

Abstract book

ORAL COMMUNICATIONS

O.1. Evaluation of mechanical and dielectric properties of some biodegradable cellulose-based composites

A.I. Barzic^{1*}, E. Turcu¹, M. Asandulesa¹, C. Tugui¹ and R.M. Albu¹

¹ “Petru Poni” Institute of Macromolecular Chemistry, Laboratory of Physical Chemistry of Polymers, Grigore Ghica Voda Alley, 41A, 700487- Iasi, Romania

Email: irina_cosutchi@yahoo.com

The scientific breakthroughs in the area of polymer science have led to important results in the area of energy harvesting [1]. Biodegradable macromolecular-based materials have introduced the benefit that they are not so harmful for the environment, regardless the type of the device where they are introduced [2,3]. This paper has the purpose to perform a theoretical evaluation of certain basic physical properties of some eco-friendly composites. The proposed materials are based on a biodegradable polymer matrix (i.e. ethyl cellulose), in which were inserted variable quantities of two sorts of highly polarizable additives, such as bentonite and carbon nanotubes. The permittivity of the continuous cellulosic phase is determined by means of the theory derived from the connectivity parameters. Afterwards, several mixing rules are employed for prediction of the dielectric properties of the composite samples. Theoretical analysis of the mechanical properties is also performed in a similar manner. The attained results display significant importance in fabrication of high-performance eco-composites having the wanted requirements for use in electrical energy storage devices.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0762, within PNCDI III

References:

- [1] S.S. Nair, S.K. Mishra, D. Kumar, POLYMER-PLASTICS TECHNOLOGY AND MATERIALS, 60, pp. 626-649 (2021).
- [2] S. Agarwal, MACROMOLECULAR CHEMISTRY AND PHYSICS, 221, 2000017 (2020).
- [3] A. Folino, A. Karageorgiou, P.S. Calabrò, D. Komilis, SUSTAINABILITY, 12, 6030 (2020)

*) Author for Correspondence: Andreea Irina Barzic, e-mail: irina_cosutchi@yahoo.com

O.2. Behaviour of composite materials with polymer matrix / metal powders

D.E.Gavrilă¹, A.Caramitu², S.Mitrea², V.Stoian¹

*¹Physics Department, Faculty of Applied Sciences, University POLITEHNICA of
Bucharest*

*²National Institute of Research and Development for Electrical Engineering ICPE-
CA Bucharest*

The interest for polymer / metal filler composite materials results from the fact that their electrical properties are close to those of metals and the mechanical characteristics and processing methods are close to those of plastics. In such composite there is the possibility of controlling the electrical and the physical characteristics, which determines a wide variety of their applications. The composites obtained may have a range of excellent properties, high electrical and thermal conductivity, high specific strength and modulus, high temperature resistance, corrosion resistance etc.

The article studies the characteristics of composite materials with polypropylene and polyethylene matrix with Fe and Al metal powders. A comparative study of the characteristics for different quantities of metal powders (3, 5, 8%) is made in connection with the dimensions of the metallic particles, the mechanical and thermal characteristics and the morphological changes of the composites. It was proved the existence of the agglomeration of particles from powders prior the preparation of the composite samples. For this reason in the article average values of their dimensions were used. The agglomerations of the particles are persistent and do not decompose in totality during extrusion and injection processing, their number increasing with increasing content of metal powders. Electrical behaviour at different frequencies was investigated at temperatures close to room temperature by Dielectric Spectroscopy. The dependence of losses on the nature of polymers, metal powders, dimensions and the amount of particles was shown. Important data were obtained for materials in which the metal powders have nano dimensions. The results obtained were correlated with changes in mechanical and thermal characteristics. Morphological analyzes of metal powders and composites were determined by DSC and SEM analyzes. Different variations of the crystallinity are observed for the two polymers. Particles with nano dimensions penetrate more easily both in the amorphous domains and in crystalline domains.

O.3.

Nanoparticles of cobalt doped magnetite for tumor treatment

Helmina Ardeleanu^{1*}, Iordana Așefănoaei¹, Dorina Creanga¹

¹ University Alexandru Ioan Cuza, Iasi, Romania
Email: ardeleanu_helmina@yahoo.com

The theoretical and practical approach of the thermal behavior of cobalt ferrite nanoparticle behavior (Co-MNPs), used in experimental biomedicine aiming tumor hyperthermia, was the main objective of this work.

The potential heating of cancerous tissue cells was investigated on the hypothesis that the tumor's center had been injected with Co-MNP aliquot. Mathematical modeling was done based on the results of the magnetometry investigation, carried out on the cobalt ferrite nanoparticle synthesized by us (1-2). Pennes' bioheat equation model, underlying the theoretical study developed in here, as the most extensively used thermal model, was applied considering the magnetization hysteresis loop area of each Co-MNP sample (for different ratio of Cobalt). Graphical representations of the temperature variation with the distance to the tumor center as resulted from the equation solution were discussed comparatively.

Further research into the modeling of heat transfer as a function of magnetic nanoparticle concentration was planned.

References:

[1] A. Sathya, $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$ Nanocubes for Theranostic Applications: Effect of Cobalt Content and Particle Size, Chem. Mater. 2016, 28, 6, 1769-1780.

[2] S Laurent, Magnetic iron oxide nanoparticles: synthesis, stabilization, vectorization, physicochemical characterizations, and biological applications, Chemical Reviews 2008, 108, 2064-2110.

