques [4]. Moreover, the shape as well as the growth direction of the nanowires can be controlled by selecting the crystallographic orientation of the semiconductor substrate used in the anodization process [5]. This control over structural formation enhances the potential for developing hybrid metal-semiconductor structures with tailored properties.

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VIRTUAL ABSTRACTS BOOK – ORAL COMMUNICATIONS

O.1. Synthesis and characterization of acrylic polymers

Ghizlene Fatima Zohra HAKEM[1*], Christelle DELAITE[2], Anne Sophie SCHULLER[2], Amina BOURICHE[1], Lamia BEDJAOUI-ALACHAHER[1].
[1]Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou Bekr Belkaid, 13000, Tlemcen, Algeria
[2]Laboratory of Photochemistry and Macromolecular Engineering (LPIM), National School of Chemistry – University of Haute Alsace - France
*E-mail: hakemghizlene3@gmail.com

The synthesis and characterization of acrylic polymers obtain by bulk polymerization, without the addition of solvents, aim to minimize environmental pollution. These polymers are developed under UV radiation using three types of acrylic monomers: one with a soft segment, another with a hard segment, and the third with a functional segment.

The characterization of the synthesized polymers is conducted using advanced techniques. Fourier-transform infrared spectroscopy (FTIR) is used to confirm the chemical structure. The FTIR spectrum confirms the successful polymerization of the acrylate monomers by the disappearance of the characteristic C=C double bond.

Thermogravimetric analysis (TGA) was performed to identify the degradation temperature of polymers and the different steps in this process.
Finally, the contact angle of our polymers was measured by varying their compositions to determine their surface wettability[1].

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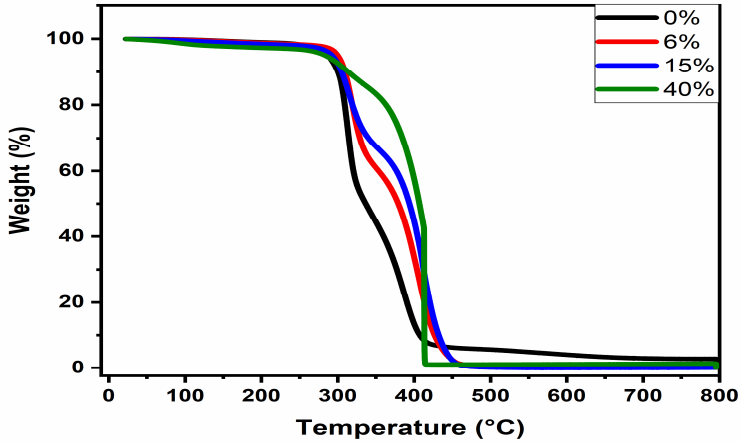

Figure 1 : Thermogravimetric analysis of polymers.

O.2. Viscoelastic and drug-release characteristics of some non-covalently crosslinked polymer hydrogels loaded with Doxycycline immersed in PBS environment

T. Staicu[1], M. Ilis[2], V. Circu[2], and M. Micutz[1*]

[1] Department of Analytical and Physical Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blvd, Bucharest 030018, Romania
Email: teos@gw-chimie.math.unibuc.ro; micutz@gw-chimie.math.unibuc.ro
[2] Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, University of Bucharest, 4-12 Regina Elisabeta Blvd, Bucharest 030018, Romania
Email: monica.ilis@chimie.unibuc.ro; viorel.circu@chimie.unibuc.ro

Polymer hydrogels as temporary depot for a wide variety of active therapeutic compounds have received growing attention during last decade in investigating them as drug-delivery and drug-release systems. This study deals with three different polymer hydrogels loaded with a broad-spectrum antibiotic (Doxycycline Hyclate), namely Pluronic F127 (a symmetric triblock copolymer: poly(ethylene oxide)-b-poly(propylene oxide)-b-poly(ethylene oxide)), PVA (poly(vinyl alcohol)) – based hydrogels (both of them physically crosslinked) and calcium alginate – based hydrogels (ionically crosslinked). Closely related to their viscoelastic characteristics revealed by oscillatory rheometry, Doxycycline release from these hydrogels into an aqueous PBS (phosphate-buffered saline) solution (pH 7.4) at 37^0C (mimicking both pH and ionic strength of extracellular fluids of mammalian and human body under physiological conditions) was assessed and rationally analyzed in terms of Peppas-type relationship (power law).

Acknowledgement
The study was supported by the grant of the Romanian Authority for Scientific Research, CNCS-UEFISCDI, project number PN-III-P2-2.1-BG-2016-0397.

* Corresponding author

O.3. Blue InGaN lasers under generation of picosecond pulses

V. Dobrovolschi[1*], S. Rusu[1], and V. Tronciu[1]

[1]Department of Physics, Technical University of Moldova, Republic of Moldova
Email: veronica.dobrovolschi@fiz.utm.md

We report in this paper the numerical results of theoretical investigations of generation of picosecond pulses by blue InGaN with saturable absorber (SA). Using the single mode rate equations, we study the influence of different geometrical and material parameters on the characteristics of output pulses. We discuss also the applications of pulses. Figure 1 shows an analytical model of investigated setup. The system consists of an InGaN active section and a SA added in longitudinal direction. The active layer is composed by three QWs, and the emitting wavelength is 405 nm. Two adimensional injected currents J_1 and J_2 are applied respectively to active section and to SA.

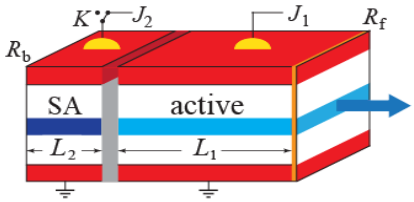

Fig.1.

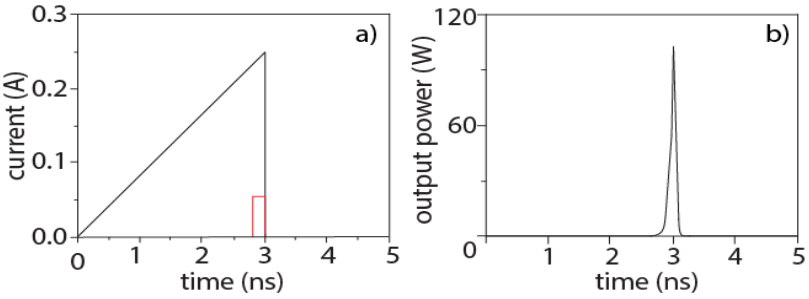

Fig. 2

To simulate the generation of pulses in setup shown in Fig. 1 we use the single mode model [1], which is given by the following rate equations for photon number S and injected carrier number n_1 in active region and n_2 in the SA

$$\frac{dn_1}{d\tau} = -(n_1 - n_{g1})S - \frac{n_1}{\tau_{s1}} + J_1, \quad \frac{dn_2}{d\tau} = -(n_2 - n_{g2})S - \frac{n_2}{\tau_{s2}} + J_2,$$

$$\frac{dS}{d\tau} = (n_1 - n_{g1} + n_2 - n_{g2})S - B_C(n_1 - n_{g1})S - G_{th}S + M(n_1 + n_2).$$

The mechanism resulting in pulse generation is Q-switching. Thus, the injected current J_1 is increased from 0 to 0.25 A (black line in Fig. 2a). At 3 ns the current is switched „off". The rectangular shape of pulse current J_2 into SA is given by red line in Fig 2a). A typical temporal behaviour of optical output power at the front facet of device is shown in Fig. 2b). We consider lasers emitting at different wavelengths between 350 and 450 nm. The results presented in this paper show the following features: we found that an increase of wavelength lead to decrease in pulse energy and maximum of the pulse. The length of the SA influences drastically features of output pulses, by decreasing its energy and peak, when SA length increases. We also found that for a very small front facet reflectivity the pulses are not generated. An increase of front facet reflectivity lead to a peak in the dependences of energy, and maximum of output pulse.

[1] V.Z. Tronciu et al Optics Communications 235 (2004) 409–414

*) Author for Correspondence: doctorand Veronica.Dobrovolschi@fiz.utm.md

O.4. Modeling and Numerical Simulation of the Evolution of Road Infrastructure Degradation

D. Craciunescu[1*], C. Racanel[1]

[1] Technical University of Civil Engineering Bucharest, Romania

Email: dan.craciunescu@phd.utcb.ro; carmen.racanel@utcb.ro

This study focuses on the modeling and simulation of road infrastructure, examining the associated types of degradation and their interdependencies. It further investigates how various degradation types impact the road structure. To develop effective road maintenance strategies, we employed a suite of mathematical prediction models, utilizing experimental data collected with the advanced Laser Crack Measurement System (LCMS) equipment. By integrating this data into predictive models grounded in mathematical distributions, we generated a series of forecasts that underscore the maintenance, and rehabilitation needs across different scenarios.

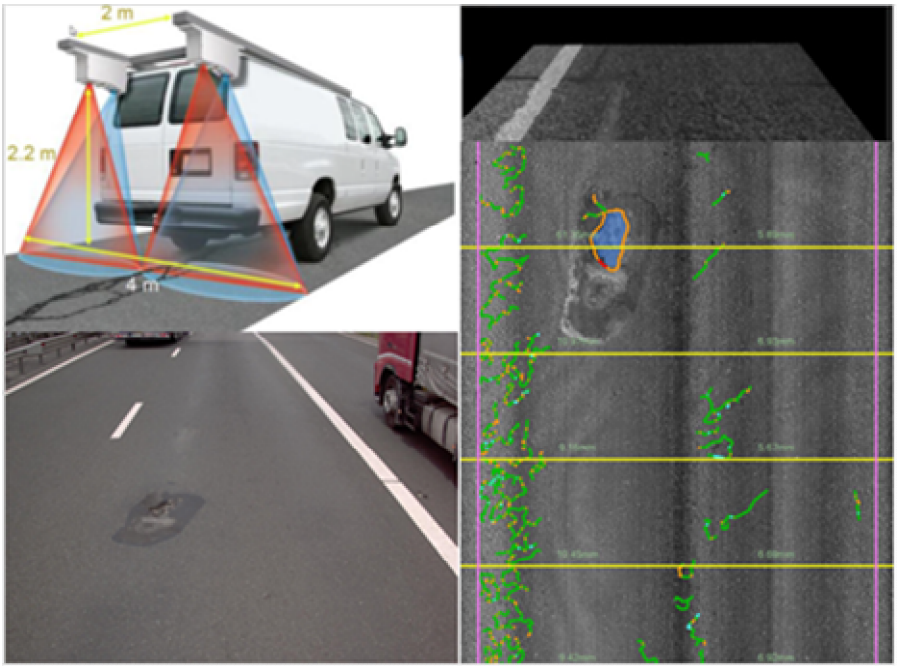

Figure 1. Advanced LCMS System. Identification of the road surface distress

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*) Author for Correspondence: dan.craciunescu@phd.utcb.ro

O.5. Two layer magnetic plasmonic nanoparticles synthesis and characterization

H. Ardeleanu[1*], D. Creanga[1], and D. Pricop[1]

[1]University Alexandru Ioan Cuza, Iasi, Romania

Email:

ardeleanu_helmina@yahoo.com

In this study, we aimed to synthesize biocompatible magnetite nanoparticles (MNPs) by tailored chemical co-precipitation method [1], followed by their stabilization in aqueous suspension with glucose and gold coating [2]. We analyzed and characterized the nanocomposites microstructurally and magnetically by different techniques: electron transmission microscopy (TEM), X-ray diffractometry (XRD) and vibrating sample magnetometry (VSM).

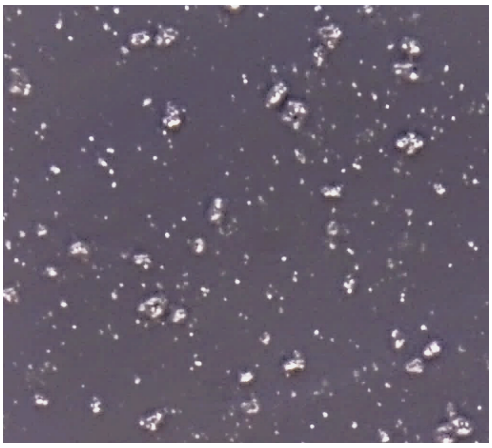

Figure 1. Plasmonic images of two layer magnetic plasmonic nanoparticles

Also, the properties given by the localized surface plasmon resonance phenomenon were revealed by UV-VIS spectrophotometry and dark-field optical microscopy (Figure 1). The nanotoxicity study demonstrated the influence of biocompatible magnetite nanocomposites on young watermelon seedlings.

