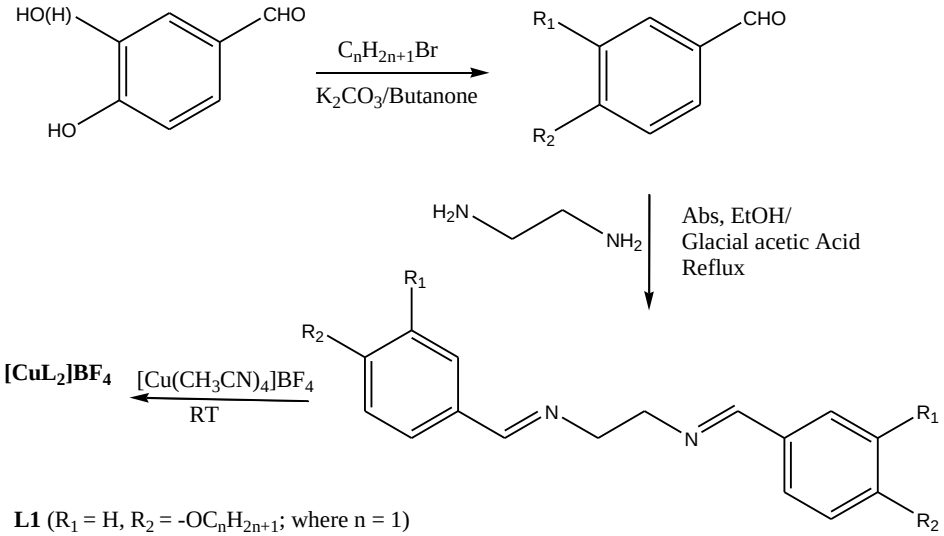
VIRTUAL ABSTRACT BOOK – POSTER SESSION PAPERS

1. Synthesis and characterization of functional materials

P.1.
Design of liquid crystals based on copper (I) complexes with Schiff bases

M. Alkali [1] and V. Cîrcu [1*]
[1] University of Bucharest, Department of Inorganic Chemistry, Romania
Email: Muhammed.alkali@s.unibuc.ro
*Corresponding author: viorel.circu@chimie.unibuc.ro

Abstract: A new set of copper(I) complexes **[CuL$_2$]BF$_4$** have been prepared from Schiff bases [ethane-1,2 diyl)bis(1-(4-(methyloxy)phenyl)methanimine **L1,** ethane-1,2-diyl)bis(1-(4-(hexyloxy)phenyl)methanimine **L2,** and ethane-1,2-diyl)bis(1-(3,4 bis(octyloxy)phenyl)methanimine **L3**]. The Schiff bases prepared for this work (**L2** & **L3**) have not been reported elsewhere from the best of our knowledge. The complexes were prepared by reacting the Schiff bases with the copper(I) precursor, **[Cu(CH$_3$CN)$_4$]BF$_4$** upon the variation of different reaction and solvent conditions. The complexes, **[Cu(L2)$_2$]BF$_4$** and **[Cu(L3)$_2$]BF$_4$** appeared as yellow oils upon which further processing was employed to afford the solid. Both the Schiff base and new copper(I) complexes were characterized with ^{1}H & ^{13}C NMR. Furthermore, preliminary investigations on the liquid crystalline property of both the complexes and the ordinary Schiff base ligands were carried out using a polarizing optical microscope.



L1 (R_1 = H, R_2 = -OC_nH_{2n+1}; where n = 1)
L2 (R_1 = H, R_2 = -OC_nH_{2n+1}; where n = 6)
L3 (R_1 = R_2, R_2 = -OC_nH_{2n+1}; where n = 8)

Figure: Scheme for the preparation of Schiff base and the corresponding copper complexes.

P.2. Synthesis, Structural Characterization and Photoluminescent studies of schiff base ligand First Row–Transition Metal Complexes

Jocelyn N. Kuate[1], Paboudam G. Awawou[1], Viorel Cîrcu[2*], Peter T. Ndifon[1*], Marilena Ferbinteanu[2]

[1] Department of Inorganic Chemistry, Faculty of Science, University of Yaounde I, Yaounde, Cameroon

Email: Jocelynjomkam@gmail.com

[2] University of Bucharest, Bucharest, Roumania

Email: viorel.circu@chimie.unibuc.ro

Nowadays, the search for new materials possessing multifunctional properties is a major challenge for material scientists. The design of metal complexes using different organic ligands has given rise to a wide range of molecular systems which find applications in optoelectronics, pharmaceutical, catalysis and biological systems [1]. However, a few reports have appeared on the prospective study of photoluminescent property of first row transition metal complexes. In the present work, the synthesis and structural characterization of a Schiff base and its first row divalent Cu(II), Co(II) and Ni(II) complexes are reported. All the synthesized compounds were characterized by physico-chemical and spectral techniques. The ligand and metals ions reacted in the 2:1 molar ratio. On the basis analytical data a square planar geometry are proposed for Ni (II) and Cu(II) and tetrahedral for Co(II) complexes, in which Schiff base acts as a bidentate ligand, coordinating to the metal ions through the azomethine nitrogen and sulphur of thiosemicarbazone moiety. The single crystal X-ray structure of Ni(II) is reported. The ligand and its metal complexes were tested for their possible photoluminescent potentials.

References:

[1] P. Ghanghas, A. Choudhary, D. Kumar, K. Poonia, Coordination metal complexes with Schiff bases: Useful pharmacophores with comprehensive biological Applications, *Inorganic Chemistry Communication*, 130, no.2, pp 1087-1100.

P.3.
Synthesis and Characterization PMMA/CaAl-Layered Double Hydroxide Nanocomposites via Solvent Blending Technical

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

[1] University Abubekr Belkaid, Faculty of Science, Macromolecules Research Laboratory (MRL),Tlemcen, Algeria.
Email: m_hamouni@yahoo.fr

[2]Institute of Electrical and Electronics Engineering, University of M'hamed-Bougara, Independence Avenue, 35000, Boumerdès, Algeria
Email: zoulisabrina@yahoo.fr

The subject of Polymer nano-composites gets the full attention of industrialists and academic researchers owing to their specific and various features such as specific surface area, pore diameter, thermal stability, mechanical and flame-retardant .
The main objective of this work is to study the effect of the concentration of nanomaterial type CaAl-HDL on the structural, rheological and thermal properties of poly-methylmethacrylate (PMMA). For that, the nanocomposites PMMA/CaAl-HDL were prepared by dispersing CaAl-HDL (with different concentration 1, 3, 5, 7 and 10 wt%) into the PMMA matrix via a solvent blending technical.
The samples obtained were analyzed by different physic-chemical analysis: Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and differential scanning calorimetry (DSC).
According to the results obtained, the thermal stability of the composites compared to pure PMMA, improves by increasing the concentration of the nanomaterial in the composites.
Key words: PMMA, HDL, solvent blending technical, nano-composites.