*) Author for Correspondence: Ardeleanu Helmina

O.4.

Dielectric features of materials based on oxide nanopowders

C.-P. Ganea*, I. Zgura, L. Frunza

National Institute of Materials Physics, 077125 Magurele, Romania

Email: paul.ganea@infim.ro

Dielectric spectroscopy (DS) is an important technique to study materials as such or in confinement, as function of frequency and temperature. In order to establish a correspondence between the composition of the samples and their dielectrical properties, we have to make a detailed analysis which allows describing the mechanisms at the molecular scale. Often this analysis is hard to be performed: The complex shape of the permittivity spectra and the important contribution of electrical conductivity require a special method of analysis. Several methods have been developed, but all these methods, although accurate, are applied with difficulty due to complicated numerical calculations.

We propose a sufficiently precise but much simpler numerical approach, with two different procedures, that can be applied for the deconvolution of complex spectra in DS. One of proposed procedures has the advantage that it uses, in most cases, non-specialized software for processing the results of DS e.g. Origin. In order to highlight the differences and advantages of the approach used, these together with other mathematical methods are presented.

In short, it is assumed a logarithmic distribution of the relaxation times

$$\varepsilon^*(\omega) = \varepsilon' - i\varepsilon'' = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \int_{-\infty}^{+\infty} \frac{g(\ln\tau)}{1 + i\omega\tau} d(\ln\tau) \quad (1)$$

An approximation is obtained for the calculation of dielectric loss only for polarization components, using logarithmic derivative of permittivity:

$$\varepsilon_{deriv}'' = -\frac{\pi}{2} \frac{\partial \varepsilon'(\omega)}{\partial(\ln\omega)} \quad (2)$$

if the electrical conduction is frequency independent. The logarithmic derivative is the starting equation for our procedures which provide us the characteristic times of the dielectric relaxation processes and, consequently, the activation energy.

The proposed procedures have recently been applied to the complicated DS experimental data for ZnO and ZnO-nematic mixture E7 composites [1] and here their results are discussed in detail.

Acknowledgements: The authors acknowledge the funding through Core Program PN19-03 (contract no. 21 N/08.02.2019), from Romanian Ministry of Education and Research and financial support under Projects No. 43/2021 (IUCN ORDER no. 365/11.05.2021).

References:

[1] I. Zgura, C.P. Ganea, et al., to be submitted 2022.

*) Author for Correspondence:

O.5.

Orbital character of two dimensional electron gas at an oxide interface

M. A. Husanu^{1*}, A. Iancu¹, D. G. Popescu¹, C. Chirila¹, C. M. Teodorescu¹

¹ *National Institute of Materials Physics, Atomistilor 405A, 077125 Magurele, Romania*

The emergence of metallic conductivity in the form of a two dimensional electron gas (2DEG) at the interface between two insulators opens the way for new avenues in oxide electronics [1]. Here we disentangle the orbital character of the 2DEG which appears at the interface between SrTiO₃ and LaAlO₃ by direct visualization of the electronic band structure [2-4]. The soft X-ray photoemission experiments performed with synchrotron radiation reveal in addition to the intrinsic electronic structure of the interface 2DEG, derived from the Ti t_{2g} orbitals, the occurrence of oxygen vacancies (OV) states manifested as defect-like non dispersive bands at ~1.5 eV below the Fermi energy. Their dimensionality is explored in angle resolved photoemission while navigating in the k_z direction of the reciprocal space where isoenergetic scans reveal their three dimensional character.

The oxygen vacancies are detrimental for high mobility devices due to the scattering of the itinerant electrons with the OVs. One way to limit such effects is to engineer the interface bandstructure such that only the bands which lie close to the contact region are occupied, while the states which experience the scattering with the OVs remain empty. This was achieved by doping the interface with transition metals with localized electronic levels below the energy of the Ti 3d ones. It is shown that the gradual filling of the bands and occupation of those protected from the scattering with OVs lead to an enhancement of the mobility by two orders of magnitude.

Keywords: X-ray Photoelectron Spectroscopy, two dimensional electron gas, high mobility interface

Acknowledgement

This work was financed by the Romanian UEFISCDI Agency under Contracts PCE 96/2021.

References:

- [1] A. Ohtomo, , H. Y. Hwang, Nature 427, 423-426 (2003)
- [2] A. Chikina et al. ACS Nano 15 (3), 4347-4356 (2021)
- [3] V. Strocov et al. Phys Rev. Mater. 3, 106001 (2019)
- [4] V. Strocov et al. Electron. Struct. 4, 015003 (2022)

*E-mail for corresponding author: ahusanu@infim.ro

O.6. Synthesis and characterization of cellulose acetate-TiO₂ polymeric membrane for water and wastewater treatment

S. Căprărescu^{1*}, V. Purcar², C. Modroga³, A. M. Dăncilă³ and O. D. Orbuleț³

¹ University Politehnica of Bucharest, Faculty of Chemical Engineering and Biotechnologies, Inorganic Chemistry, Physical Chemistry and Electrochemistry Department, Ghe. Polizu Street, no. 1-7, 011061 Bucharest, Romania

Email: simona.caprarescu@upb.ro

² National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, Splaiul Independentei no. 202, 6th District, 060021, Bucharest, Romania

³ University Politehnica of Bucharest, Faculty of Chemical Engineering and Biotechnologies, Analytical Chemistry and Environmental Engineering Department, Ghe. Polizu Street, no. 1-7, 011061 Bucharest, Romania

In the last years, polymeric membrane that contains different types of natural or synthetic polymers and metal oxide nanoparticles have been synthesized [1-3]. These polymeric membranes were successfully used in the various membrane processes for different water and wastewater treatment [4-6].