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*)AuthorforCorrespondence: Helmina Ardeleanu

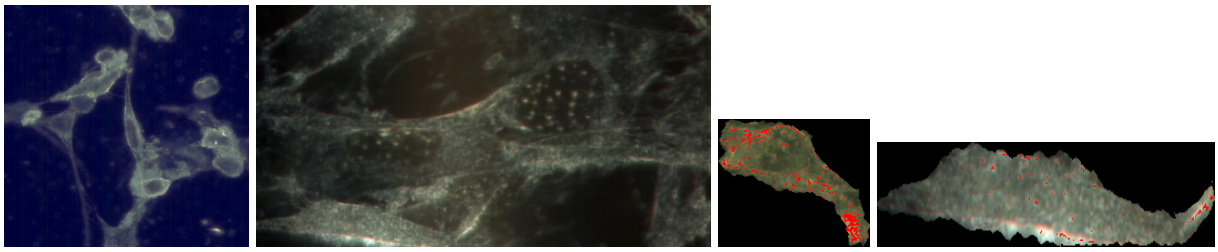
O.6. Hyperspectral images for digital detection of codelivery nanoparticles incorporated in malignant cells

Ionela N. Irimescu[1], Nicolae Tarba[2], Roxana C. Popescu[3], Simona Ionita[4], Mihaela Deaconu[5], Cosmin C. Mustaciosu[6], Eugen Scarlat[7], AnaMaria Pleava[5], Daniela Berger[8], Diana I. Savu[6], Mona Mihailescu[7,9]

[1]*Applied Sci. Doct Sch, Nat Univ Politehnica Bucharest, Medist Imaging & Point of Care*
[2]*Computer Sciences Doctoral School, Physics Department, Politehnica Bucharest, Romania*
[3]*Depart of Bioeng and Biotech, Faculty of Med Eng, Politehnica, Bucharest Romania*
[4]*Chemical Engineering Doctoral School, Nat. Univ of Sci and Tech Politehnica, Bucharest*
[5]*CAMPUS Research Institute, Nat. Univ of Sci and Tech Politehnica, Bucharest Romania*
[6]*Horia Hulubei" National Institute for Research and Development in Physics and Nuclear Engineering, Department of Life and Environmental Sciences, Magurele, Romania*
[7]*Physics Department, Nat. Univ of Sci and Tech Politehnica, Bucharest, Romania*
[8]*Dep of Inorganic Chem, Physical Chemistry & Electrochem, Politehnica Bucharest, .Romania*
[9]*Fundam Sci Appl in Eng Res Cent., Nat. Univ. of Sci. and Tech. Politehnica Bucharest*
ionela.irimescu@stud.fsa.upb.ro

Hyperspectral images HSI contain in each pixel spectral information (400-600nm) linked with the chemical composition of the investigated samples and are used as input data to our developed digital tool which count the incorporation percentage of nanoparticles NPs in cultured cells (breast cancer cells of human origin (BT474) and human dermal fibroblasts (BJ). Our NPs as codelivery system were obtained by functionalization of MCM-41 mesoporous silica carrier through an amidation reaction. Then, the carrier was loaded with resveratrol from an ethanolic solution, followed by their impregnation with doxorubicin aqueous solution.

HSI of investigated cells incubated with codelivery nanoparticles were recorded (Fig. 1, 2) and spectral fingerprint of NPs were saved in spectral library as spectral vectors with 468 values following a standard procedure in ENVI software. To find which pixel corresponds with the same spectral fingerprint, we compare the angles between spectral vectors and the ones under a threshold angle are colored in red. Our developed tool segments each cell and counts the red pixels inside its contour and its area (Fig. 1 c, d).



a) b) c) d)

Figure 1.

Acknowledgments The research was financed by contract 576PED/2022. HSI are due to Europ. Reg. Develop Fund through Competitiv. Operat Program 2014-2020, Priority axis 1, INOVABIOMED

O.7.Study of swelling behaviour of an acrylic hybride material

A. ZEHOUANI[1]*, L. BEDJAOUI-ALACHAHER[1]

[1]Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou

Bekr Belkaid, 13000, Tlemcen, Algeria

*E-mail : aymen_zehouani@yahoo.com

This study examines the swelling behavior of a hybrid material made from isobornyl acrylate and various metal-organic frameworks (MOFs), which were synthesized via photopolymerization. The incorporation of MOFs aims to enhance material properties and expand applications in separation and adsorption [1-2]. We evaluated the swelling kinetics and equilibrium swelling ratios, highlighting the influence of MOF type and loading, as illustrated in **Figure 1**. Results indicate that swelling behavior is significantly affected by solvent type, with toluene generally inducing greater swelling than methanol due to its lower polarity and higher solubility parameter. Furthermore, different MOFs alter the polymer's affinity for each solvent, demonstrating the importance of MOF structural characteristics and surface properties. These findings enhance the understanding of interactions between hybrid materials and solvents, facilitating the design of responsive materials for specific applications.

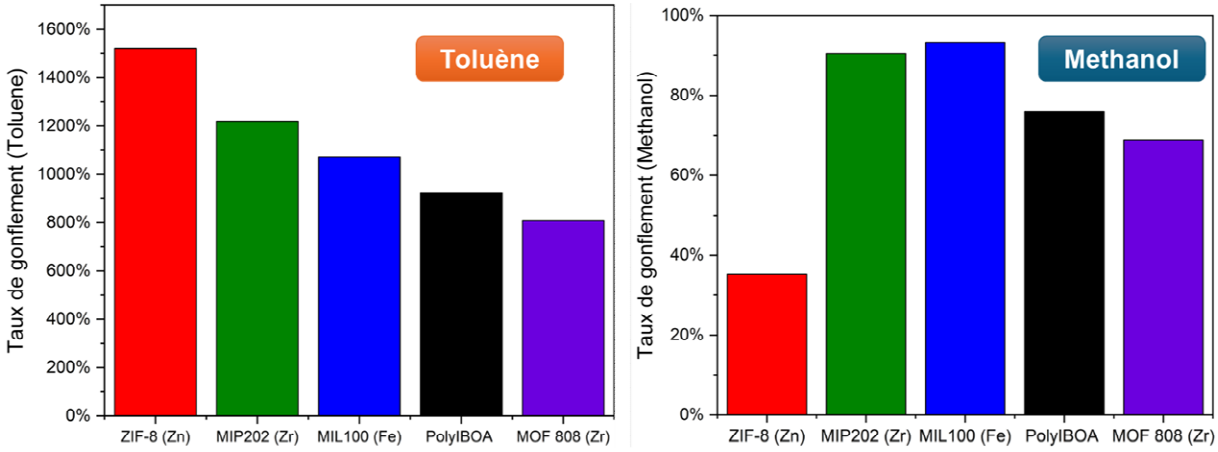


Figure 1. Swelling Ratios of Hybrid Materials in Toluene and Methanol

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O.8. Influence of Mg in Ni-based Takovite Catalysts and its Derivatives on Catalytic Activity over two Reactivity Cycles of Dry methane Reforming

Zoulikha Abdelsadek[1,2],
zoulisabrin@yahoo.fr, z.abdelsadek@univ-boumerdes.dz
Patrick J. Masset[3]
patrick.masset@technallium.com
[1]Institute of Electrical and Electronics Engineering, University of M'hamed-Bougara, Independence Avenue, 35000, Boumerdès, Algeria
[2]Laboratory of Sciences of Materials and Chemical Processes (LSMPC), USTHB, B.P. 32 El-Alia, 16111 Bab-Ezzouar, Algeria
[3] Technallium Engineering & Consulting, Fliederweg 6, D-92449 Steinberg am See, Germany

Abstract:

Nickel-based catalysts derived from the HT hydrotalcite structure (or layered double hydroxides: LDH) were labeled takovite NiAl-LDH and its derivative Mg@NiAl-LDH (Mg@takovite) where Ni was partially substituted by Mg. The solids were prepared by the co-precipitation method under alkaline conditions at pH = 11 [1, 2].

Calcined and non-calcined samples were characterized by various techniques such as X-ray diffraction (XRD), Fourier transform infrared (FTIR), Raman spectroscopy, Brunauer-Emmett-Teller (BET), Atomic Absorption Spectroscopy (AAS), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), thermogravimetry (TGA/DTAS) and programmed temperature reduction (TPR-H_2). As part of an industrial initiative, the catalysts were tested in the dry reforming reaction of methane at atmospheric pressure, using two cycles at different temperatures (cycle 1: 500°C to 700°C, cycle 2: 700°C to 500°C). The aim of this comparative study is to examine the reactivity of the catalysts in two different cycles, in particular for the second where catalytic activity was tested at low temperature, i.e. 500°C, the temperature required for industrial, economic and energy interest.

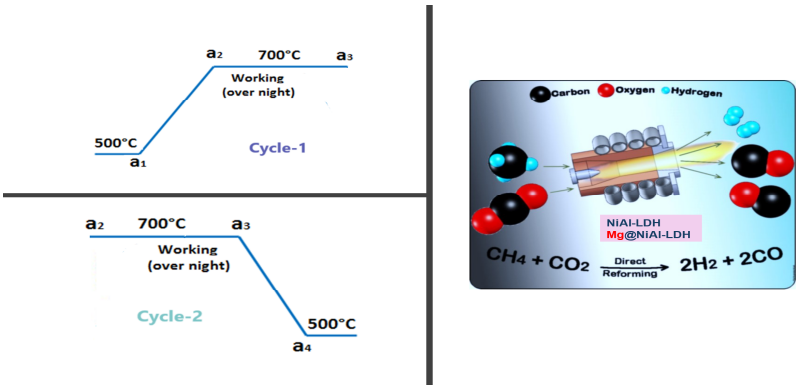

Figure 1: Methane dry reforming cycle in the presence of NiAl-LDH and Mg@NiAl-LDH

Under the same conditions, the Mg@NiAl-LDH catalyst showed high activity and stability with minimal carbon deposition, particularly for the second cycle 2 and at a low temperature of 500°C.

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[2] Z. Abdelsadek, S. Gonzales-Cortes, D. Halliche, O. Cherifi, P.J. Masset, ", IOP Conference Series Earth and Environmental Science 1167(1) (2023) 012031 - https://doi.org/10.1088/1755-1315/1167/1/012031

*) Author for Correspondence: Zoulikha ABDELSADEK

O.9. Luminescent heteroleptic dinuclear copper(I) complexes with phosphine and N-benzoyl thiourea ligands

Cosmin A. Tudor[1*], Monica V. Iliș[1] and Viorel Cîrcu[1]

[1] University of Bucharest, Faculty of Chemstry, Romania
Email: cosmin.tudor@s.unibuc.ro

This study explores a new series of dinuclear copper(I) complexes that use S-donor N-acyl thioureas alongside triphenylphosphine ligands. While traditional research has focused on expensive precious metals, copper has emerged as a promising alternative for luminescent materials due to its affordability, availability, and low toxicity. The luminescent properties of copper(I) complexes, particularly those exhibiting phosphorescence and thermally activated delayed fluorescence (TADF), suggest their potential for applications in organic light-emitting diodes (OLEDs).

In this research, a series of heteroleptic copper complexes were synthesized, resulting in light yellow to orange microcrystalline powders. Characterization techniques, including NMR spectroscopy, revealed that the N-acyl thiourea ligands bind to copper through sulfur, demonstrating strong interactions with the metal. X-ray diffraction analysis of one complex showed a distorted tetrahedral structure around the copper atom, with bond lengths and angles comparable to those reported in prior studies.[1]

Photophysical analysis indicated absorption patterns in the UV-Vis range that align with ligand-centered transitions, and the solid-state emission spectra revealed a range of emission wavelengths from 574 to 588 nm. Cyclic voltammetry tests showed distinct redox behavior among the complexes. Overall, this research not only enhances the understanding of copper(I) complexes using thiourea ligands but also supports their potential as efficient luminescent materials in next-generation electronic devices.