References:

[1]: BARIK, Sunita, BADAMALI, Sushanta Kumar, BEHERA, Lingaraj, et al. Mg–Al LDH reinforced PMMA nanocomposites: A potential material for packaging industry. Composite Interfaces, 2018, vol. 25, no 4, p. 369-380.
[2]: KUMAR, Manish, CHAUDHARY, Vivek, SURESH, Kelothu, et al. Synthesis and characterization of exfoliated PMMA/Co–Al LDH nanocomposites via solvent blending technique. Rsc Advances, 2015, vol. 5, no 50, p. 39810-39820.
[3]: NOGUEIRA, Telma, BOTAN, Rodrigo, WYPYCH, Fernando, et al. Synthesis and characterization of LDHs/PMMA nanocomposites: Effect of two different intercalated anions on the mechanical and thermal properties. Journal of Applied Polymer Science, 2012, vol. 124, no 3, p. 1764-177.

2. Nanomaterials, metamaterials and nanoelectronics

P.4. Diameter modulated GaAs nanowire arrays via crossing crystallographic pores

Elena I. Monaico

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

The morphologies and properties of the produced porous semiconductor materials are determined by the mechanisms of the pore growth during electrochemical etching of the bulk semiconductor wafers [1]. Depending on the mechanism of growth, pores with different characteristics are formed in terms of their shape, velocity of growth, etc. On the other hand, the pore growing mechanism depends on the characteristics of the initial bulk semiconductor material and the specific anodizing conditions [2,3].

Only crystallographically oriented pores were reported up to now in GaAs crystals subjected to anodization. The main feature of the crystallographically oriented pores, in contrast to current line oriented pores, consists in their ability to intersect each-other and grow at low applied potentials or current densities. The formation of GaAs nanowire arrays aligned perpendicular to the substrate surface was reported for (111)B oriented GaAs substrates in 1M HNO_3 electrolyte via one step anodization [2].

It will be reported that at optimized electrochemical parameters, the growth of perpendicular nanowires to the surface occurs with simultaneous growth of tilted pores intersecting them. As a result, diameter modulated nanowires are obtained due to the penetration of tilted pores through nanowires. The proposed approach is feasible for obtaining GaAs diameter modulated nanowires along the length as long as 200 μm. The tree-dimensional modulation of diameter, including the functionalization with magnetic materials, will give the possibility to increase the area of their applications.

References:

[1] Monaico, E.; Tiginyanu, I.; Ursaki, V. Porous Semiconductor Compounds. *Semicond. Sci. Technol.* **2020**, *35*, 103001, doi:10.1088/1361-6641/ab9477.

[2] Monaico, E.I.; Monaico, E.V.; Ursaki, V.V.; Honnali, S.; Postolache, V.; Leistner, K.; Nielsch, K.; Tiginyanu, I.M. Electrochemical Nanostructuring of (111) Oriented GaAs Crystals: From Porous Structures to Nanowires. *Beilstein J. Nanotechnol.* **2020**, *11*, pp. 966–975, doi:10.3762/bjnano.11.81.

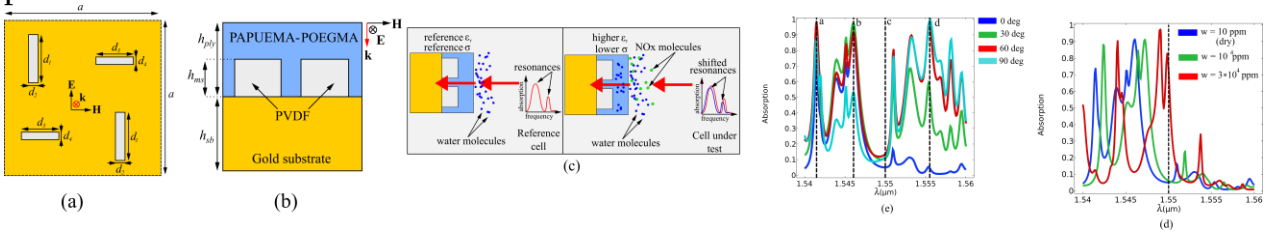
[3] Monaico, E.I.; Monaico, E.V.; Ursaki, V.V.; Tiginyanu, I.M. Evolution of Pore Growth in GaAs in Transitory Anodization Regime from One Applied Voltage to Another. *Surf. Engin. Appl.Electrochem.* **2021**, *57*, pp. 165–172, doi:10.3103/S106837552102006X.

P.5. Atmospheric and Biological Nitrous Oxides Sensors Based on Triggerable-Response Metasurfaces

O. Dănilă[1*], B. M. Gross[2]

[1] University Politehnica of Bucharest, 060042 Bucharest, Romania
Email: octavian.danila@upb.ro
[2] City University of New York, 10031 New York, United States of America
Email: gross@ccny.cuny.edu

We present simulations on a promising NOx gas sensor configuration featuring a metasurface-analyte architecture that is able to detect NOx gases by exploiting triggered hydrophillicity of the poly(oligo(ethylene glycol) methyl ether methacrylate) - POEGMA polymer. Our sensor design is based on a metasurface architecture [1-3] composed of a set of rod-like PVDF elements deposited on a gold substrate. On top of the metasurface, we have deposited an analyte layer with designated thickness. The analyte layer is made up of POEGMA polymer which has been functionalized with a NOx-responsive poly(2-(3-(2-aminophenyl) ureido)ethyl methacrylate) or PAPUEMA monomer [4,5]. This functionalization makes the POEGMA polymer respond to humidity only if NOx molecules are present in the vicinity of the monomer. In this approach, a new class of gas sensors that rely on humidity as a critical input rather than as a parasitic effect can
be developed. Initial proof of concept comparisons to existing sensors will be provided.