The main goal of the present study was to synthesize the polymeric membrane based on cellulose acetate-TiO₂ nanoparticles by the phase inversion technique. The polymeric membrane was characterized through the Fourier Transform Infrared Spectroscopy (FTIR), microscopy analysis, and Electrochemical Impedance Spectroscopy (EIS). The FTIR spectra of the obtained polymeric membrane showed that the incorporation of TiO₂ nanoparticles into the polymer matrix chains lead to the modification of the absorption band intensities. The microscopy analysis of the polymeric membrane containing TiO₂ nanoparticles showed that the nanoparticles were uniformly distributed in the polymer matrix. The impedance results indicated that the TiO₂ induced a higher protonic conductivity. The obtained polymeric membranes could be used in the various membrane processes for the removal of different target pollutants (e.g., metallic ions, dyes, microorganisms) from waters and wastewaters.

References:

- [1] F. Galiano, K. Briceno, T. Marino, A. Molino, K.V. Christensen, A. Figoli, JOURNAL OF MEMBRANE SCIENCE, 564, 2018, pp. 562-586.
- [2] L.Y. Ng, A.W. Mohammad, C.P. Leo, N. Hilal, DESALINATION, 308, 2013, pp. 15-33.
- [3] M. Zahid, A. Rashid, S. Akram, Z. Rehan, W. Razzaq, JOURNAL OF MEMBRANE SCIENCE & TECHNOLOGY, 8, 2018, pp. 1-20.
- [4] E.O. Ezugbe, S. Rathilal, MEMBRANES, no. 10, 2020, 89.
- [5] S. Căprărescu, R. G. Zgârian, G. T. Tihan, V. Purcar, E. E. Totu, C. Modroga, A.-L. Chiriac, C. A. Nicolae, POLYMERS, 12, no. 8, 2020, 1792.
- [6] S. Căprărescu, C. Modroga, V. Purcar, A. M. Dăncilă, O. D. Orbuleț, POLYMERS, 13, no. 11, 2021, 1875.

*) Author for Correspondence: simona.caprarescu@upb.ro

Acknowledgements: This work was supported by the INCDCP ICECHIM Bucharest 2019-2022 Core Program PN. 19.23–Chem-Ergent, Project No.19.23.03.01.

O.7. FORMAL ACTIVITIES TO LEARN ABOUT NEW MATERIALS AND TECHNOLOGIES USED IN MAKING SENSORS AND ACTUATORS

L.C Farcas^{1,2*}, C. Enachescu¹

¹Alexandru Ioan Cuza University of Iasi, Faculty of Physics, Iasi, Romania

²"St. John of La Salle" Technological High School, Pildești, Romania

Email: lidycera@yahoo.com

The teaching of physics may be made easier and more efficient and pleasant for (young) students by using a wide variety of devices based on sensors, actuators and microcontrollers can be made. Therefore, in order to satisfy their practical needs, the physics teachers should be motivated to build themselves such devices.

The paper describes how practical solutions can be found for the realization of sensors, actuators and experimental physics devices that meet the needs of students and support the efforts of teachers to introduce new technologies into the learning process as a factor of inspiration and motivation for students who wish to pursue a career in engineering.

In the Technological High School "St. John of La Salle" Pildești from Neamț county, using a series of materials that anyone has at their disposal and the simplicity of the Arduino microcontroller and the open-source community, we have developed a series of tools that can be used in physics experiments, activities and laboratories to investigate, measure and analyze the phenomena of physics. The formal activities are carried out within a Curriculum in local development (CDL) and have as their starting point the educational resources made available by the great company Microsoft in the Microsoft Education section. As the finality of the practical activities carried out within the CDL, the students made a sensor from a Cu wire used to demonstrate Faraday's law. The sensor can also be used as a metal detector in certain environments, as the coil has a "receiver" behavior of magnetic field lines produced various devices that generate magnetic fields.

The impact of the activities carried out within the CDL on the students was analyzed in two stages: firstly the attitude of the students was studied using non-verbal language - body language, while the second stage of the analysis consisted in the application of a satisfaction questionnaire in order to identify the students interested in participation to this type of activities but also the satisfaction of involvement in such activities

References:

[1] M. G. Lodico, D. T. Spaulding, K. H. Voegtle, *Methods In Educational Research - From Theory to Practice*, First Edition, Jossey-Bass, San Francisco, SUA, 2006, pp.5

[2] S. Alapati, S. Yeole, *Development of flex sensor array to identify damage on sheet metal*, International Journal of Engineering Science and Technology, Vol. 9 No.10 Oct 2017, pp 967-974

[3] *A Guide to Conductivity Measurement – Theory and Practice of Conductivity Applications*, Mettler-Toledo AG, Analytical, pp 6-12

*) Author for Correspondence: lidycera@yahoo.com

O.8. Structure–property relationships in photopolymerizable systems : Effect of composition and resulting physical properties of acrylates based copolymers

D. Bendeddouche^{1*}, G F-Z. HAKEM¹, U. MASCHKE ², L. BEDJAOUI-ALACHAHER¹

¹ Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou Bekr Belkaïd Tlemcen, 13000, Tlemcen, Algeria