This work is a continuation of research started a few years ago and incorporates a greater diversity in the nature of the ligands, as well as the structure of the compounds themselves: from mononuclear in previous work to dinuclear complexes in the present study [1].

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*) Author for Correspondence

O.10. Study of Liquid Crystals based on Ionic Copper(I) Complexes with Benzoyl thiourea ligands using BF_4^- and PF_6^- as counterions.

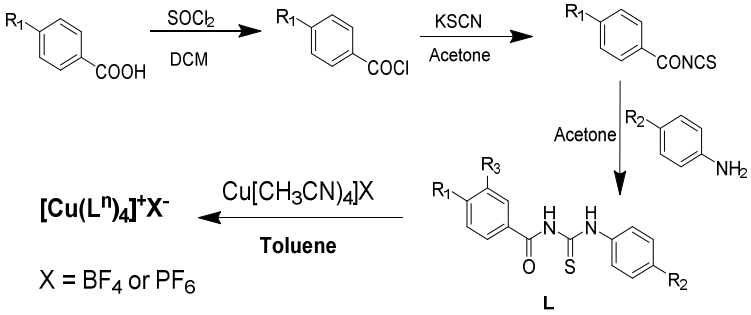
Muhammed ALKALI [1*], **Viorel CIRCU** [1], **and Monica ILIS** [1]

[1]*Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, University of Bucharest, Boulevard Regina Elisabeta Nr. 4-12, 030018 Bucharest, Romania*

**Corresponding author: Muhammed.alkali@s.unibuc.ro*

Introduction: Liquid crystals are generally referred to as substances that integrates the structure and properties of solid and liquid states, this intriguing combination gives liquid crystals the ability to induce certain properties that have gained useful applications in the displays of devices as well as in sensors, smart windows, optical switches, etc. [1]. There are liquid crystalline materials based on copper(I) complexes prepared with various ligands including ionic complexes with different counter ions [2] however in this ongoing study, we have made attempts to prepare liquid crystals of ionic complexes with Benzoyl thiourea (BTU) ligands having a tetrahedral core varying BF_4 and PF_6 as the counterions.

Synthetic strategy: All the compounds in this ongoing research were prepared based on the reaction scheme provided in figure **1**. The ligands were synthesized by slight modification in methodology previously employed in our laboratory [3]. Each BTU ligand prepared was reacted with the Cu(I) precursors $Cu[(CH_3CN)_4]BF_4$ and $Cu[(CH_3CN)_4]PF_4$ in a 4:1 ratio in Toluene by stirring for 2 hours at room temperature and products were precipitated out by treating the concentrated solution with heptane. The structure of the prepared compounds was characterized by NMR (^1H, ^{13}C and ^{31}P) while the liquid crystalline properties were investigated via a combination study of use of a polarizing optical microscope (POM) and Differential scanning calorimetry (DSC).



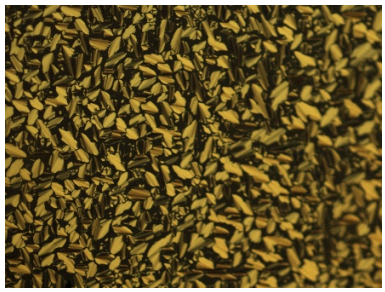


Figure 1: Reaction scheme for the prepared compounds and one example of PM picture showing the SmA texture.

References:

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VIRTUAL ABSTRACTS BOOK – POSTER SESSION PAPERS

1. Synthesis and characterization of functional materials

P.1. Synthesis of ternary compounds (Max-phases) in low-voltage pulsed discharge plasma

V. Mihailov[1], S. Ivashcu[1] N. Kazak[1*], E. Ovchinnikov[2] and A. Ianachevici[1]

[1]Institute of Applied Physics, Moldova State University, Moldova
Email: valentin.mihailov@gmail.com
[1]Institute of Applied Physics, Moldova State University, Moldova
Email: natalia.kazak@ifa.usm.md
[1]Institute of Applied Physics, Moldova State University, Moldova
Email: sergiu.ivascu@gmail.com
[1]Institute of Applied Physics, Moldova State University, Moldova
Email: ianakevici@yahoo.com
[2]Grodno State University named after Yanki Kupaly, Belarus
Email: ovchin_1967@mail.ru

Triple compounds, also known as Max-phases, are of particular scientific and practical interest due to their distinctive combination of properties that are characteristic of both metals and ceramics. Among the numerous Max-phases that have been synthesized to date, those based on titanium (Ti_2AlC, Ti_2AlN, Ti_3AlC_2, Ti_3SiC) are of particular interest with regard to the degree of their properties.
The metallurgical methods employed to obtain these materials are associated with the use of sophisticated technological equipment and high energy costs. In the present study, the synthesis of ternary compounds was conducted on components that were subjected to intensive wear, employing the electrospark alloying (ESA) method as the synthesis technique. This method is founded upon the phenomenon of polar transfer of material from the processing electrode (anode) to the part (cathode), which occurs when electric pulses are discharged between them. The ESA technology is straightforward, and the requisite equipment is modest in size, dependable, and transportable. The use of compact electrodes and powders of the materials that constitute ternary compounds: Ti, Al, graphite as a source of carbon and silicon carbide (SiC) were employed to obtain MAC-phase layers on metal surfaces. The powder mixtures were introduced into the plasma channel of the pulse discharge via a hollow titanium electrode or into the treatment zone on its side. The energy parameters of the ESA process were optimized, specifically the energy value of the electric pulses and the average operating current. The energy value at which quality coatings were obtained was found to be in the range of 0.9 to 3.0 J, while the average current was found to be in the range of (1.2-2.0) A.

This work was supported by the National Agency for Research and Development, Moldova within the projects No. 20.8009.5007 and No. 20.8009.5007.7BL.

ACKNOWLEDGMENTS
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*) Author for Correspondence: N. Kazak

P.2. Synthesis and Characterization of olive oil capped nickel sulphide: influence of treatment temperature and precursor source on optical and photocatalytic properties

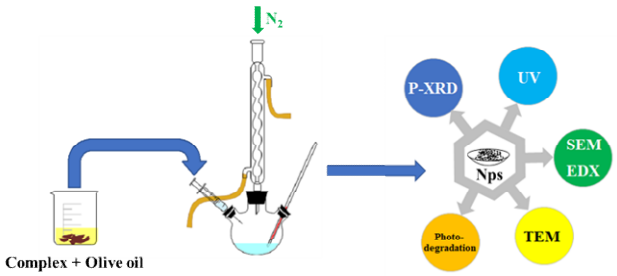
Jocelyn N. Kuate[1,2,3], Paboudam G. Awawou[1], Sunder N. Dhuri[3], Peter T. Ndifon[1*], Viorel Cîrcu[2*]

[1] University of Yaounde I, Yaounde, Cameroon
Email: Jocelynjomkam@gmail.com

[2] University of Bucharest, Bucharest, Roumania
Email: viorel.circu@chimie.unibuc.ro

[3]University of Goa, Taleigao Plateau, India

Since many decades, the design of nanoparticles has aroused of lot of interest due to their nanoscale properties [1]. To this end, different synthetics routes like physical, chemical and green synthetic route has been developed. Among these technics, chemical route has gained a lot of interest since it allows more control over size, shape and stoichiometry. However, the design of the most protocols raises concerns about their effectiveness in producing high-quality nanomaterials considering financial and environmental impacts since they are using toxic and harmful solvents (TOPO, HDA, DDA…etc). Hence, the look toward non-toxic or an eco-friendly solvent constitutes the first step to greener synthesis via chemical route. In this piece of work, we reported olive oil capped nickel sulphide nanoparticles using hot injection route. The effect of treatment temperature and precursors sources were evaluated on crystallinity and optical properties of the as-prepared nanoparticles.



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P.3. INVESTIGATING THE BEHAVIOR AND PROPERTIES OF PHOTOPOLYMERIZABLE COPOLYMERS BASED ON ACRYLATES

Djazia BENDEDDOUCHE[1*], Christelle DELAITE[2], Anne Sophie SCHULLER[2], Ulrich MASCHKE[3], Lamia BEDJAOUI-ALACHAHER[1]

[1] *Laboratoire de Recherche sur les Macromolécules (LRM), Université de Tlemcen 13000, Algérie*
[2] *Laboratoire de Photochimie et d'Ingénierie Macromoléculaires (LPIM), Université de Haute-Alsace 68100, Mulhouse, France*
3 Unité Matériaux Et Transformations (UMET), Université de Lille 59000, Lille, France
** djazia.bendeddouche@univ-tlemcen.dz*

Abstract:

Acrylic polymers are renowned for their wide-ranging applications [1, 2]. A series of UV-curable copolymers was synthesized via radical polymerization under an inert atmosphere and is primarily composed of two monomers: isobornyl acrylate (IBOA) and 2-ethylhexyl acrylate (2-EHA). This association is a key focus to understand the chemical structure and mechanical performance, facilitating the design of tailored materials for specific applications. Thermal analysis by DSC shows a single glass transition temperature (Tg), while tensile testing provides insights into stiffness and elasticity. FTIR analysis confirms the successful formation of the copolymer backbone (Figure). These results demonstrate that the copolymerization approach and the strategic introduction of 2-EHA allow for the fine-tuning of IBOA properties.

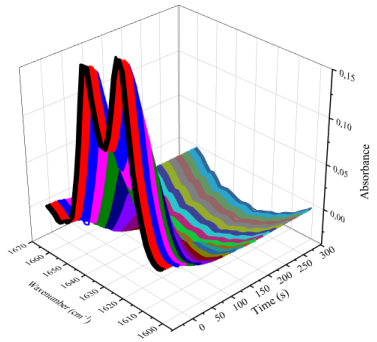

Figure : FTIR analysis of evolution of the absorption band at 1635 cm^{-1}

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2. Nanomaterials, metamaterials and nanoelectronics

P.4. Aero-GaN and ZnO Microtetrapods Functionalized with Metal Nanodots for Photocatalytic Degradation of Tetracycline

V. Ciobanu[1,2*], T. Galatonova[1], P. Urbanek[3], T. Braniste[1,2], F. Doroftei[1], M. Masar[3], P. Suly[3], V. Ursaki[1,2], B. Hanulikova[3], T. Sopik[3], V. Sedlarik[3], I. Kuritka[3] and I. Tiginyanu[1,2]

[1] Centre of Advanced Research in Bionanoconjugates and Biopolymers, "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania, Email: vladimir.ciobanu@cnstm.utm.md; tudor.braniste@cnstm.utm.md; tighineanu.ion@icmpp.ro;
[2] National Centre for Materials Study and Testing, Technical University of Moldova, Chisinau, Moldova. Email: tatiana.galatonova@cnstm.utm.md
[3] Centre of Polymer Systems, Tomas Bata University in Zlin, tr. Tomase Bati 5678, CZ 760 01 Zlin, Czech Republic

This study reports on the fabrication of a novel photocatalyst material characterized by ultra-porous structures formed from interconnected hollow microtetrapods of gallium nitride (GaN) or zinc oxide (ZnO). The specific surface area was estimated to be about 0.2 m^2/gr and 4.7 m^2/gr for ZnO and aero-GaN, respectively, according to BET measurements. The photocatalytic efficiency of these nanomaterials, enhanced with noble metal nanodots, was validated through the complete degradation of tetracycline under both UV and solar light exposure. Given its substantial surface area and improved chemical stability compared to traditional ZnO, the 3D aero-GaN/ZnO composite emerges as a promising candidate for photocatalytic applications and filtration systems. The schematic of the experiment and the photocatalytic performance of the aeromaterials are shown in figure 1.