(a) (b) (c) (e) (d)

Figure 1: (a),(b) Structure of the metasurface; (c) Operation principle and (d),(e) Simulated spectra

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REFERENCES

[1] Smith, D. R.; Padilla, W. J.; Vier, D. C.; Nemat-Nasser, S. C. and Schultz, S., PHYSICAL REVIEW LETTERS, 84(18), pp. 4184 – 4187, 2000.
[2] O. Danila, JOURNAL OF QUANTITATIVE SPECTROSCOPY AND RADIATIVE TRANSFER, 254, 107209, 2020.
[3] O. Danila, D. Manaila-Maximean, MATERIALS, 14(9), 2201, 2021.
[4] J. Hu, M. R. Whittaker, H. Duong, Y. Li, C. Boyer and T. P. Davis, ANGEWADTE CHEMIE, 53, pp. 7779-7784, 2014
[5] J. Hu, M. R. Whittaker, Y. Li, J. F. Quinn and T. P. Davis, POLYMER CHEMISTRY, 6(13), pp. 2407-2415, 2015.

*) Author for Correspondence:

P.6.
MID-INFRARED RADIATION CONTROL WITH METAL-DIELECTRIC MICROSTRIP NANOANTENNAS

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

[1] Faculty of Mechanics and Mechatronics, University Politehnica of Bucharest, Bucharest, Romania
Email: alexandra.grigore@stud.upb.ro
[2] Faculty of Electronics, Telecommunications and Information Technology, University Politehnica of Bucharest, Bucharest, Romania
Email: ana.barar@upb.ro
[3]Faculty of Applied Sciences, University Politehnica of Bucharest, Bucharest, Romania
Email: doina.manaila@upb.ro
[4]Faculty of Applied Sciences, University Politehnica of Bucharest, Bucharest, Romania
Email: octavian.danila@upb.ro

ABSTRACT: We report theoretical assessments on a metal-dielectric metasurfacebased nanoantenna operating in the 7-10 THz range. Our design is a continuation of previously published work [1,2]. The metasurface is highly responsive to the external electromagnetic field and exhibits a high dynamic range for reflection and absorption. The metasurface is addressable by means of input polarization, and can be used in a series of terahertz applications, from dichroic filters to tunable switches and absorbers.

REFERENCES:

[1] O. Danila. SPECTROSCOPIC ASSESSMENT OF A SIMPLE HYBRID SI-AU METASURFACE-BASED SENSOR IN THE MID-INFRARED DOMAIN, Journal of Quantitative Spectroscopy and Radiative Transfer, **254**(107209), 2020.

[2] O. DanilA, D. Manaila-Maximean, A. Barar, and V. A. Loiko. NON-LAYERED GOLD-SILICON AND ALL-SILICON FREQUENCY-SELECTIVE METASURFACES FOR POTENTIAL MID-INFRARED SENSING APPLICATIONS, Sensors, **21**(16), 5600, 2021.

*) Author for Correspondence: Octavian Dănilă, email: octavian.danila@upb.ro

P.7. METAL-DIELECTRIC FREQUENCY-SELECTIVE SURFACES IN THE TERAHERTZ WINDOW

C. Coman[1], A. Bărar[2], D. Mănăilă-Maximean[3] and O. Dănilă[4,*]

[1] Faculty of Mechanics and Mechatronics, University Politehnica of Bucharest, Bucharest, Romania
Email: cosmin.coman@stud.upb.ro
[2]Faculty of Electronics, Telecommunications and Information Technology, University Politehnica of Bucharest, Bucharest, Romania
Email: ana.barar@upb.ro
[3]Faculty of Applied Sciences, University Politehnica of Bucharest, Bucharest, Romania
Email: doina.manaila@upb.ro
[4] Faculty of Applied Sciences, University Politehnica of Bucharest, Bucharest, Romania
Email: octavian.danila@upb.ro

ABSTRACT: We report theoretical investigations on a modified split ring resonator metasurface architecture, designed to operate in the THz regime. The spectral response of the metasurface is evaluated as a function of variations in the values of the internal ring radius size and linear input polarization state, in terms of reflection, absorption and induced phase, for gold- and copper-polyamide configurations. The configuration is adapted from previous work [Dan21a, Dan21b]. The plasmonic behavior of the surface is evaluated by means of electric field maps taken at frequencies corresponding to the highest resonance peaks.

REFERENCES

[1] O. Danila. SPECTROSCOPIC ASSESSMENT OF A SIMPLE HYBRID SI-AU METASURFACE-BASED SENSOR IN THE MID-INFRARED DOMAIN, Journal of Quantitative Spectroscopy and Radiative Transfer, **254**(107209), 2020.
[2] O. DanilA, D. Manaila-Maximean, A. Barar, and V. A. Loiko. NON-LAYERED GOLD-SILICON AND ALL-SILICON FREQUENCY-SELECTIVE METASURFACES FOR POTENTIAL MID-INFRARED SENSING APPLICATIONS, Sensors, **21**(16), 5600, 2021.

*) Author for Correspondence: Octavian Dănilă, octavian.danila@upb.ro

3. Materials for Sustainable Energy

P.8. Design and theoretical investigations of a MAPbI3/Silicon carbide fractal metasurface for photovoltaic applications

A. Bărar[1,2] and H. Ge[2]

[1] Polytechnic University of Bucharest, Bucharest, Romania
[2] New York University, New York, USA
Email: ana.barar@upb.ro

A very efficient method for optical loss reduction in thin-film solar cell is the use of light trapping metasurfaces. Light trapping consists of incident light absorption, followed by its re-emission and confinement within the active layer of the cell. Thus, the light's optical path in the active layer is increased, leading to an increase in free charge carrier generation and device efficiency. Light trapping metasurfaces allow solar cell thickness reduction and improve device performance. The first approaches used plasmonic structures, such as light trapping metallic nanoparticles embedded in the semiconducting active layer of the cell [1], or corrugated metal back surfaces with light coupling properties [2]. Plasmonic structures were also designed for tandem solar cell configurations, where each semiconducting active layer is separated by nanostructured metal contact that couple different wavelengths of the incident light in the corresponding semiconductor layers [3, 4]. In more recent approaches, non-resonant dielectric nanoscatterers, based on different geometries, are grown on the top surface of the solar cell. According to their geometry and the materials that are used in their fabrication, these metasurfaces exhibit different light-management functions, such as light coupling and trapping [5], which consists of light absorption by the metasurface, and re-emission of photons of lower wavelength than the absorbed wavelength.