Email^{1*}: djazia.bendeddouche@univ-tlemcen.dz

² University of Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Materials and Transformations Unit, Lille, France

Photoinitiated linear polymers were formed by copolymerization of isobornyle acrylate (IBoA) with 2-ethylhexyle acrylate (2-EHA). The copolymers were elaborated by varying the weight proportion of monomers. The developed poly (IBoA-co-EHA) was characterized by Fourier Transform Infrared - Attenuated Total Reflexion (FTIR-ATR) (Figure 1) and Proton Nuclear Magnetic Resonance (¹H NMR) spectroscopy for structural analysis. Their physical properties were evaluated by the Differential Scanning Calorimetry (DSC) and the Dynamic Mechanical Analysis (DMA). Depending on weight proportion of monomers, the glass transition temperatures (T_g) from DSC and DMA varied respectively from 202 to 313 K and 317 to 350 K. This evolution has been modeled theoretically by applying the equations of Fox, Gordon Taylor and Brekner-Schneider-Cantow, on the experimental data of the DSC. The effect of composition on copolymer structure and resulting physical properties such as stiffness increased with the addition of (IBoA), due to their large cyclic side groups [1,2].

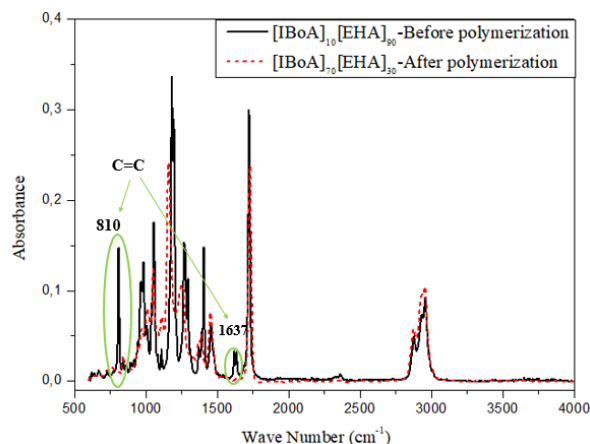


Figure 1. FTIR spectra of Cop[IBoA]₇₀[EHA]₃₀, Before and After polymerization.

References:

- [1] N. Zeggai, COMPOSITE SCIENCE AND TECHNOLOGY, 219, 109213 (2022).
- [2] D. Merah, JOURNAL OF POLYMER RESEARCH, 29, 279 (2022).

O.9. Corrosion protection of metallic substrates by silane-based coatings

D. Bala^{1,*}, A. Sfetcu¹, M.A. Tănase^{1,2}, L.O. Cintează¹

¹University of Bucharest, Faculty of Chemistry, Department of Physical Chemistry, 4-12
Regina Elisabeta, 030018 Bucharest, Romania

²INCDCP-ICECHIM Bucharest, 202 Spl. Independentei, 6th district, Romania

dbala@gw-chimie.math.unibuc.ro, alexandru.sfetcu@s.unibuc.ro, maria.a.tanase@gmail.com,
ocinteza@gw-chimie.math.unibuc.ro,

The corrosion protection of three silane-based coatings on copper and aluminium substrates was investigated in 3.5 % NaCl solution. For this purpose, tetraethoxysilane (TEOS), vinyltriethoxysilane (VTES) and (3-glycidoxypropyl)trimethoxysilane (glyTES) were coated onto a Cu and Al substrates by the sol–gel deposition method. The prepared films were compared with others embedded with zinc oxide (ZnO) nanoparticles. The corrosion behavior of uncoated and coated copper and aluminium plates was evaluated using linear sweep voltammetry. The corrosion parameters, including the corrosion potential (E_{corr}), corrosion current density (I_{corr}), polarization resistance (R_p), and corrosion rate (CR), obtained for the treated metallic supports, are determined for bare and coated copper and aluminium plates. The results revealed significantly lower values of the corrosion rates and current density, higher corrosion resistances for all the protected surfaces. The best anticorrosive performance was obtained for the ZnO film-coated plate [1, 2]. The hydrophobicity of films was characterized by contact angles measurements.

[1] L. O. Cinteza, D. Bala, C. Tablet, E. Alexandrescu, R. Somoghi, V. Purcar, C. Gifu, R. Ianchis, C. Petcu, JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS, 2017, 19 (11-12), 800.

[2] C.L. Nistor, C.I. Mihaescu, D. Bala, I.C. Gifu, C.M. Ninciuleanu, S.G. Burlacu, C. Petcu, M.G. Vladu, A. Ghebur, L. Stroea and L.O. Cinteza, COATINGS, 2022, 12, 253

O.10.

Physical and chemical properties of cyano-containing polyimide/azo-chromophore systems designed for flexible electronic products

I. Stoica^{1*}, E.-L. Epure², A. I. Barzic¹, M. Asandulesa¹, C. Ursu¹, I. Mihaila³,
A.-D. Diaconu¹, I. Sava¹

¹ "Petru Poni" Institute of Macromolecular Chemistry, Iasi-700487, Romania

² Faculty of Chemical Engineering & Environmental Protection, "Gheorghe Asachi"
Technical University, Iasi - 700050, Romania

³ Integrated Center of Environmental Science Studies in the North-Eastern Development
Region (CERNESIM), "Alexandru Ioan Cuza" University of Iasi, Iasi - 700506, Romania