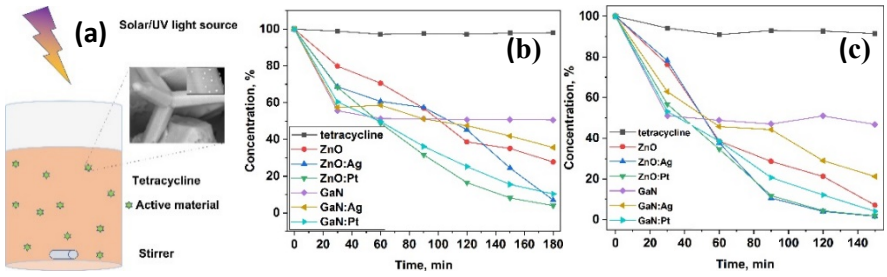

Figure 1. The schematic of the experiment (a); photocatalytic performance of the materials under visible (b) and UV irradiation (c)

Acknowledgments
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*) Author for Correspondence: Vladimir Ciobanu, vladimir.ciobanu@cnstm.utm.md

P.5. Morphology Investigation of Gold Membranes Deposited by Electrochemical and Sputtering Techniques

Elena I. Monaico*

National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Republic of Moldova
Email: elena.monaico@cnstm.utm.md

In this study, the morphology of gold layers deposited by pulsed electrochemical deposition on GaAs substrates was investigated using Atomic Force Microscopy (AFM). By adjusting the pulse duration, it was demonstrated that pores can be introduced in deposited Au layers [1]. According to previous studies, the deposition process follows the hopping electrodeposition mechanism [2,3]. For comparison, the study was also conducted on thin Au layers deposited by sputtering. The surface roughness of the bulk GaAs substrate, sputtered Au layer on GaAs, and Au layer deposited by pulsed electrochemical deposition on GaAs was determined to be 4 nm, 34 nm, and 65 nm, respectively. By reducing the pulse duration from 300 µs to 100 µs, it was demonstrated that the surface roughness of the Au film could be controlled, decreasing from 65 nm to 30 nm. Furthermore, during the anodization process of the GaAs substrate thought the Au film deposited by pulse electrochemical deposition, detachment of the gold membrane at an optimized anodization voltage was demonstrated. The ability to control the roughness of the Au films is significant for optimization of the materials performance in electronic and optoelectronic devices.

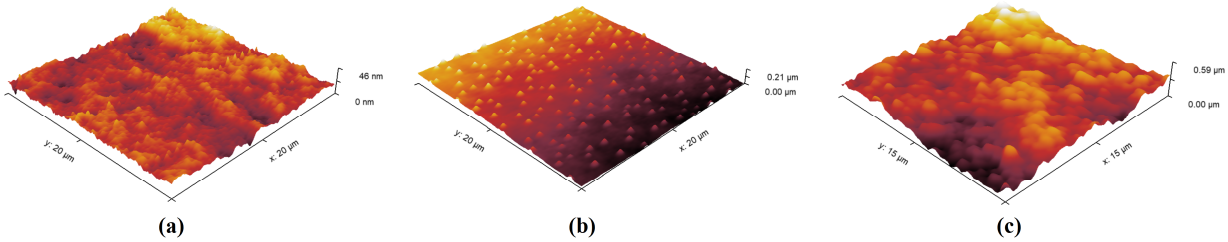

Figure 1. 3D AFM topology image of (a) bulk GaAs substrate; Au film deposited on bulk GaAs by sputtering (b) and (c) pulsed electrochemical deposition technique

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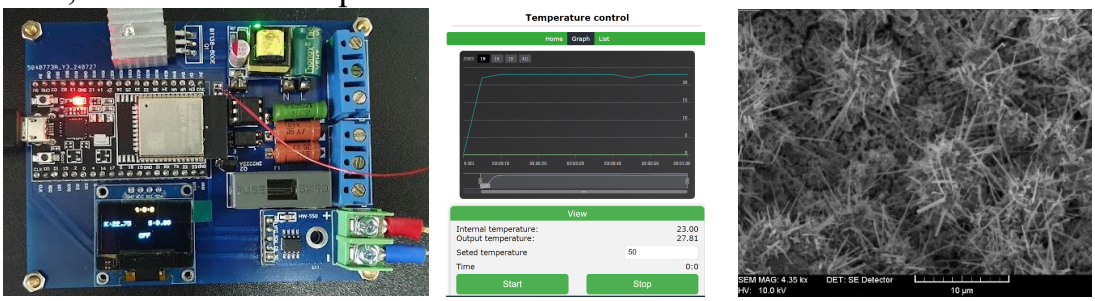
P.6. Remote-Controlled Temperature Setup Designed for ZnO Nanostructures Fabrication

C. Creciunel*, V. Ciobanu and E.V. Monaico

National Center for Materials Study and Testing, Technical University of Moldova
Email: creciunel.catalin@mib.utm.md (C.C.); vladimir.ciobanu@cnstm.utm.md (V.C.); eduard.monaico@cnstm.utm.md (E.V.M.)

In this work, an optimized remote temperature control and monitoring system is proposed and developed for thermal treatment process. Particularly, Zn foils were used in experiments in order to fabricate ZnO nanostructures. Zinc oxide is an important material with multiple applications that can be synthesized through various methods, including thermal treatment [1], electrochemical etching [2,3], etc. To perform the thermal treatment, a control circuit was developed based on the ESP32 microcontroller presented in Fig. 1a. This setup ensures galvanic isolation using an optotriac and optotransistor to control the 220V signal via the BT138 triac. The software solutions are implemented with FreeRTOS, allowing the creation of a graph that tracks the temperature inside the reactor, the time elapsed since the target temperature was reached, and the option to set the desired duration (Fig. 1b). After the thermal treatment, the zinc foils were analyzed using SEM (Fig 1c), EDX, and XRD techniques.



(a) (b) (c)

Figure 1. (a) Real photo of the elaborated device; (b) Web interface; (c) SEM image of the obtained ZnO nanostructures after annealing process of Zn foil.

Acknowledgements: This work was partially supported by the "Young Researchers" project #24.80012.5007.12TC and by the institutional subprogram #02.04.02.

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P.7. Electrochemical Impedance Spectroscopy for Non-Enzymatic Glucose Detection Using ZnO Nanowire Arrays: Substrate Impact Analysis

Simon Busuioc*, Eduard V. Monaico

National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Republic of Moldova

E-mail: simon.busuioc@cnstm.utm.md
eduard.monaico@cnstm.utm.md

The goal of this work is to develop a cost-effective, highly selective, and sensitive non-enzymatic glucose sensor utilizing zinc oxide (ZnO) nanowire arrays for biomedical applications. ZnO nanostructures have attracted significant attention due to their excellent chemical stability, biocompatibility, and unique electrochemical properties. This work explores the glucose sensing performance of ZnO nanowires grown on different substrates, such as Zn-based seed layer and gold-covered seed layer, with a detailed analysis of their electrochemical behavior via Electrochemical Impedance Spectroscopy (EIS). The investigation focuses on understanding how nanowire morphology, determined by substrate properties and growth conditions, impacts their electrochemical performance, building upon previous studies in related porous semiconductor compounds [1,2].

Distinct impedance shifts were observed with each 100 µM increment in glucose concentration, reaching a maximum tested concentration of 500 µM. The Nyquist and Bode plots demonstrated a relationship between glucose concentration and the sensor's electrochemical response, indicating high sensitivity and repeatability of the ZnO nanowire-based sensor.

Acknowledgments: The work was supported by the institutional subprogram 02.04.02 no. 4/FI «Development of technologies and investigation of the properties of layered semiconductor compounds, hybrid nanostructures and laser sources».

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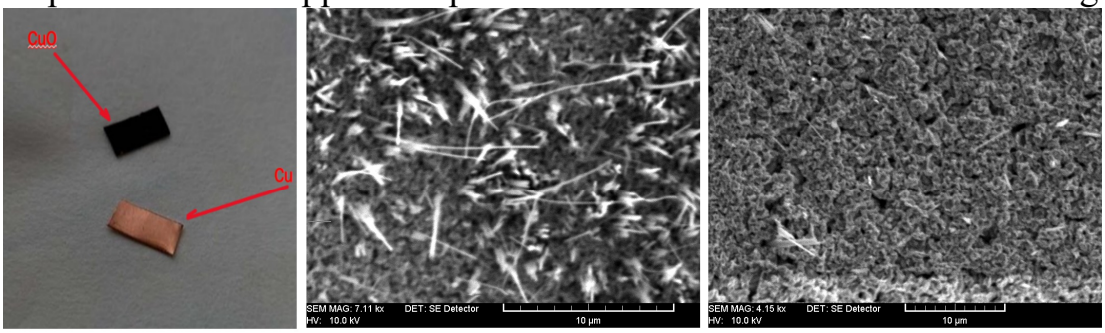
P.8. Impact of Thermal Treatment Temperature on Copper Oxide Formation from Copper Films

A. Mamoico*, and E.V. Monaico

National Center for Materials Study and Testing, Technical University of Moldova, Republic of Moldova
Email: mamoico.alin@mib.utm.md (A.M.); eduard.monaico@cnstm.utm.md (E.V.M.)

This study investigates the effects of thermal treatment (TT) in air [1] on the morphology and chemical composition of copper oxide (CuO) films using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) [2]. The results demonstrate that the temperature of TT significantly influences the formation of CuO structures. Nanowires were predominantly obtained at temperatures up to 500 °C. However, as the temperature increased, mixed structures of nanowires and CuO layers were formed. A drastic reduction in the number of CuO nanowires was observed at 800 °C. Chemical composition analysis confirmed the formation of CuO. Furthermore, the influence of a gold layer deposited on the copper film prior to thermal treatment was also investigated.



(a) **(b)** **(c)**

Figure 1. (a) Photo of the copper film before and after thermal treatment indicating the formation of CuO. SEM images of Cu films after thermal treatment at temperature of 500 °C (b) and 800 °C (c).

Additionally, it was demonstrated that the obtained CuO films can be detached from the copper substrate through rapid cooling. In contrast, at slow cooling maintaining the sample in the oven until reaching 150 °C before removal, results in the formation of a CuO layer on the copper substrate.

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P.9. Tunable Reflection and Absorption in the Mid-Infrared Using Metal-Dielectric Microstrip Nanoantennas

A. Grigore [1], O. Dănilă [2], A. Bărar [3] , D. Mănăilă-Maximean [4]

[1] Faculty of Electronics, Telecommunications and Information Technology, 1-3 Iuliu Maniu Boulevard, 061071 Bucharest, Romania; alexandra.grigore00@stud.mec.upb.ro

[2] Physics Department, 'Politehnica' University of Bucharest, 313 Splaiul Independentei,060042 Bucharest, Romania; octavian.danila@upb.ro

[3] Electronic Technology and Reliability Department, 'Politehnica' University of Bucharest,313 Splaiul Independentei, 060042 Bucharest, Romania; ana.barar@upb.ro

[4] Physics Department, 'Politehnica' University of Bucharest, 313 Splaiul Independentei,060042 Bucharest, Romania; doina.manaila@upb.ro

We present theoretical evaluations of a metal-dielectric metasurface nanoantenna designed for operation within the 2-6 THz range. This innovative metasurface exhibits high sensitivity to external electromagnetic fields and offers a broad dynamic range for reflection and absorption. By utilizing input polarization, the metasurface can be selectively addressed, enabling a wide array of terahertz applications, including dichroic filters, tunable switches, and absorbers.

P.10. Deep Learning-Driven Predictive Modeling for Metasurface Behavior

A. ILIE[1*], O. DĂNILĂ[2], and D. MĂNĂILĂ-MAXIMEAN[3]

[1] National University of Science and Technology Politehnica, Bucharest, Romania
Email: alexandra.ilie0407@stud.fils.upb.ro

[2] National University of Science and Technology Politehnica, Bucharest, Romania
Email:

Metasurfaces are engineered materials designed to control electromagnetic waves, finding applications in areas like wireless communications, imaging, and sensing. Traditional simulation methods to compute the electromagnetic response of metasurfaces are computationally expensive, especially as metasurface patterns, such as PLG (Polygonal) geometries and PLR (Polygonal Ring) [1] patterns with concentric polygons, become more intricate. By developing predictive models, we aim to learn how the structural geometry of these patterns influences their spectral response, offering a faster and more efficient alternative to simulations. This approach facilitates rapid design and optimization of metasurfaces, enabling real-time predictions and adjustments, which are crucial for advancing metasurface applications in cutting-edge technologies.

In this work, we introduce a Convolutional Neural Network (CNN) [2] model, enhanced with residual connections and Fourier transformations, to predict the reflection spectra of metasurfaces. Our CNN architecture is designed to capture spatial features from complex metasurface patterns, while residual connections mitigate vanishing gradients, promoting stability and convergence across layers.