This paper reports the design and simulation of a methylammonium lead iodide (MAPbI3) fractal metastructure on a silicon carbide (SiC) substrate. The simulated spectral response of the structure, under incident UV-VIS radiation, is presented and discussed, for potential photovoltaic cell performance enhancement.

References:

[1] Rand, B. P., Peumans, P. & Forrest, S. R. Long-range absorption enhancement in organic tandem thin-film solar cells containing silver nanoclusters. *J. Appl. Phys.* 96, 7519–7526 (2004).

[2] Berini, P. Plasmon–polariton waves guided by thin lossy metal films of finite width: bound modes of symmetric structures. *Phys. Rev. B* 61, 10484–10503 (2000).

[3] Fahr, S., Rockstuhl, C. & Lederer, F. Metallic nanoparticles as intermediate reflectors in tandem solar cells. *Appl. Phys. Lett.* 95, 121105 (2009).

[4] Yao, Y., Liu, H. & Wu, W., Spectrum splitting using multi-layer dielectric meta-surfaces for efficient solar energy harvesting, Appl. Phys. A, 115 (2014).

[5] Garnett, E.; Yang, P. Light Trapping in Silicon Nanowire Solar Cells. Nano Lett. 2010, 10, 1082−1087.

*) Author for Correspondence: A. Bărar, email: ana.barar@upb.ro

4. Electronic, photonic and optoelectronic materials

P.9. General Characterizations As-S-Sb-Te Nanostructured Semiconductors

O. Iaseniuc[1]*, M. Iovu[1], S. Rosoiu[2], M. Bardeanu[2], L.-B. Enache[2], G. Mihai[2,3], O. Bordian[1], V. Verlan[1], I. Culeac[1], I. Cojocaru[1], M. Enachescu[3,4]

[1] Institute of Applied Physics, Str. Academiei 5, MD-2028 Chisinau, R. Moldova
Email: oxana.iaseniuc@gmail.com
[2]Center for Surface Science and Nanotechnology, University Politehnica of Bucharest
Splaiul Independentei 313, 060042, Bucharest, Romania
Email: marius.enachescu@upb.ro
[3]S.C. NanoPRO START MC S.R.L., Mitropolit A. I. Street 40, 110310 Pitesti, Romania
[4]Academy of Romanian Scientists, Ilfov Street, 3, 50044 Bucharest, Romania
Email: secretariat@aosr.ro

Investigation of the chalcogenide glasses of As-S-Sb-Te system are important for their contribution in semiconductor physics, as well as for a wide range of technical applications, such as infrared optics, acousto-optic and all-optical switching devices, ovonic devices, holographic recording media, diffractive optics, photonic crystals, gas sensors, etc. [1-2].

Thin films of As_2S_3-Sb_2S_3-Sb_2Te_3 nanostructured polycrystalline and amorphous materials have been characterized using X-Ray diffraction (XRD), micro-Raman spectroscopy, Scanning Electron microscopy (SEM) and Energy-Dispersive Spectroscopy (EDS) methods.

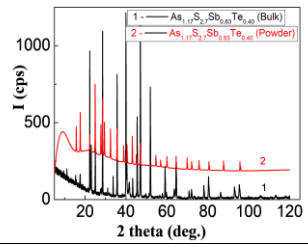

Figure 1. X-Ray Diffraction patterns bulk and powder samples.

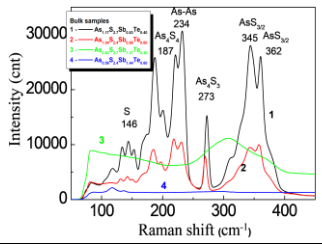

Figure 2. Micro-Raman spectra of bulk samples.

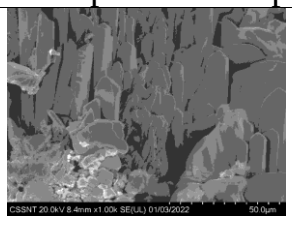

Figure 3. SEM analysis mapping of the polycrystalline bulk samples.

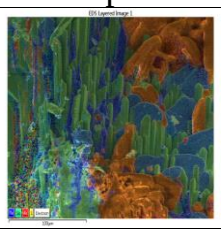

Figure 4. EDX mapping of the polycrystalline bulk samples.

[1] M. Popescu, A. Andriesh, V. Ciumash, M. Iovu, S. Shutov, D. Tsyiuleanu, „PHYSICS OF CHALCOGENIDE GLASSES", Ed.Bucuresti, Stiinta, in Romanian, 487 (1996).
[2] D. Tsiuleanu, M. Ciobanu, „ROOM TEMPERATURE A.C. OPERATING GAS SENSORS BASED ON QUATERNARY CHALCOGENIDES, SENSORS AND ACTUATORS", B, 223, pp.95-100 (2016).
*) Author for Correspondence: O. Iaseniuc

P.10. Rashba coupling in metallic states at the Ni-doped Ge interface

D.G. Popescu[1*], L. Borcan[1], A. Iancu[1], A. Rostas[1], C. Ruxandra[1], V. Strocov[1], M.A. Husanu[1]

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

Ferromagnetic Ni-doped Ge are obtained by epitaxial growth onto Si(111) wafer at high temperatures in a dedicated Molecular Beam Epitaxy chamber from properly outgassed Knudsen cells in ultra-high vacuum (better than 10^{-8} Pa base pressure) [1]. The samples are characterized by X-ray photoelectron spectroscopy after properly cleaning using flash annealing. The 7x7 reconstruction of Si(111) is confirmed by the low energy electron diffraction. The Rashba spin-orbit interaction leads to lifting of the spin degenacy at the surface due to space inversion symmetry breaking [2]. It is visible in Angle-Resolved Photoelectron Spectroscopy measurements performed at a synchrotron facility. This feature act on the Rashaba spin-orbit interaction resulting into spin polarized states confirmed by ab-inito calculations. The experiments and density functional theory simulations validate the spin–orbit coupling at the interface. These results could represent a progress into the spin field-effect transistor applications.