Thermostable and flexible polymer films have been intensively used in the field of electronics. A great deal of attention was ascribed to polyimides (PIs), which are recognized for displaying advantageous combination of chemical resistance, mechanical strength and good insulation abilities [1], properties highly desirable for application in flexible electronics [2]. Given the aforementioned context, this work had the goal to design novel supramolecular PI systems by blending the cyano-containing PI precursor with certain azo-chromophores and investigate their chemical and physical properties. The thermally treated samples were examined from structural point of view. All the polymers under investigation revealed a very good thermal stability. Dielectric properties were also evaluated. The capacity of the PI films to develop surface relief gratings under UV laser exposure was assessed via Atomic Force Microscopy, which highlighted the role of azo-chromophore type on the generated micro/nano patterns onto the surface of the film samples. The impact of the intrinsic factors on the micro and nano scale compartment, determined by isomerization was explored by molecular dynamics simulations. The results are discussed in regard to the applicability of the attained PI systems as flexible supports for electronic products.

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number TE 25/9.05.2022 within PNCDI III (code PN-III-P1-1.1-TE-2021-1044).

References:

- [1] A. Sezer Hicyilmaz, A. Celik Bedeloglu, SN APPLIED SCIENCES, 3, pp. 363 (2021).
- [2] I. Sava, I. Stoica, I. Topala, I. Mihaila, A.I. Barzic, POLYMER, 249, pp. 124829 (2022).

*) Author for Correspondence: Iuliana Stoica, e-mail: stoica_iuliana@icmpp.ro

O.11. Technology for obtaining the amorphous luminophore composition $\text{As}_2\text{S}_3:\text{Eu}(\text{DBM})_3\text{Phen}$

M. Iovu^a, V. Verlan^{a*}, O. Bordian^a, I. Culeac^a, A. A. Popescu^{b*}, and D. Savastru^b

^{a)} *Institutul de Fizică Aplicată, Str. Academiei 5, MD-2028 Chisinau, R. Moldova*

^{b)} *Institutul National de Cercetare-Dezvoltare pentru Optoelectronica INOE 2000, Str. Atomistilor 409, Magurele, Romania.*

^{*}) *Author for Correspondence: vverlan@gmail.com; apopescu@inoe.ro;*

The aim of the work is to obtain the amorphous luminophore composition based on As_2S_3 and $\text{Eu}(\text{DBM})_3\text{Phen}$ with enhanced luminescence properties.

Thin films of the amorphous composition $\text{As}_2\text{S}_3:\text{Eu}(\text{DBM})_3\text{Phen}$ were obtained on optical glass substrate by the method of simultaneous thermal co-evaporation in vacuum ($2 \cdot 10^{-5}$ mm. Hg) from two tantalum evaporators: "quasi-closed" for As_2S_3 [1] and cross-shaped for $\text{Eu}(\text{DBM})_3\text{Phen}$. Transparent amorphous films were obtained with thicknesses in the range of $125 \div 1000$ nm.

On Fig.1. is shown the sample of the amorphous composition $\text{As}_2\text{S}_3:\text{Eu}(\text{DBM})_3\text{Phen}$ with two different thicknesses: $0.9 \mu\text{m}$ on the left and $3 \mu\text{m}$ on the right side. Upon illumination with violet light ($450 - 500$ nm) abundant red color luminescence appears. On Fig. 2 the photoluminescence (PL) spectrum upon excitation with blue laser is presented. The PL maximum is at 614 nm and its half-width is less than 10 nm, which can be considered as laser luminescence. The material has intense narrow-band red luminescent at room temperature.

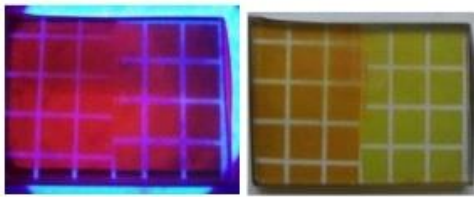


Fig. 1. Thin film network (left) and Red luminescence (write).

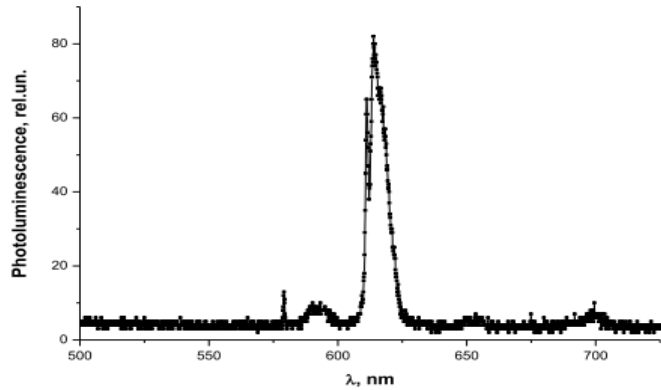


Fig. 2. PL spectrum of the material: $\lambda_{\text{ex}}=405\text{nm}$, $T=300$ K.

This work was funded by ANCD Moldova through projects 20.80009.5007.14, 22. 80013.5007.6BI, and by the Romanian Ministry of Research, Innovation and Digitalization, grant number [PN-III-P4-PCE-2021-0585].

Reference

[1] A. A. Popescu, M. Mihăilescu, C. Negutu et. all., "Preparation of chalcogenide bulk and thin films and their characterization using optical methods", U.P.B. Sci. Bull., Series A, Vol. 76, No. 3, pp.214 -222.

O.12.