We chose to train the model in the frequency domain, leveraging the Fourier transformation to preprocess the data. This approach allows the model to focus on frequency-dependent characteristics intrinsic to the electromagnetic response of metasurfaces, such as resonance patterns, which are challenging to interpret in the time domain. By working directly with frequency components, the model can more effectively capture the nuances of spectral behavior that define a metasurface's interaction with electromagnetic waves.

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3. Materials for Sustainable Energy

P.11. Theoretical study of the effect of active layer thickness on the performance of perovskite solar cells

A. Bărar[1*], O. Dănilă[1], D. Mănăilă-Maximean[1]

[1] National University of Science and Technology POLITEHNICA of Bucharest, Bucharest, Romania
Email: ana.barar@upb.ro
octavian.danila@upb.ro
doina.manaila@upb.ro

For the past decade, perovskite solar cells have been one of the main research niches in the field of photovoltaic technology. Their simple and cost-effective fabrication technology, put together with their record-breaking power-conversion efficiencies, makes them an ideal candidate for wide-spread solar energy harvesting. However, several crucial drawbacks, such as chemical instability and high sensitivity to humidity, have hindered their mass-production and their introduction in the energy industry. Also, their performance as solar energy converters are dependent on their structural thickness. For thicker active layers, the power-conversion efficiency will increase, but the device will become brittle and more susceptible to damage. However, with thinner active layers, the device will be more flexible, but the power-conversion efficiency will decrease. Therefore, a balance must be struck to optimize both power-conversion efficiency and mechanical flexibility of the device.
This work is a theoretical study of several perovskite solar cell architectures, with a focus on finding a direct relationship between their power conversion efficiency and the active layer thickness. The study also looks at the effect that the thickness has on the cell's device parameters, such as short-circuit current, open-circuit voltage, series and shunt resistance.

P.12. Maximizing Solar Photovoltaic Energy Efficiency: MPPT Techniques Investigation

A-M. Badea[1], D. Manaila-Maximean[1,2], D. Craciunescu[1*], and L. Fara[1,2]

[1] National University of Science and Technology "Politehnica", Bucharest, Romania
[2] Academy of Romanian Scientists, Bucharest, Romania

Email: ana_maria.badea1210@stud.fsa.upb.ro; doina.manaila@upb.ro; dan.craciunescu@renerg.pub.ro; lfara@renerg.pub.ro

This investigation presents a comprehensive study focused on understanding and optimizing the behavior of a photovoltaic (PV) generator. The study explores MPPT algorithm optimization of the PV generator, including a deep analysis of the shading effect for the illuminated area of the PV system, in order to assess its response to rapidly changing weather conditions, specifically variations in solar irradiance and temperature. The study presents various techniques for Maximum Power Point Tracking (MPPT) and analyzes their capabilities and performance metrics. The research methodology involves a combination of simulated and experimental data to understand how PV panels behave under different shading conditions. Furthermore, the study proposes an optimized configuration and advanced MPPT algorithms to enhance system performance in the presence of partial shading. The findings and strategies outlined in this study could be adapted and applied to various types of PV modules.

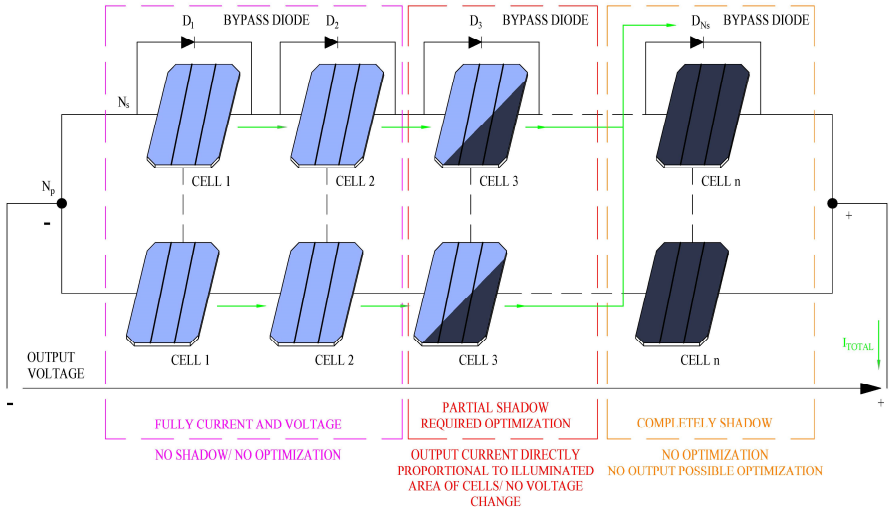

Figure 1. Behavior of the PV generator under shading effect

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*) Author for Correspondence: dan.craciunescu@renerg.pub.ro

4. Electronic, photonic and optoelectronic materials

P.13. First-principles Characterization of the Structural and Electronic Properties of MgF_2 Crystal Doped with Divalent Nickel

N.M. Avram[1,2*], E-L. Andreici Eftimie[1], and M.G. Brik[2,3]

[1] West University of Timisoara, Timisoara, Romania
Email: nicolae.avram@e-uvt.ro; andreicilaura@yahoo.com
[2] Academy of Romanian Scientists, Bucharest, Romania
[3] Institute of Physics, University of Tartu, Tartu, Estonia
Email: mikhail.brik@ut.ee

Magnesium fluoride is a material with a high transparency in a large energy spectrum from UV to IR consequently has numerous applications (filters, mirrors lenses, light polarizers, etc.). The rutile-type structure of MgF_2 bulk crystal doped with divalent nickel ($3d^8$ electronic configuration) has new properties with different technological applications like quantum electronics, optical thermometry, bioimaging et al. Due to its technical significance, several authors have studied the mechanical, optical and spectral properties of Ni^{2+}:MgF_2 system. The aim of this paper is to present some new theoretical results regarding characterizations of structural and electronic properties of investigated system, stemming from density functional theory (DFT), using localized Gaussian-type basis sets [1]. We combined this method with multireference *ab initio* ones *via* the complete active space self-consistent field (CASSCF) and n-electron valence second order perturbation theory (NEVPT2) using Orca software [2]. The one-particle and many particle energy levels, d-d transitions and magnetic sublevels have been done. From the ab initio ligand field theory (AILFT) protocol [3], the B and C Racah parameters, the spin-orbit coupling constant and the ligand field parameters of the angular overlap model (AOM) were accurately extracted [4]. The spin Hamiltonian parameters (SHPs), which characterize the magnetic properties of the doped crystal, including gyromagnetic factors and axial zero-field splitting have been reported. Additionally, we have extended the AILFT protocol, incorporating the 2p shell electrons in our calculations, all with subsequent comparison with experimental data or existing theoretical results in the literature. The calculations proposed in this paper could be a predictive formalism for further characterizations of other optical materials.

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*Author for Correspondence:

P.14. Influence of Exfoliation on the Photoluminescence Properties of Layered Gallium Selenide Single Crystals

E. Cristea[1*], V.V. Zalamai[2] and E.V. Monaico[2]
[1] Department of Telecommunications and Electronic Systems, Faculty of Electronics and Telecommunications, Technical University of Moldova, Chisinau, Republic of Moldova, ecaterina.cristea@srco.utm.md
[2] National Center for Materials Study and Testing, Technical University of Moldova, Chisinau, Republic of Moldova, andrei.tiron@scec.utm.md, victor.zalamai@cnstm.utm.md and eduard.monaico@cnstm.utm.md

With the discovering of graphene [1], interest in obtaining 2D materials based on various semiconductors has increased. The gained interest appears to various layered semiconductor materials such as SnSe, SnS, SnS_2, $SnSe_2$, GaS and GaSe. Among these materials, gallium selenide has the weakest Van der Waals bonds, which allows obtaining layers of nanoscale sizes. In addition, this material has pronounced nonlinear properties and can be used in terahertz region. In gallium selenide single crystals, 4 excitonic series and photoluminescence are observed [2].

The main objective of the work was to obtain nano-sheets of various sizes and study the effect of their sizes on the morphology and luminescent properties. Nano-sheets were obtained by exfoliation of a thin GaSe layer from the bulk material using adhesive tape. Then the tape was dissolved in acetone, and the resulting layers were broken up by ultrasound. Another method involved mechanical exfoliation followed by fracturing of the layer using ultrasound in water, thereby avoiding the influence of acetone and adhesive residue from the tape on the investigation. Size separation of the obtained GaSe nanostructures was achieved through centrifugation. Photoluminescence (PL) spectra of the resulting nanoparticle solutions were excited using lasers with wavelengths of 325 nm, 450 nm, and 532 nm, and recorded by a high-aperture MDR-2 spectrometer.

A solution of nanosheets of varying sizes in water and acetone was prepared. In the PL of a GaSe single crystal, a narrow line of about 2 eV is observed, associated with band-to-band transitions or possibly with free excitons. In the GaSe nanosheets, the same line is observed, but shifted toward higher energies.

Acknowledgments:
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P.15. Optical and Structural Analysis of Thulium-Doped CaF_2 Crystals: Segregation Coefficients of Tm^{3+} and Tm^{2+} Ions

C.Schörnig[1*], M.Ștef[1], P Veber[1], D. Vizman[1,2], M. Poienar[2] and G.Bușe[2]

[1] Faculty of Physics, West University of Timisoara 300223, Timisoara, Romania
[2] ICAM, West University of Timisoara 300223, Timisoara, Romania
E-mail: carla.schornig76@e-uvt.ro

Rare-earth doped fluorite crystals are recognized for their very good optical properties, making them integral to the development of solid-state lasers, amplifiers, and quantum memory devices. Among these materials, CaF_2 crystals doped with TmF_3 stand out due to their excellent spectroscopic characteristics. The distribution of dopants within these crystals plays a significant role in their luminescence properties, making the determination of the segregation coefficient for laser-active centers in the host material essential [1].

This study investigates the distribution of Tm^{3+} and Tm^{2+} ions in TmF_3-doped CaF_2 crystals and determines the segregation coefficient using optical absorption methods.

The crystals were grown in the Crystal Growth Laboratory using the vertical Bridgman method. crushed CaF_2 optical UV-VIS windows (Crystran Ltd., UK) and supra-pure grade TmF_3 (Merck) were used as raw materials. Transparent, colorless crystals, 10 mm in diameter and 5-6 cm in length, were obtained in graphite crucibles under vacuum (~10^{-3} Torr) using a shaped graphite furnace [2]. These crystals exhibited no visible inclusions or cracks, and the segregation coefficient values indicated that they were of high quality, suitable for laser applications.

The segregation coefficients of Thulium ions (Tm^{3+} and Tm^{2+}) were determined for crystals with different TmF_3 concentrations. For Tm^{3+} ions, the characteristic segregation coefficients were close to unity, indicating a homogeneous distribution within the crystals. In contrast, for Tm^{2+} ions, the segregation coefficient for CaF_2:1 mol% TmF_3 crystals was 1.03, suggesting a slightly higher dopant concentration at the crystal's start. However, for CaF2:5 mol% TmF_3 crystals, the segregation coefficient was less than one, showing that these impurities tended to accumulate towards the crystal's end [3].

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*) Author for Correspondence: Carla Schörnig, E-mail: carla.schornig76@e-uvt.ro

P.16. Hybrid materials based on liquid crystals doped with double cyclopalladated complexes

Daiana G. Mitrea[1], Monica Iliș[1], Doina Mănăilă-Maximean[2] and Viorel Cîrcu[1*]

[1]Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, University of Bucharest, Bucharest, Romania
Email: daiana.mitrea@drd.unibuc.ro, *viorel.circu@chimie.unibuc.ro
[2]Department of Physics, National University of Science and Technology Politehnica Bucharest, Bucharest, Romania

The organometallic complexes have gained a significant interest due to their interesting photoluminescent properties, in terms of optical and sensing applications. For development of organic light emitting diodes (OLEDs), various systems based on Ir(III) or Pt(II) complexes were studied. An interesting alternative that can be taken into account is represented by cyclopalladated compounds that display remarkable photophysical properties due to the strong ligand field imposed by the cyclometalated organic ligands. Especially, hybrid materials based on luminescent liquid crystals were investigated, as they exhibit photoluminescence and anisotropy properties leading to linearly or circularly polarized emission. Therefore, our interest consisted in preparing luminescent mixtures containing a liquid crystal, a Pd(II) complex and a chiral dopant. First of all, the double cyclopalladated compounds based on Schiff base derivatives and N-benzoylthiourea (BTU) ligands were obtained and characterized [1]. Then, the selected Pd(II) complexes were used to prepare different liquid crystals mixtures (the concentration of each component was varied until the best composition was reached). Regarding the desired properties, the most promising mixtures (E7 doped with Pd(II) complexes and chiral dopants) were incorporated into a polymeric matrix through the emulsification solvent diffusion method (ESD)[2]. These hybrid materials were investigated concerning their luminescence and polarized emission properties at room temperature (Figure 1).