Keywords: X-ray Photoelectron Spectroscopy, metal-semiconductor interface, Rashba spin-splitting

Acknowledgement

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References:

[1] G.A. Lungu, N.G. Apostol, L.E. Stoflea, R.M. Costescu, D.G. Popescu, C.M. Teodorescu, *Materials 6*, 612-625 (2013)

[2] S. Oyarzun, A.K. Nandy, F. Rortais, J.C. Rojas-Sanchez, M.T. Dau, P. Noel, P. Laczkowski, S. Pouget, H. Okuno, L. Vila, C. Vergnaud, C. Beigne, A. Marty, J.P. Attane, S. Gambarelli, J.M. George, H. Jaffres, S. Blugel, M. Jamet, *Nature Communications* 7, 13857 (2016)

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

P.11. Lamellar liquid crystals from luminescent palladium(II) complexes with mixed ligands

T.A. Ilincă[1], M. Iliș[1], M. Micutz[2], and V. Cîrcu[1*]

[1] University of Bucharest, Inorganic Chemistry Department, Bucharest, Romania
Email: theodora.ilinca@drd.unibuc.ro
[2] University of Bucharest, Department of Physical Chemistry, Bucharest, Romania

Emissive properties were reported for a series of metallomesogens based on palladium(II) complexes, having the metal ion in a cyclometallated surrounding [1-3]. By judicious design, new palladium(II) complexes with mixed ligands were obtained. These complexes were investigated for their liquid crystalline properties by a combination of differential scanning calorimetry (DSC) and polarizing optical microscopy (POM); thermogravimetric analysis (TGA) was used to study the thermal stability. The formation of these palladium(II) complexes as well as their structure were attributed by ^{1}H and ^{13}C NMR spectroscopy and IR spectroscopy. All palladium(II) compounds behave as luminescent materials in solution, in the solid state and liquid crystalline state. The melting temperatures of the palladium(II) complexes depend on the BTU co-ligand and were found in the range of 85-220°C. The results of the thermogravimetric analysis show that the complexes have a high thermal stability up to 260°C. These complexes show a yellow-orange solid-state emission at room temperature.

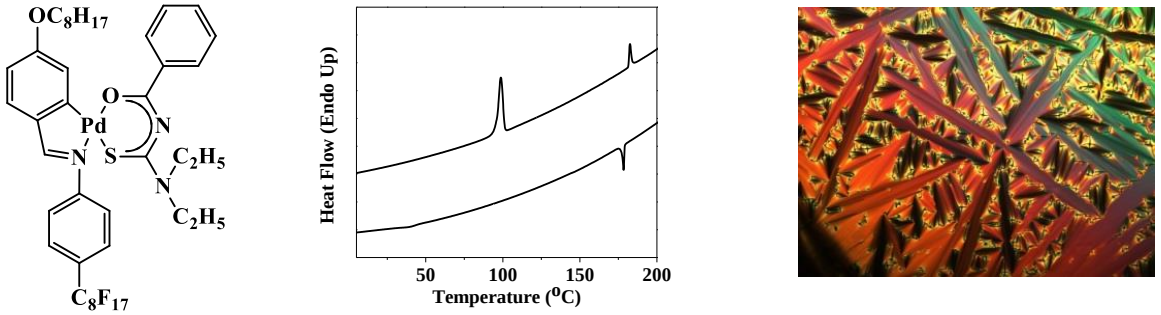

Figure 1. Structure, DSC traces and POM picture showing SmA texture at 170°C for a palladium(II) complex.

References:

[1] M. Iliș, D. Batalu, I. Pasuk and V. Cîrcu, Journal of Molecular Liquids, 2017, 233, 45-51.
[2] M. Iliș, M. Micutz and V. Cîrcu, Journal of Organometallic Chemistry, 2017, 836, 81-89.
[3] M. Micutz, I. Pasuk and M. Iliș, Journal of Molecular Liquids, 2017, 243, 151-156.

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

P.12. THE MAGIC OF THE CHOLESTERIC LIQUID CRYSTALS

A. Albu and V. Cîrcu*

University of Bucharest, Romania
Email: anastasia.albu@s.unibuc.ro

Why would someone want to study cholesteric liquid crystals? Because, over the years, these proved to be very useful in a lot of different applications (like making a variety of sensors [1] and thermometers), but also, there is a strong relationship between cholesteric liquid crystals and life [2]. Even though they are studied by scientists for more than 100 years (since 1888), cholesteric liquid crystals still keep a lot of secrets away from humanity and don't stop to impress us with their beautifulness and properties. So, wanting to get to know more about these mysterious liquid crystals, we prepared two mixtures containing three cholesteric compounds in different proportions, for which we analyzed the variation of the color and texture with the temperature, using polarized microscopy (POM). The selective reflection of the two mixtures was recorded by variable temperature UV-VIS spectroscopy. Also, we studied the capacity of the mixtures to polarize the light, using a pair of glasses with polarized lenses, being able to discover the full magic of the cholesteric liquid crystals mixtures prepared.

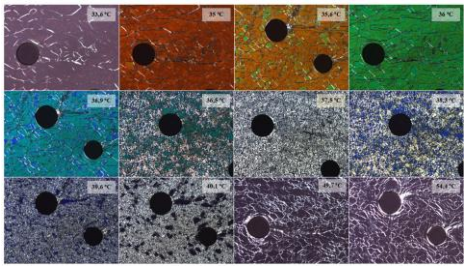

Figure 1 – Variation of color and texture with temperature for one of the mixtures

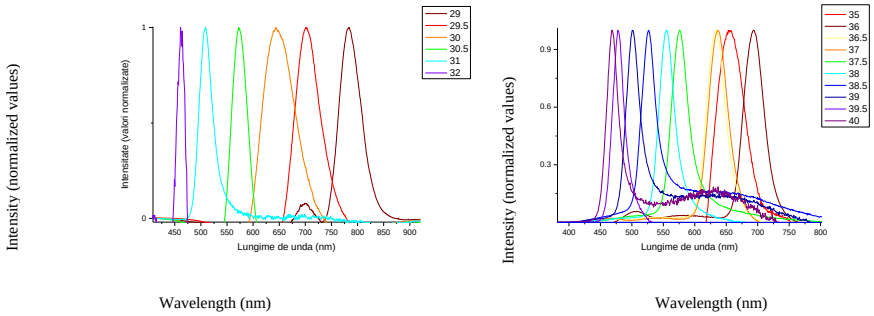

Figure 2 – Selective reflection for both mixtures analyzed

References:

[1] Mulder, D.J., Schenning, A.P.H.J, Bastiaansen, C.W.M., Chiral-nematic liquid crystals as one dimensional photonic materials in optical sensors. J. MATER. CHEM., 2 (2014), 6695-6705.
[2] Mitov, M., Cholesteric liquid crystals in living matter. SOFT MATTER, 13(2017), 4176-4209.