Light-emitting materials based on nematic liquid crystals doped with double cyclopalladated complexes

Daiana G. Mitrea¹, Monica Iliș¹, Doina Mănăilă-Maximean², Viorel Cîrcu^{1*}

¹Department of Inorganic Chemistry, University of Bucharest, Bucharest, Romania
Email: daiana.mitrea@drd.unibuc.ro, *viorel.circu@chimie.unibuc.ro

²Department of Physics, University Politehnica of Bucharest, Bucharest, Romania

In the past decade, the organometallic complexes with photoluminescent properties have attracted a significant attention, due to their possibility to be used in the manufacturing of various sensing or optical devices. A promising alternative to the well-known triplet emitters such as Ir(III) or Pt(II) complexes can be considered the luminescent Pd(II) complexes. Cyclopalladated compounds have impressive photophysical properties due to the strong ligand field imposed by the cyclometalated organic ligands, which make them suitable for practical applications in the design of red-shift emitters and OLEDs. Particularly, a tremendous attention was given to luminescent liquid crystals (LLCs) since they are exceptional materials that can display both photoluminescence and anisotropy leading to linearly or circularly polarized emission. In this regard, we were interested to prepare nematic LLC based on Pd(II) complexes. Thus, a series of double cyclopalladated complexes based on imine derivatives and N-benzoylthiourea (BTU) ligands was synthesized and characterized [1]. Further, the obtained Pd(II) compounds were used for the microencapsulation of luminescent liquid crystal (E7 Merck doped with Pd(II) complexes) into poly(methyl methacrylate Merck) by the emulsification solvent diffusion method (ESD) [2]. These complexes were investigated regarding their luminescence and polarized emission properties at room temperature (Figure 1).

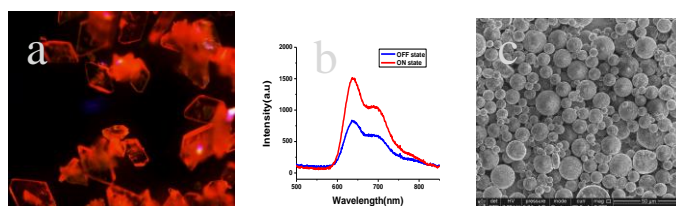


Figure 1. a) Solid state emission of the Pd(II) complex upon UV irradiation; b) Effect of the applied voltage on the PL intensity for the E7+5% Pd (II) complex mixture filled in a planar ITO cell; c) SEM picture of spherical microcapsules.

References:

[1] M. Micutz, M. Iliș, T. Staicu, F. Dumitrașcu, I. Pasuk, Y. Molard, T. Roisnel, V. Cîrcu, Dalton Transactions, 2014; 43, pp.1151-1161.

[2] M. R. Sharifimehr, K. Ayoubi, E. Mohajerani, Journal of Molecular Liquids, 2020, 313, pp. 113576.

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

O.13. Features of self-pulsating InGaN lasers

E. Grigoriev*, S.Rusu, V.Tronciu

Department of Physics, Technical University of Moldova, Chisinau Moldova

*Email: eugeniu.grigoriev@fiz.utm.md

In recent years, due to applications in medicine, blue and blue-violet light lasers (450 and 405 nm) seem to represent an interesting approach for several clinical treatments [1]. In this paper we present theoretical results of the influence of blue light laser parameters on self-pulsations. We studied the influence of the thickness of the saturation absorber, the length of the laser, as well as the lifetime of the charge carriers on the self-pulsation region in terms of several parameters. Figure 1 shows a setup of the investigated laser which consists of the InGaN active layer and a saturation absorber. Both the active layer and the saturation absorber are composed of 3 quantum wells of the InGaN type. The thickness of the active region and saturation absorber is 18 nm and the wavelength is 405 nm. The length of the active layer is 650 μm .

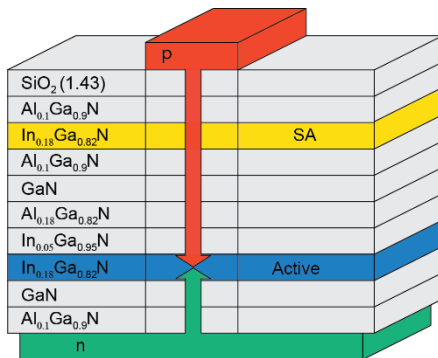


Figure 1. Schematic of the InGaN laser.

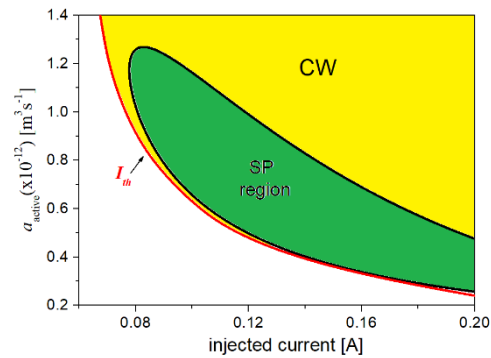


Figure 2 Self-pulsation region.

The theoretical model used to describe the laser dynamics is based on the model proposed in [2]. Fig. 2 shows the curve (black line) calculated for the region with self-pulsations in the plane: the differential amplification coefficient depending on the current injected in the active region. The red line in Fig. 2 represents the border between the operating regions of the laser in "off" and "on" mode. We discuss the possible variations of the differential amplification coefficient. The yellow region marked with CW corresponds to the operating mode of the laser with continuous waves. In the case when the parameter values correspond to green regions, the laser manifests self-pulsations. As mentioned above, the influence of absorber thickness, laser length, as well as the lifetime of the charge carriers on the performance of the self-pulsation regime was also investigated.