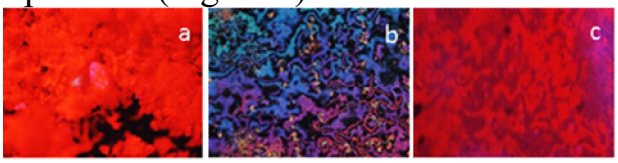

Figure 1. Picture of Pd(II) complex upon UV irradiation (a); Optical micrographs of the nematic schlieren textures of E7 with 4% Pd(II) complex in polarized and UV light (b,c).

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*) Author for Correspondence: viorel.circu@chimie.unibuc.ro

P.17. Liquid crystalline and gel properties of luminescent palladium(II) complexes with benzoylthiourea ligands

Theodora A. Ilincă[1], Monica Iliș[1], Marin Micutz[2], and Viorel Cîrcu[1*]

[1] University of Bucharest, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Bucharest, Romania
Email: viorel.circu@chimie.unibuc.ro
[2] University of Bucharest, Department of Analytical and Physical Chemistry, Bucharest, Romania

Metallomesogens - liquid crystals incorporating metal ions - with luminescent properties present a great interest for their promising applications in the electrooptical devices. Emissive properties were reported for a series of metallomesogens based on palladium(II) complexes, having the metal ion in a cyclometallated surrounding. By judicious design, new palladium (II) complexes with high quantum yields and luminescence lifetimes can be obtained [1,2].
The design and development of new luminescent metallogels formed by cyclometalated palladium(II) complexes in protic solvents were investigated by a combination of differential scanning calorimetry (DSC), polarized optical microscopy (POM) and rheology. Cyclometalated palladium(II) complexes based on imine ligand and ancillary benzoylthiourea (BTU) ligand show red emission in solid and gel state. The formation of a lyotropic liquid crystal phase was observed for complex bearing shorter alkyl groups on BTU ligand. Dynamic rheology measurements (frequency sweep in the 5 - 90°C range) on the 1-decanol solution of palladium(II) complexes highlighted their ability of supramolecular self-association to generate 3D networks and gel-formation as a final result.

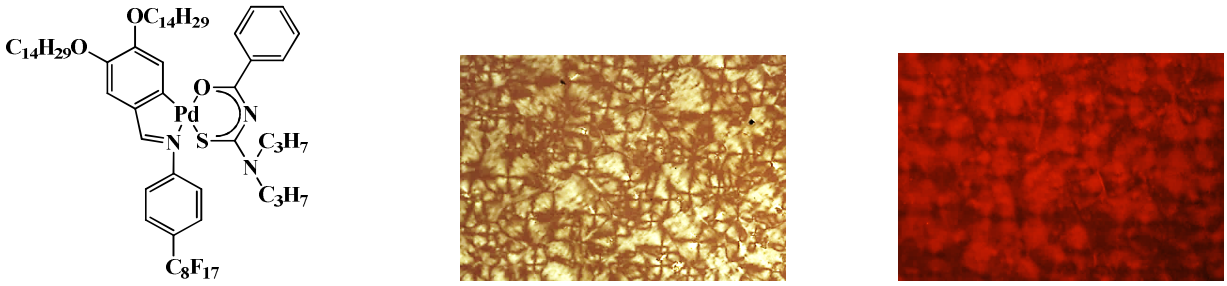

Figure 1. Structure and lyotropic liquid crystal phase of palladium compound (5% gel) in normal polarized light and by irradiation with UV light.

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*) Author for Correspondence

P.18. Thermo Responsive Surfaces Design Using Cholesteric Liquid Crystals

Cosmin A. Alexe[1,2*], C. Gaidău[2], Monica V. Iliș[1], V. Cîrcu[1]

[1] University of Bucharest, Faculty of Chemistry, Bucharest, Romania
Email: cosminandrei.alexe@yahoo.com
[2] National Research and Development Institute for Textiles and Leather (INCDTP) – Bucharest, Romania

The synthesis of liquid crystals, which have unique properties because of their supramolecular responsive structure, has found use in a variety of technologies. The most well-known of these include light modulators, lasers, erasable optical disks, electronic slides, flat panel electronic displays, optical imaging and recording, and more [1]. An intriguing platform for creating sensors or thermoresponsive surfaces was discovered in the phase transition of liquid crystals. Although the synthesis and characterization techniques of liquid crystals are extensively documented in the literature [2], leather surface finishing is hardly ever applied. The objective of the presentation is to produce leather surfaces with thermochromic response for future applications in flexible and wearable sensors as well as for a variety of aesthetic impacts.

The dispersion according to the invention is prepared by mixing 0.5 g of cholesteric liquid crystals with 0.05 g of NOA65 photopolymer dissolved in 5 mL of dichloromethane, when a homogeneous mixture is obtained that is dosed over 20 mL of PVA 3% under magnetically stirring, at 400 RPM, and irradiated with UV light at a wavelength of 365 nm for 20 minutes, then add 20 ml of 3% PVA and increase the magnetic stirring speed to 1000 RPM, under UV light, when a homogeneous, thermochromic dispersion is obtained (Figure 1), which after 20 minutes is deposited by scraping on various surfaces, which is then dried at room temperature, when a glossy, flexible, thermochromic film is formed.

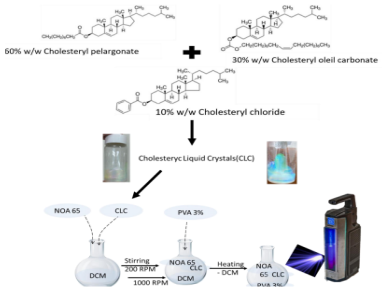

Figure 1.

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*) Author for Correspondence:

5. Materials science

P.19. Enhanced Spin Asymmetry in $SrTiO_3$ (011) and $SrTiO_3$ (001): Insights from Spin-Resolved Photoelectron Spectroscopy

L.E. Borcan[1,2,*], D.G. Popescu[1], A.C. Iancu[1,2], C.M. Teodorescu[1], M.A. Husanu[1,*]

[1] National Institute of Materials Physics, Atomiștilor 405A, 077125 Măgurele, Ilfov, Romania
[2] University of Bucharest, Faculty of Physics, Atomiștilor 405, 077125 Măgurele, Ilfov, Romania
*Email: larisa.borcan@infim.ro, ahusanu@infim.ro

This study investigates the spin asymmetry of atomically clean $SrTiO_3$ (001) and $SrTiO_3$(011) using low energy electron diffraction (LEED), core level X-ray photoelectron spectroscopy (XPS), and spin-resolved photoelectron spectroscopy. The $SrTiO_3$(011) sample exhibit a significantly higher spin asymmetry—approximately four times greater than that observed in $SrTiO_3$ (001) - partial neutralization of O_2 (4–) or SrTiO(4+) end layers. Missing electrons from O 2*p* states in the case of O_2 terminations (or additional electrons on Ti 3*d* states in the case of SrTiO terminations) enable robust atomic spins. The parallel analysis of core level shifts for surface atoms and amplitude of spin asymmetry suggests that 50% of the oxygens from the surface SrO layer of $SrTiO_3$(001) have a $2p^5$ configuration with an unpaired electron (the rest are in $2p^6$ configuration), while in the case of O_2 terminated $SrTiO_3$(011) about 50% of surface oxygens have a $2p^5$ configuration and 50% of surface oxygens are neutral ($2p^4$), yielding a net charge per O_2 surface unit cell of (–1) instead of (–4). The magnetization seems to be oriented along the rows formed by the (4 × 1) reconstruction, in the $[0\bar{1}1]$ in-plane direction.

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*) Author for Correspondence:

P.20. Temperature-Dependent CO Adsorption on $BaTiO_3$(001): Mechanisms, Surface Stability, and Potential for Gas Sequestration

A.C. Iancu [1,2,*], C.M. Teodorescu[1], D.G. Popescu[1,*]

[1] National Institute of Materials Physics, Atomiștilor 405A, 077125 Măgurele, Ilfov, Romania
[2] University of Bucharest, Faculty of Physics, Atomiștilor 405, 077125 Măgurele, Ilfov, Romania
*Email: alexandru.iancu@infim.ro, dana.popescu@infim.ro

This study investigates the reversible adsorption and desorption of carbon monoxide (CO) on BaO-terminated $BaTiO_3$(001) surfaces using photoelectron spectroscopy. CO is adsorbed in non-dissociated form, with adsorption geometry varying according to temperature. Below room temperature, CO adsorbs atop surface barium atoms, while at room temperature, it adsorbs atop surface oxygen, and at high temperatures, CO forms a "hollow" site adsorption involving coordination with three oxygen atoms. The adsorption rate increases by 30% at lower temperatures, with approximately one CO molecule adsorbed per 10 surface unit cells. CO is completely desorbed when the substrate is heated above the Curie temperature, indicating the pivotal role of ferroelectric polarization in the adsorption process. The $BaTiO_3$(001) surface remains stable through repeated CO adsorption and desorption cycles, suggesting its potential for applications in controlled CO removal. The study also suggests that the interaction of CO with $BaTiO_3$ enhances surface polarization, as evidenced by an increase in surface band bending. Theoretical investigations are encouraged to further explore the adsorption mechanisms and potential applications for CO sequestration and other gases.

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*) Author for Correspondence:

P.21. PHOTO DEGRADATION OF ORGANIC COMPOUND DRIVEN BY PRISTINE AND Pt-MODIFIED TiO_2

A. Ilie[1*], C. Anastasescu[1], L. Predoana[1], J. Pandele[1], A. Rusu[1], S. Preda[1], D. Culita[1], I. Balint[1] and M. Zaharescu[1]

[1] *"Ilie Murgulescu" Institute of Physical Chemistry of the Romanian Academy, 060021 Bucharest, 202 Spl. Independentei, 6th district, Romania*

Email: *asandulescu@icf.ro*

Keywords: *photocatalytic oxidation, organic compound oxidation, TiO_2 modified with noble metals, photodegradation*

Introduction: Photocatalytic oxidation of organic matter conducted by sunlight is of great importance in several respects: (i) it involves low costs, (ii) it is able to clean water and air [1], and (iii) is an alternative route relative to selective synthesis of high value-added oxygenated products [2].

Materials and methods: Materials used: ethanol, TiO_2 and Pt/TiO_2 powders (obtained by sol-gel method). The reaction products of gas phase oxidation processes were analyzed by gas phase chromatography (GC-TCD and GC-FID).

Results: Both support and noble metals play an important role in light absorption, charge separation and the formation of carbon dioxide which are analyzed for light-induced oxidation of ethanol on the noble metal (Pt) loaded with TiO_2. The presence of platinum nanoparticles on TiO_2 can mainly trigger the red shift of light absorption edge and separation of the photo generated charges.