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

P.13. Linear birefringence of uniax anisotropic inorganic crystals measured by ellipsometric means

Delia Anne Marie Androne[1], Cristina Nechifor[2], Mihai Postolache[3], Dan Gheorghe Dimitriu[4], Dana Ortansa Dorohoi[4]

[1]Faculty of Geography and Geology, Alexandru Ioan Cuza University of Iasi, 700056, Iasi, Romania
[2]Faculty of Machine Manufacturing and Industrial Management, Gheorghe Asachi University, 700050, Iasi, Romania
[3]Faculty of Automatic Control and Computed Engineering, Gheorghe Asachi University, 700050, Iasi, Romania
[4]Faculty of Physics, Alexandru Ioan Cuza University of Iasi, 700056, Iasi, Romania

There are some optical methods (interferometric, refractometric, or compensatory) for estimating the refractive indices and the linear birefringence of the uniaxial layers. Now a simple ellipsometric method for determining the linear birefringence of the thin anisotropic layers is described. This method consists in establishing the inclination of the axes of the polarization ellipse relative to the principal axes of the anisotropic uniax layer. The relation between the inclination angles of the polarization ellipse axes relative to the principal axis of the anisotropic layer at the exit and the azimuth of the incident linearly polarized light at the entrance of the layer permits to estimate (with good precision) the phase difference introduced by the uniax anisotropic layer between the ordinary and extraordinary components of light. The results of measurements for four inorganic crystals from Carpathian Mountains (quartz, calcite, tourmaline and Island Spat) are given in this communication. The results are compatible with those obtained by other methods for crystals with similar structure and symmetry.

Corresponding author: Dana Ortansa Dorohoi

5. Materials science

P.14. The study of thermal properties of conducting polymers (polypyrrole) using molecular dynamic.

S. Ammour[1*], M. Hamouni[1] and L. Bouzid[2]

[1] University of Abou Bebr Belkaid, Tlemcen, Algeria
Email: phs.ammour@gmail.com
[2] University of science and technology, Mohamed Boudiaf , Oran, Algeria

In this work, the thermal properties of polypyrrole (PPY) is investigated using molecular dynamics simulation.
Conducting polymers, especially polypyrrole has attracted many scientists due to its high electrical conductivity, environmental stability and ease of preparation [1].
Because of the important number of atoms in polymer chain, the molecular dynamic (MD) is applied in the computer simulation. This method is based on the choice of the force field, which plays an important role on the final results [2]. In our study, we have chosen COMPASS as a force field.
The PPY polymer structure with 20 repeat units is embedded in a periodic cell (Figure 1). Then a series of molecular dynamics is using with the NVT and NPT canonical ensemble. Finally, the curve of specific volume versus temperature is plotted in order to pick up the glass transition temperature Tg. In polymer system, the Tg is a very important value and the theory of free volume proposed by Fox and Florry is the most used procedure [3].

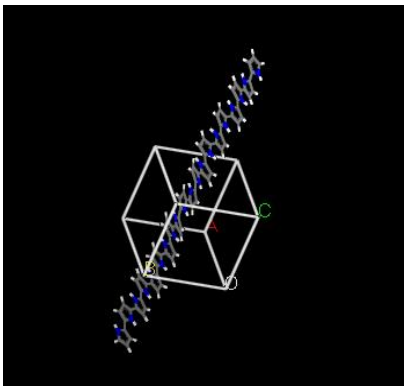

Figure 1. Molecular model of PPY

The simulated glass transition temperature is compared with others experimental and theoretical values (table 1). From this comparison, we can say that our methods give good results. All molecular dynamic simulation were computed by Materials Studio 6.0 software package of Accelerys.

	SIMULATED TG (MD)	EXPRIMENTAL TG
PPY	375.63 K	384.85 k[4] 370.32 K[5]

Table 1: Simulated and experimental Tg of PPY.

References:

[1] B. Scrosati, Science and Applications of Conducting Polymers (Chapman and Hall, London, 1993).
[2] L. Bouzid, S. Hiadsi, M. O. Bensaid, and F. Z. Foudad,"Molecular dynamics simulation studies of the miscibility of PMMA/PS polymer blend," Chinese Journal of Physics, 2018.
[3] M. J. He, H. D. Zhang, and W. X. Chen, Polymer Physics, Fu Dan University Press, Shanghai, 2007.
[4] T. Tikish, A.kumar and J.Kim. study on the miscibility of polypyrrole and polyaniline polymer blends, Advanced in materials science and engineering, 2018.

*) Author for Correspondence: S. Ammour.

P.15. An overview of fusion-relevant tungsten dust synthesis via RF (13.56 MHz) plasma discharge

V. Marascu[1*], C. Stancu[1], C. Constantin[1,2*], A. Bonciu[3], V. Satulu[1], and G. Dinescu[1]
[1]Low Temperature Plasma Department, National Institute for Laser, Plasma and Radiation Physics, RO-077125, Magurele, Romania
Email: valentina.marascu@inflpr.ro; cristian.stancu@inflpr.ro; catalin.constantin@inflpr.ro; veronica.satulu@inflpr.ro; gheorghe.dinescu@inflpr.ro;
[2]Faculty of Physics, University of Bucharest, RO-077125, Magurele, Romania
[3]FOTOPLASMAT Department, National Institute for Laser, Plasma, and Radiation Physics, RO-077125, Magurele, Romania
Email: anca.bonciu@inflpr.ro

Fusion-related domain plays an important role in achieving green energy via thermonuclear plasma, by using deuterium and tritium as the primary fuel. In this line, scientific concerns are undergoing for analyzing the impact of the plasma upon the inner walls of the fusion facilities (tokamaks inner walls, e.g., ITER tokamak.) [1-3]. Herein, various plasma lab-scale systems are used for many scientific studies: plasma diagnosis, plasma-material interaction, dust synthesis, analyses, etc. In our paper, we highlight an overview, of the field of tungsten material behavior during He, H_2, D_2, and Ar plasma lifetime interaction, in the view of surface material changes, and dust formation [4-6]. Herein, both, the tungsten material and the plasma were analyzed. SEM, EDS, XPS, statistical analyses [5,6], and contact profilometry methods were used to investigate tungsten surfaces and dust. OES measurements were used for plasma diagnosis. Our material results have shown similar behavior to the materials used in the fusion-related domain.