[1] Carlo Fornaini Reza Fekrazad Jean-Paul Rocca Shiyong Zhang Elisabetta Merigo Use of Blue and Blue-Violet Lasers in Dentistry: A Narrative Review, Journal of Lasers in Medical Sciences, Vol. 12 (2021), p. e31.

[2] Yamada, M., A theoretical analysis of self-sustained pulsation phenomena in narrow-stripe semiconductor lasers, IEEE J. Quantum Electron., vol. 29, pp. 1330–1336, May 1993.

O.14.

Design and Simulations of Perovskite-Based Solar Cells with Efficiencies Over 30%

S. H. M. A. Hussein^{1,2}, A. Drăgulescu^{3*}

¹ Faculty of Engineering in Foreign Languages, Politehnica University of Bucharest, 1-3 Iuliu Maniu Blvd., Spl. Independenței 313, sector 6, RO-060032, Bucharest, Romania

² ARRK Research & Development SRL, Str. Fabricii De Chibrituri 13-21, Cluj-Napoca, Cluj, Romania

Email: seifhesham96@gmail.com

³ Department of Electronic Technology and Reliability, Politehnica University of Bucharest, 1-3 Iuliu Maniu Blvd., Spl. Independenței 313, sector 6, RO-060032, Bucharest, Romania

Email: dragulescu@yahoo.com

Recently, numerous efforts have been directed towards improving the efficiency of perovskite-based solar cells, as a viable competitor of the ones based on silicon. In this paper, we designed and simulated five different solar cells with perovskite, either alone or in combination with other materials (silicon, copper indium gallium selenide), with the purpose of obtaining high values of the power conversion efficiency (PCE), after performing a suitable selection of compatible materials for the layers and finding the optimum values for the doping concentrations and thicknesses of the active layers. The highest values of the PCE (36.83%, 34.19% and 33.31%) were obtained for solar cells with an active layer of p-type perovskite, n-type perovskite and a combination of perovskite and silicon, respectively. These results are higher than for the perovskite-based solar cells in literature and offer promising perspectives for future practical implementation of such solar cells with efficiencies higher than the traditional technologies based on silicon.

References:

- [1] Messmer, C., Schön, J., Lohmüller, S., Greulich, J., Luderer, C., Goldschmidt, J. C., Bivour, M., Glunz, S. W., Hermle, M., "How to make PERC suitable for perovskite–silicon tandem solar cells: A simulation study", *Prog. Photovolt. Res. Appl.* 30, 1023–1037 (2022).
- [2] Khattak, Y. H., Vega, E., Baig, F., Soucase, B. M., "Performance investigation of experimentally fabricated lead iodide perovskite solar cell via numerical analysis", *Materials Research Bulletin* 151, 111802 (2022).
- [3] Salah, M. M., Zekry, A., Shaker, A., Abouelatta, M., Mousa, M., Saeed, A., "Investigation of Electron Transport Material-Free Perovskite/CIGS Tandem Solar Cell", *Energies* 15, 6326 (2022).
- [4] Jošt, M., Köhnen, E., Al-Ashouri, A., Bertram, T., Tomšič, Š., Magomedov, A., Kasparavicius, E., Kodalle, T., Lipovšek, B., Getautis, V., Schlatmann, R., Kaufmann, C. A., Albrecht, S., Topič, M., "Perovskite/CIGS Tandem Solar Cells: From Certified 24.2% toward 30% and Beyond", *ACS Energy Lett.* 7(4), 1298–1307 (2022).

*) Author for Correspondence

O.15. Nanoscale Imaging of Polymer Coated Gold Nanoparticles with Scattering-type Scanning Near-Field Optical Microscopy

Stefan G. Stanciu¹, Denis E. Tranca¹, Giulia Zampini², Radu Hristu¹, George A. Stanciu¹, Xinzhong Chen^{3,4}, Mengkun Liu^{3,4}, Harald A. Stenmark⁵, and Loredana Latterini²

¹Center for Microscopy-Microanalysis and Information Processing, Politehnica University of Bucharest, Romania.

²Department of Chemistry, Biology and Biotechnology, Perugia University, Italy.

³Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA.

⁴National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York, USA.

⁵Department of Molecular Cell Biology, Institute for Cancer Research, Oslo University Hospital, Oslo Norway

Gold nanoparticles (Au NPs) represent one of the most popular types of nanomaterials as they are stable, easy to synthesize in various shapes and sizes with reproducible procedures and, well bio-compatible when delivered for therapeutic purposes¹. As polymers are also highly tailorable and widely used in many biomedical topics, using these materials to coat Au NPs significantly augments the number of applications of both materials classes, together with their efficiency², given the multivalence of their interplay. In this work we investigate polymer coated Au-NPs with scattering-type Scanning Near-Field Optical Microscopy (s-SNOM), **Fig. 1**, an emerging optical characterization technique capable to provide optical information at nanoscale resolution³. s-SNOM amplitude and phase images were acquired in the visible frequency range, under illumination with 532nm, a wavelength falling in the absorption band of the investigated instances made of an Au core covered by composite polymeric shells, consisting of polystyrene sulfonate (PSS) and poly(diallyldimethylammonium chloride) (PDDA), of different thicknesses. Our results can facilitate studies and applications in nanomedicine and nanotechnology where the precise positioning of AuNPs with nanoscale resolution is needed. Such applications can also benefit of other opportunities offered by s-SNOM, such as quantitative dielectric function mapping⁴. Additionally, the results presented here can be relevant for other NPs comprised of different polymeric-shell metallic core combinations. We discuss as well perspectives for augmenting s-SNOM imaging with artificial intelligence.