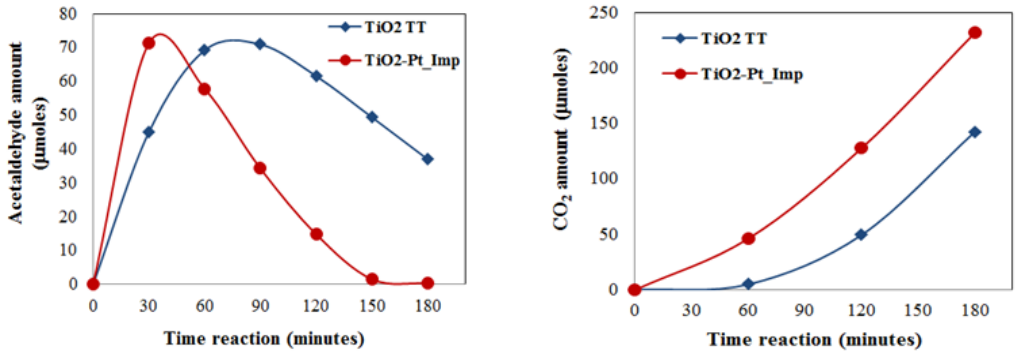

Figure 1. Solar light-driven ethanol oxidative conversion

Conclusions: This study reveals the light-initiated photooxidative pathways for an organic substrate over TiO_2 charged with noble metal. The analysis of the complex phenomena associated with the photocatalytic reactions focuses on the formation of carbon dioxide, the separation of the light generated charges by platinum adition, as well as on the oxidative conversion reaction mechanism of ethanol.

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*) Author for Correspondence: *asandulescu@icf.ro*

P.22. MORPHOLOGY AND DYNAMICS OF THE PLASMA PLUME DURING LASER PROCESSING FOR THE DETECTION OF STRUCTURAL DEFECTS

Robert RADU[1*], Sabin MIHAI[2,3], Diana CHIOIBASU[2], Andrei C. POPESCU[2], Cristina STAN[1]

[1]Faculty of Applied Sciences, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest,
Email: radurobert@yahoo.com
[2] Center for Advanced Laser Technologies (CETAL), National Institute for Laser, Plasma and Radiation Physics (INFLPR), Ilfov, 077125 Magurele, Romania
[3]Faculty of Industrial Engineering and Robotics, National University of Science and Technology Politehnica Bucharest, 060042 Bucharest, Romania

The theme revolves around the study of the morphology and dynamics of the plasma plume resulting from the deposition of composite material with a nickel alloy metal matrix IN718 (INCONEL) and a dispersed phase in form of TiC (titanium carbide) particles in specific composition/mixing ratios, using the Laser Melting Deposition (LMD) technique. This research aims to examine the relationship between the irradiated area and the resulting plasma to early detect formations of particles cluster and to monitor the plasma's evolution in real-time for characterizing the homogeneity of composite materials fabricated using the LMD technique. Thus, through the direct monitoring described, using a high-speed imaging camera, there is potential to develop a real-time quality characterization method for the deposited materials, based on plasma plume variation image analysis. This approach would allow for identification of clusters of unmelted titanium carbide particles within the sample volume, which could lead to a decrease in mechanical strength, and facilitate the production of composite material parts with a homogeneously spread reinforcing phase [1].

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*) Author for Correspondence: radurobert@yahoo.com

P.23. REMOVAL OF Eosin (Y) DYE FROM WASTEWATER USING POLYACRYLAMIDE HYDROGEL ADSORBENTS: EQUILIBRIUM ANALYSIS AND APPLICATION OF ADSORPTION ISOTHERM MODELS

Chouikhi Manel Safia[1], Salah HAMRI[1,2] , Zakia HADJOU BELAID[1], Fayçal DERGAL[2], Djahida LERARI[2].

[1]Macromolecular Research Laboratory (LRM), Department of Physics, Faculty of Sciences, University of Abou Bekr Belkaid, PB 119,13000 Tlemcen, Algeria
[2]Center for Scientific and Technical Research in Physico-chemical Analyzes (CRAPC), PB384, Bou-Ismail, RP Tipaza 42004, Algeria

manelsafia.chouikhi@univ-tlemcen.dz

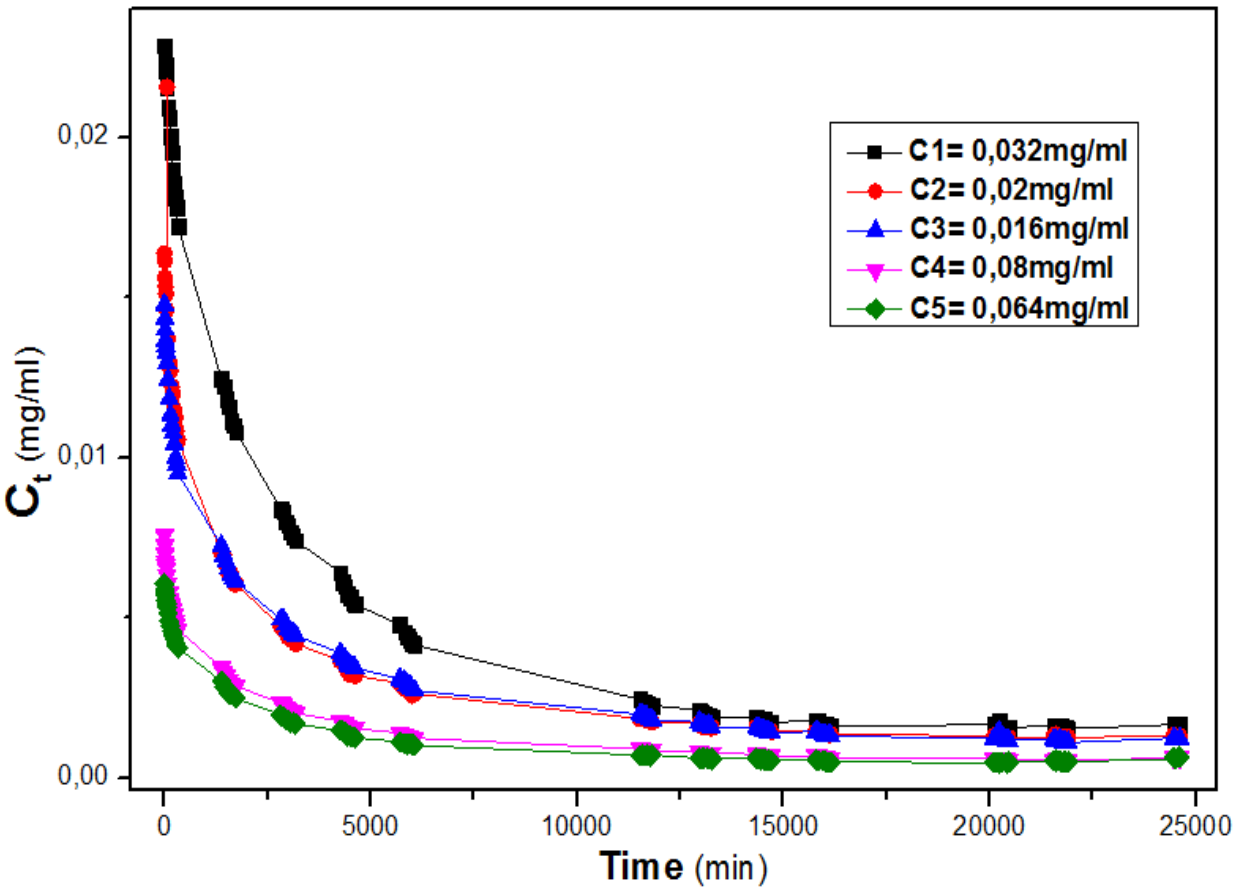
The removal of dyes from wastewater through adsorption has gained significant research interest in recent years. This is due to the recognition of hydrogel-based adsorbents as promising tools for dye removal, as they are easy to use and cost-effective **[1]**.

The objective of the present study was to design and develop a super adsorbent hydrogel based on acrylamide monomer for effectively removing dyes such as eosin (Y) from polluted water sources. Acrylamide was selected as the monomer due to its structural properties. As it contains both a polar amide group and a carbon-carbon double bond, acrylamide can strongly interact with polluting dyes through electrostatic and Van der Waals forces, facilitating adsorption.

The acrylamide-based hydrogels were synthesized using a simple and scalable radical polymerization method. A photoinitiator was used to trigger polymer chain growth, while a crosslinker allowed a treelike, three-dimensional network structure to form within the hydrogel. This porous network structure is beneficial for adsorption, providing a large surface area for dye molecules to interact with **[2]**.

Testing showed the super adsorbent hydrogels exhibited exceptionally high adsorption capacity for eosin (Y) with over 98% elimination efficiency. Adsorption isotherm models provide important insights into the adsorption process between adsorbents and adsorbates. By fitting experimental data to models like Langmuir, Freundlich and Temkin, parameters can be derived to characterize the maximum adsorption capacity and surface properties. This helps understand adsorption behavior and optimize adsorbent design for efficient pollutant removal from wastewater in various applications **[3]**.

In summary, this study developed a novel super adsorbent hydrogel for highly effective dye removal from wastewater. The acrylamide-based material demonstrated great potential through its low-cost synthesis and very high adsorption performance, showing promise for scaling up water purification



applications. Further optimization has the potential to improve adsorption capacity and kinetics even more.

Figure 1: Variation in the concentration of eosin adsorbed as a function of time.

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6. Biomaterials and organic materials

P.24. A More Detailed Mathematical Simulation of the Swelling Step of a Pulsatory Liposome

D. R. Radnef-Constantin[1*], D. Popescu[2], and V. I. R. Niculescu[3]

[1] Institutul Astronomic al Academiei Romane, Bucharest, Romania
Email*: ghe12constantin@yahoo.com
[2] "Gheorghe Mihoc-Caius Iacob" Institute of Mathematical Statistics and Applied Mathematics, Department of Mathematical Modelling in Life Sciences, Calea 13 Septembrie 13, Bucharest, Romania
Email: dghpopescu@gmail.com
[3] National Institute for Lasers, Plasma and Radiation Physics, Atomistilor 409, Magurele, Ilfov, Romania
Email: filo_niculescu@yahoo.com

In this paper we consider a pulsatory liposome. An large unilamellar liposome (lipid vesicle) filled with aqueous solution of osmotic solute is introduced in an aqueous medium of large dimensions. Due to the osmosis process the liposome swells to a critical size, when a transbilayer pore suddenly appears. Through this pore a part of the internal solution leaks and the liposome relaxes and returns to its initial size. The swelling starts again and the liposome begins a new cycle and so on. The operation of the pulsatory liposome is a dynamic and cyclic process. It can be considered as a biophysical engine. For each cycle, the swelling of the liposome is described by a differential equation and its relaxing is described by three differential equations [1–5]. This system of differential equations can be integrated using numerical methods In this paper we deal with the mathematical modeling both by analytical and statistical regression methods for the swelling stage of the pulsatory liposome. The osmotic solvate can be a pharmacological substance. At each cycle, a quantity of pharmacological substance is released. So, the pulsatory liposome can release substances with a medical effect in a controlled manner to diseased sites.

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P.25. Long-Term Monitoring of Black Carbon in Măgurele, Romania: A Source Apportionment Approach with the AE33 Aethalometer

A. V. Dandocsi[1,2*], J. Vasilescu[1], L. Belegante[1] and C. Stan[2]

[1] National Institute of Research and Development for Optoelectronics INOE 2000, Magurele, Romania
Email: andrei.dandocsi@inoe.ro
[2] National University of Science and Technology POLITEHNICA Bucharest, Romania

Black carbon (BC), commonly known as soot, is a critical component of atmospheric pollution and significantly influences Earth's climate system [1]. Formed through the incomplete combustion of fossil fuels and biomass, BC contributes to positive climate forcing [2] and poses considerable health risks [3]. This study utilizes the AE33 aethalometer, which employs an advanced multi-wavelength absorption technique to measure BC concentrations. The aethalometer works by directing light beams through a filter where aerosol particles accumulate, causing a decrease in transmitted light intensity. By measuring this attenuation at multiple wavelengths, the instrument can estimate the mass concentration of BC. A key feature of the AE33 is its dual spot technology, which enables simultaneous measurements of light absorption at two distinct points on the filter. In this research, the built-in source apportionment model developed in [4] is applied to separate BC emissions from traffic and biomass burning sources. Measurements were conducted at a peri-urban ACTRIS National Facility located in Măgurele, Romania (44.344°N, 26.012°E, 77 m a.s.l.). The dataset consists of approximately a decade of continuous monitoring, from 2014 to 2024.