Acknowledgment: This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them. Part of this work was supported by grants from the Romanian Ministry of Research, Innovation and Digitalization, CCCDI - UEFISCDI, in the frame of Nucleus Program INFLPR LAPLAS VI 16N/2019.

References:

- C. Grisolia.; et al. https://doi.org/10.1016/j.jnucmat.2008.12.192
- C. Grisolia; et al. https://doi.org/10.1016/j.jnucmat.2014.10.089
- E.A. Hodille, et al. https://doi.org/10.1088/1741-4326/ac0f37
- C. Stancu, *et al.* https://doi.org/10.1007/s00339-017-1235-4
- V. Marascu, *et al.* https://doi.org/10.3390/app10196870
- V. Marascu, *et al.* https://doi.org/10.1088/2053-1591/ab955d
- V. Marascu, et. al., https://doi.org/10.1063/1.4944292
- V. Marascu, et. al., DOI: 10.21279/2457-144X-21-034

*) Author for Correspondence: catalin.contantin@inflpr.ro; valentina.marascu@inflpr.ro

P.16. Thermo-Mechanical Properties of Plasticized Poly(lactic acid) Films

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

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

Nowadays, polymeric materials, commonly known as plastics, have become ubiquitous. They are used across a wide range of sectors including packaging, textiles, agriculture, building and construction, medicine, electronics and so on. However, most plastics are derived from crude oil and just a small amount of them are being recycled and reused. Over the last few decades, increasing interest has been given to biobased and biodegradable polymers in order to reduce the dependence on fossil resources on one side and mitigate waste disposal problems on the other side. Among currently available biopolymers, poly(lactic acid) (PLA) is the most promising one. It is a compostable thermoplastic derived from 100 % renewable sources such as corn. Besides its ecological benefits, PLA shows interesting physical and mechanical properties and good processability with conventional melt-processing techniques (injection molding, extrusion, thermoforming). However, the usage of PLA is restricted because of its high brittleness and poor thermal stability. One way to overcome these shortcomings is by plasticizing. In our work, PLA is plasticized by polyethylene glycol (PEG). PLA films with various contents of plasticizer (1-20 %) are prepared by solvent casting method. The obtained films are analysed using differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The obtained results show an improvement of the ductility and the melt crystallization of PLA with increasing PEG content.

P.17. THE EFFECT OF ALUMINOSILICATE INDUSTRIAL WASTE ON THE PROPERTIES OF POLYPROPYLENE REINFORCED WITH GLASS FIBER

George-Mihail Teodorescu[1], Zina Vuluga[1*], Andreea Ioniţă[1], Florin Oancea[1], Jenica Paceagiu[2], Cristi-Andi Nicolae[1], Raluca Augusta Gabor[1]

[1]INCDCP-ICECHIM Bucharest, 202 Spl. Independentei, 6th district, Romania

[2] CEPROCIM S.A., 6 Preciziei, 062203, Bucharest, Romania

**Corresponding author: (zvuluga@icechim.ro)*

Introduction: Automobile manufacturers face great challenges as regulations of automobile fuel consumption and CO_2 emission become stricter year by year. Glass fiber-reinforced polymers are still considered as a main solution material for lightweight automobile parts, such as body panels, doors, roofs, frame segments, and seating systems [1,2]. The addition of ash powder into the polymer system provides a cheaper filler for the final product thus reducing the cost of the car part and also provides usefulness to a waste material [3]. The purpose of this paper is to study the effect of ash powder on the properties of polypropylene composite formulations that are regularly used in industries such as automotive and the possibility of reducing the glass fiber content in the final compositions.

Materials And Methods: A commercial high flow polypropylene (PP), maleinized PP (PPMA), masterbatch with 60% long glass fiber (G), aluminosilicate power plant ash in the form of powder with particle sizes <90 microns (C), dispersion agent, poly(propylene glycol adipate) (P) and a thermoplastic elastomer, poly[styrene-b-(ethylene-co-butylene)-b-styrene] (E). Samples based on PP, with 25-30 wt.% G, with and without 1 and 5% treated C, 2.5 wt.% PPMA and 20 wt.% E, were prepared in dynamic conditions through melt processing methods. The mechanical tensile and impact properties of the obtained samples were tested with Instron and Zwick devices, dynamic mechanical and thermal properties were performed with DMAQ800, TGAQ5000 and DSCQ2000 and nanomechanical tests were performed on a TI Premier system.

Results And Discussion: Nanomechanical, mechanical and dynamic mechanical analysis showed a high stiffness for the composites based on PP with 25-30 wt.% G, commonly used in the automotive industry. A decrease of reduced modulus and hardness is observed for the composites with ash content compared to PP with G and G-E content. A similar decrease is observed from mechanical and dynamic mechanical properties where the young modulus and storage modulus of the composites with ash are lower compared to PP with glass fiber and elastomer. However, the impact strength of the final composites with ash content has increased by 55% for the composite with 1 wt.% C and with 60% for the composite with 5 wt.% C compared to PP with 25 wt.% G. The same final composites have increased toughness compared to PP-30 G (38% and 46%) and PP-G-E (21% and 31%). TGA analysis showed that the composite PP-G-E has lower thermal stability (almost 20^{o}C) compared to PP-25 wt.% G and PP-30 wt.% G whereas, with the addition of ash powder, the final composites with ash content have increased thermal stability by almost 10^{o}C. DSC analysis showed that the melting temperature is similar for all samples however the melting enthalpy decreases drastically for the final composites, especially for 5 wt.% C compared to the PP-G sample due to the interaction between the components.

Conclusion: The glass fiber content of PP composite can be reduced by the addition of ash. The addition of ash greatly increases the mechanical and nanomechanical properties of a polypropylene/glass fiber composite, as a result of achieving a synergistic effect between the components.