Keywords: scattering-type scanning near-field optical microscopy; polymer coated Au nanoparticles

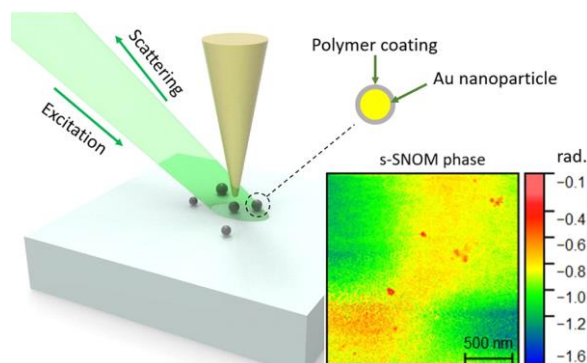


Figure 1: s-SNOM phase imaging of PSS/PDDA coated Au NPs⁵.

References:

- Elahi, N., Kamali, M., Baghersad, M.H., (2018) *Talanta*, 184, 537-556.
- Capek, I. (2017) *Advances in Colloid and Interface Science*, 249, 386-399.
- Chen, X., Hu, D., Mescall, R., You, G., Basov, D.N., Dai, Q., Liu, M., (2019) *Advanced Materials*, 31, 1804774.
- Stanciu, S.G., Tranca, D.E., Pastorino, L., Boi, S., Song, Y.M., Yoo, Y.J., Ishii, S., Hristu, R., Yang, F., Bussetti, G., Stanciu, G.A., (2020) *ACS Applied Nano Materials*, 3, 1250-1262
- Stanciu, S.G., Tranca, D.E., Zampini, G., Hristu, R., Stanciu, G.A., Chen, X., Liu, M., Stenmark, H.A. and Latterini, L., (2022). *ACS omega*, 7(13), 1353-11362.

O.16. Rheological aspects on some hydrogels e-beam crosslinked

T. Staicu¹, M. Demeter², M. Ilis³, V. Circu³, and M. Micutz^{1*}

¹ Department of 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 National Institute for Lasers, Plasma and Radiation Physics (INFLPR), Atomiștilor 409, 077125, Măgurele, Romania

Email: maria.dumitrascu@inflpr.ro

³ Department of Inorganic Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blvd, Bucharest 030018, Romania

Email: monica.ilis@g.unibuc.ro; viorel.circu@g.unibuc.ro

Nowadays, hydrogels are receiving increasing attention mainly due to their applicability in biomedicine (cell culture, contact lenses, wound dressings, drug delivery), as superabsorbents (with equilibrium swelling of at least 1000%) or for solid surfaces cleaning (in the case of solvent-sensitive surfaces). Apart from the methods of morphostructural characterization, hydrogels are almost mandatorily to be studied rheologically, including the pre-hydrogel state prior to crosslinking. Several sorts of novel composite polymer-based aqueous compositions, both in viscous and hydrogel state, were investigated by dynamic rheometry at room temperature in the region of linear viscoelasticity. Their rheological behavior revealed particular dependencies of specific quantities (loss and storage moduli, loss tangent, dynamic viscosity) as a function of the formulations chosen, the irradiation dose and the frequency of the applied oscillatory deformation.

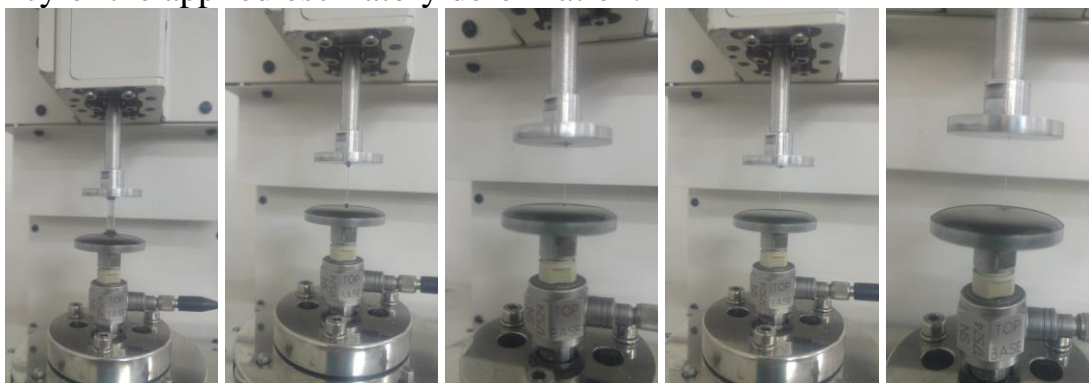


Figure 1. Time evolution of a polymer-based pre-hydrogel after rheological measurements and during detaching it from the upper plate of rheometer at the same gap between plates (18500 μm) and different values of flow time (from left to right: 0, 5, 20, 30, 145 min)

Acknowledgement

The study was supported by grants of the Romanian Authority for Scientific Research, CNCS-UEFISCDI, project numbers PN-III-P2-2.1-BG-2016-0397 and PN-III-P1-1.1-PD-2021-0552.

* Corresponding author