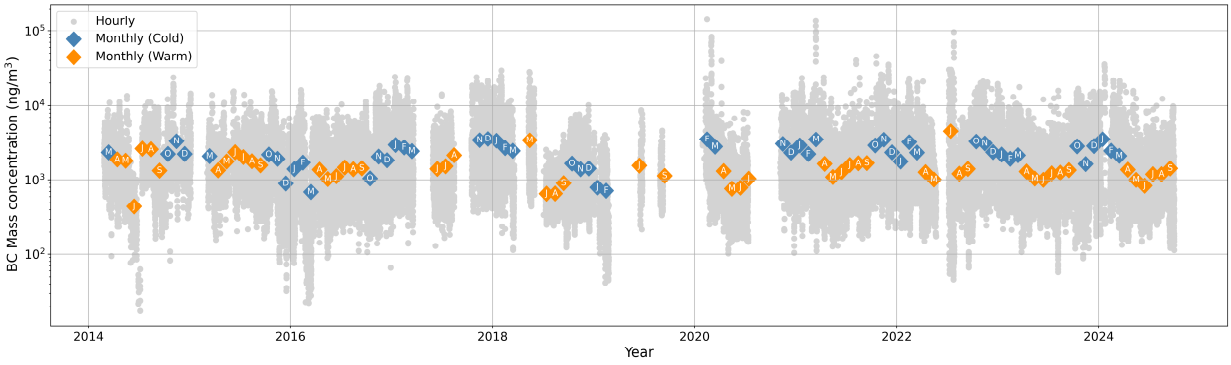

Figure 1. BC concentrations timeseries, monthly and hourly means

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*) Author for Correspondence: Andrei-Valentin Dandocsi

P.26. Amyloid beta improved surfaces for development of biomedical applications

Sara Nistor[1], Mihaela Beregoi[2], Corina Ciobotaru[2], Monica Enculescu[2], Liviu Nedelcu[2], Cristina Busuioc[3], Adrian Enache[2]

[1]Faculty of Medical Engineering, National University of Science and Technology Politehnica of Bucharest, 060042 Bucharest, Romania, E-mail: sara.nistor@stud.fim.upb.ro
[2]National Institute of Materials Physics, Atomistilor Str. 405A, 077125 Magurele, Romania,
[3]Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology Politehnica of Bucharest, 060042 Bucharest, Romania

Nanostructured and biocompatible materials play a pivotal role in medical applications due to their unique properties such as large surface area, high surface energy, spatial confinement, and not harmful to the human body. When fabricated from conductive materials, these can stimulate cell proliferation, differentiation and tissue functionalities by promoting the transmission of natural bioelectric signals or electrical stimulation to cells and tissues that are electrically isolated. Considering these properties, one of the biomedical applications of conductive nanostructured materials address to neuronal cells, mainly due to the complexity of the nervous system and inefficiency of conventional repair methods.

Our study tries to support this kind of applications through the development and fabrication of novel conductive and biocompatible nanostructures materials to be further used in application involving neuronal cells. Thus, several conductive solid and flexible surfaces were fabricated using different types of glass, an electrospun polymeric nanofibers-based mesh and magnetron sputtering method for gold deposition. Scanning electron microscopy and X ray diffraction techniques were employed for a selection of conductive nanostructured materials to be used in further studies on living cells. To increase the biocompatibility and cell adhesion of cells at the selected samples, their surfaces were modified with different high ordered structural biomolecules such as poly-Lysine, collagen or amyloid peptides. Using the fibroblast L929 and the neuroblastoma SH-SY5Y lines as cellular model, the MTS assay, fluorescence and scanning electron microscopy investigations it was demonstrated that the new developed nanostructured surfaces are favorite candidates to be integrated in complex devices for cellular electrostimulation.

P.27. Rutin loaded Human Serum Albumin nanoparticles for intracellular targeted drug delivery

G. Chilom[1 *], Sorina Iftimie[1], E. Balan[1,] T. Enache[2,] [1]M. Enculescu, and D. Oprea[1, 2]

[1]University of Bucharest, Romania
Email: office@g.unibuc.ro
[2]National Institute of Materials Physics, Magurele, Romania
Email: secretariat@infim.ro

Abstract

A drug delivery system using folic acid-rutin-conjugated human serum albumin nanoparticles (HSA-FA-Ru NPs) were developed to target and destabilize HT-29 adenocarcinoma cells through the delivery of rutin, a chemotherapeutic drug. Unconjugated human serum albumin nanoparticles (HSA NPs) and the L929 fibroblast cell line were used as controls. The NPs were synthesized using an optimized desolvation method and characterized by Atomic Force (AFM) and Scanning Electron Microscopy (SEM). The analysis showed that the NPs were spherical, uniformly distributed, and had diameters below 100 nm. Time stability studies, using UV-Vis spectroscopy, revealed that the NPs maintained 68% stability for over 30 days. The effects of the NPs on the cell lines were assessed using an *in vitro* MTS viability assay. Results showed that, after 24 hours of incubation, the viability of HT-29 cells decreased significantly compared to L929 cells. Fluorescence microscopy revealed that while the nucleus and cytoskeleton of both cell lines remained intact after 24 hours of exposure to HSA NPs and HSA-FA-Ru NPs, a notable aggregation of NPs on the surface of HT-29 cells was observed, particularly in the presence of HSA-FA-Ru NPs. The selective reduction in HT-29 viability suggests that these NPs could serve as a promising alternative to conventional colorectal cancer treatments, improving targeting and minimizing damage to healthy cells.

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*) Author for Correspondence: Bratu Oprea Daniela; email: daniela.oprea@infim.ro

P.28. Effect of Annealing and Plasticization on the Crystallinity, Thermal and Dynamic Mechanical Properties of Poly(lactic acid)

L. Benkraled[1*], A. Zennaki[1] and A. Berrayah[1]

[1] Laboratoire de Recherche sur les Macromolécules (LRM), University of Tlemcen, Algeria
Email: linabenkraled@gmail.com

Recently, there has been an increasing interest in biopolymers to substitute petroleum-based plastics in many applications. Among commercially available biopolymers, poly(lactic acid) (PLA) is the most promising. Besides being environmentally friendly material, PLA is easy-processable and offers good mechanical properties. However, PLA suffers from high brittleness, poor thermal resistance and slow crystallization kinetics which limit its widespread use. The purpose of this work is to improve the properties of PLA by thermal annealing and plasticization. PLA was plasticized with polyethylene glycol (PEG-400) at a content of 10 wt%. The plasticized and non-plasticized films were prepared by the solvent casting method and annealed at various temperatures ranging from 80 to 120 °C. The films were analyzed with differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The results showed that the crystallinity and heat resistance were improved by annealing for all samples, but the plasticized films showed higher crystallinity. The crystalline structure of PLA was also dependent on the annealing temperature and the plasticizer addition.

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*) Author for Correspondence: linabenkraled@gmail.com

P.29. Bionanocomposite films with antioxidant activity for safe food preservation

Sarra Benaissa[1*], Kamal Benmansour[2]

[1]Lboratory of Macromolecules LRM / Abou Bekr Belkaid, Tlemcen, Algeria
[2]Laboratory of Macromolecules LRM/ Abou Bekr Belkaid, Tlemcen, Algeria
*sarahbena439@gmail.com, kamaldz@yahoo.fr

In the context of plastic pollution and human health risks, researches about biodegradable packaging have increased in order to eliminate environmental hazards. Biopolymers are widely used for this purpose for its interesting properties such as biocompatibility, antioxidants, antibacterial activity and thermal stability. However they present low characteristics compared to petroleum polymers. Hence additives such as essential oils, plants extracts and nanoparticles are added.
In this work we intended to make biofilms using a polysaccharide as the main matrix and silver nanoparticles as antioxidants agents, and examine their properties.

Thus silver nanoparticles are obtained using plant extract as a reducing and stabilizing agent, the particle size distribution analysis reveal a size of 78nm,50nm,43nm and 37nm and a zeta potential of -12.8mv,-13.2mv,-14.1mv and -20mv respectively for the four samples. The UV-Vis confirms the presence of a plasmonic bound around 400nm-500nm.
In the matter of the fabrication of the biofilms, certain amounts of nanosized particles are added to the biopolymer. The FTIR analysis verify the main characteristic functions OH, CH, CO, NH, NH2 and COC stretching's of the films, the UV-Vis demonstrate a good UV properties and opacity for the nanocomposites compared to the plain polymer, the mechanical tests also reveal an enhanced properties. The study of antioxidant activity shows an upgrade for the bionanocomposites, these results are very promising for a safer food packaging and medicine.

Keywords: nanoparticles, bionanocomposites, light barrier, antioxidant activity, packaging

7. Methods for material characterization

P.30. Reinforcement of Polymethyl Methacrylate (PMMA) with Modified MgAl Layered Double Hydroxides: A Study of Optical and Thermal Properties

W. Haffaf [1*], M. Hamouni[1], and Z. Abdelsadek[2]

[1] University Abubekr Belkaid, Faculty of Science, Macromolecules Research Laboratory (MRL),Tlemcen, Algeria.
[2] Institute of Electrical and Electronics Engineering, University of M'hamed-Bougara, Independence Avenue,35000, Boumerdès, Algeria

*Email :wissemhaffafdz@gmail.com

Polymethyl methacrylate (PMMA) is widely used in applications requiring optical transparency ; however, its thermal and mechanical limitations restrict its use in demanding environments. To address these limitations, layered double hydroxides (LDH) can be introduced as reinforcing agents [1-3]. This study examines the effect of incorporating modified MgAl-LDH on the structural, optical, and thermal properties of PMMA.

Two PMMA-based composites were prepared by dispersing 3 wt % and 5 wt % of modified MgAl layered double hydroxides (LDH) into PMMA matrix via a solvent blending technical. The resulting nanocomposites were characterized using various analytical techniques, including Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), UV-Visible spectroscopy and thermogravimetric analysis (TGA).

FTIR spectroscopy confirmed the formation of interactions between the PMMA and the modified LDH, while XRD analysis indicated the formation of an intercalated structure within the PMMA matrix. UV-Visible spectroscopy demonstrated that the polymer's optical transparency was retained, and TGA result indicated a modest improvement in the thermal stability of the PMMA-LDH nanocomposites compared to neat PMMA.

Key words: PMMA, Modified MgAl-LDH, Optical Transparency, Thermal Stability.

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P.31. Modeling of Phase Diagrams of Polysiloxane/Nematic Liquid Crystal Systems. Study of the Effect of Molecular Weight.

Yamina BOUAYED-KAZI AOUEL[1], Amina BOURICHE[1], Ulrich MASCHKE[2], Lamia BEDJAOUI-ALACHAHER[1]

[1] Research Laboratory on Macromolecules (LRM), Faculty of Sciences, Aboubakr Belkaïd University, 13000 Tlemcen, Algeria.

y_kazi2002@hotmail.fr

[2] *Materials and Transformations Unit – UMET (CNRS UMR No. 8207), Building C6, University of Lille 1 - Sciences and Technologies, 59655 Villeneuve d'Ascq Cedex, France*.

l_bedjaoui@yahoo.fr>

Abstract

Polymer and liquid crystal mixtures have numerous applications in optical fields, including switchable glazing and display screens [1-3]. Most applications rely on specific electro-optical responses that depend on both phase behavior and thermodynamic properties, as well as the morphology and dimensions of the liquid crystals. A detailed study of these properties is necessary to better understand and enhance performance under practical conditions.

This work aims to establish theoretical models that can explain experimental phase diagrams of mixtures composed of linear and isotropic polymethylphenylsiloxane (PMPS) with molecular weights of Mw = 9600 and 70900 g/mol, and a nematic liquid crystal (LC) E7. E7 exhibits a broad nematic range, from a glass transition temperature (Tg) of 213 K to a nematic-isotropic transition temperature (TNI) of 334.7 K, with no other transitions in between. A combination of the Flory-Huggins theory for isotropic mixing and the Maier-Saupe theory for nematic order [4,5] was used to establish these diagrams. Depending on the nature of the polymer, its molecular weight, and the nature of the liquid crystal, a variation in the isotropic phase region is observed.

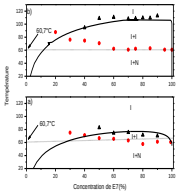

Figure 1: Phase diagrams of the PMPS9600/E7 (a) and PMPS70900/E7 (b) systems obtained experimentally.

Keywords: Phase diagram, Flory-Huggins theory, Maier-Saupe.

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