Acknowledgments: The work on this paper was supported by UEFISCDI Romania through the framework of project POC 2016 SECVENT, P_40_352, MySMIS: 105684

REFERENCES: [1] Kim, D.-H., et al., Strain rate dependent mechanical behavior of glass fiber reinforced polypropylene composites and its effect on the performance of automotive bumper beam structure. Composites Part B: Engineering, 2019. 166: p. 483-496.

[2] Luo, G., et al., Coupling effects of glass fiber treatment and matrix modification on the interfacial microstructures and the enhanced mechanical properties of glass fiber/polypropylene composites. Composites Part B: Engineering, 2017. 111: p. 190-199.

[3] Nath, D., et al., Structure-property interface correlation of fly Ash-isotactic polypropylene composites. Journal of Materials Science, 2009. 44: p. 6078-6089.

6. Biomaterials and organic materials

P.18. Liquid Crystal based bacterial infection biosensor

Cavaco, Gonçalo [1]; Soares, Maria Simone [2]; Grilo, Inês R. [1]; Pina, Ana Sofia [3]; Roque, Ana Cecília [1]; Marques, Carlos [2]; Miragaia, Maria [3]; Sobral, Rita G. [1] and Almeida, Pedro L. [4,5*]

[1] UCIBIO, School of Sciences and Technology, University NOVA of Lisbon, Lisbon, Portugal
[2] I3N and Physics Department, Aveiro University, Aveiro, Portugal
[3] ITQB, University NOVA of Lisbon, Lisbon, Portugal
[4] I3N - CENIMAT, School of Sciences and Technology, University NOVA of Lisbon, Lisbon, Portugal
[5] Lisbon's Superior Institute of Engineering, Polytechnic Institute of Lisbon, Lisbon, Portugal * Author for Correspondence: pla@fct.unl.pt

A powerful indicator of bacterial infection is the presence of free parts of the bacterial cell wall, as these molecules are unique to bacteria and released during bacterial growth by the action of autolytic enzymes. Accordingly, the presence of peptidoglycan components, muropeptides in sterile body fluids can be the reflection of an infection. We are developing a non-invasive biosensor to identify bacterial infections at early stage, by detecting the presence of muropeptides in body fluids, using the binding capacities of an amidase protein of the pathogen *Staphylococcus aureus* [1,2].

The basic arrangement of this microfluidic system is a double-chambered cell composed of a chemically activated glass surface to which the active protein domains are immobilized. The activated surface is able to induce an homeotropic alignment of the nematic liquid crystal. In contact with the analyte sample, the surface-immobilized proteins will bind to muropeptides, if present. To detect the presence of peptidoglycan and thus a bacterial infection, the sensor cell is then filled with the nematic liquid crystal and the test results are observed using two cross-polarizers, to visualize the interaction of the incident light with the liquid crystal molecules [3,4]. These biosensors have a large number of point-of-care applications, namely in medical appointments, at hospital admission and emergency departments, at inpatients bedside, in blood banks screening and even in remote regions with no available health-care facilities or electrical energy.

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References:

[1] T. Oshida, et al. *Proc Natl Acad Sci U S A*, **92**, 285-289 (1995).

[2] F.M. Büttner, et al. *J. Biol. Chem*, **289**, 11083-11094 (2014).

[3] V. K. Gupta, et al., *Science*, **279**, 2077-2080 (1998).

[4] T. Kato, *Science*, **295**, 2414-2418 (2002).

P.19. Potential of aliphatic polyesters as hot embossing substrates

G. M. Oprica[1], A. N. Frone[1], M. Mihailescu[2], A. R. Gabor[1], C. A. Nicolae[1], and D. M. Panaitescu[1*]

[1] National Institute for Research and Development in Chemistry and Petrochemistry, Bucharest, Romania
Email: madalina_oprica@yahoo.com
[2] University Politehnica of Bucharest, Romania
Email: mona.mihailescu@upb.ro

Hot embossing of thermoplastic polymers is a cost-effective method to transfer microstructure patterns from a master mold onto a polymeric substrate [1]. This is a widely used technique in microstructure fabrication, for example in the manufacture of holographic security features [2]. Polymethylmethacrylate and polycarbonate are usually employed as substrates for hot embossing. However, these synthetic polymers are derived from petroleum hydrocarbons, which are hazardous to the environment and more and more expensive.

In this work, polylactic acid (PLA) and poly(3-hydroxybutyrate) (PHB) biopolymers were tested as possible substrates in the hot embossing process. The advantages of PLA and PHB are multiple due to their bio-based origin and minimal impact on the environment. Plate samples with a thickness of 1 mm were obtained from several commercial PLA sorts (PLA 4043, PLA 2002 and PLA 2500) from Nature Works (USA) by compression molding. These plates were characterized by dynamic mechanical analysis using a DMA equipment and a controlled ramp force mode to establish the suitable temperature and pressure ranges for embossing. Hot embossing tests were also carried out with a small mark in the compression molding press using different temperatures from 25 to 70 °C and pressures between 5 and 25 bars. The characterization of these embossed plates by optical microscopy and enhanced darkfield hyperspectral microscopy showed a clear connection between the temperature and pressure during embossing and the quality of the optical image after embossing.

References:
[1] L. Peng, Y. Deng, P. Yi, X. Lai, JOURNAL OF MICROMECHANICS AND MICROENGINEERING 2014, 24, 013001.
[2] S. S. Deshmukh, A. Goswami, MATERIALS TODAY: PROCEEDINGS 2020, 26, pp. 405–414.

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*) Author for Correspondence: panaitescu@icechim.ro

P.20. A parallel between plasma irradiation of nanocellulose water suspensions and silane grafting as surface treatments of nanocellulose

C. D. Usurelu[1], A. N. Frone[1], C. A. Nicolae[1], A. R. Gabor[1], S. Vizireanu[2], V. Satulu[2], C. Stancu[2], S. M. Teodorescu[3], and D. M. Panaitescu[1*]

[1] National Institute for Research and Development in Chemistry and Petrochemistry, Bucharest, Romania
Email: catalina.usurelu@icechim.ro
[2] National Institute for Laser, Plasma and Radiation Physics, Ilfov, Romania
Email: sorin.vizireanu@inflpr.ro
[3] University Politehnica of Bucharest, Romania
Email: mircea.teodorescu@upb.ro

Cellulose, the most abundant organic polymer on Earth, is biodegradable and biocompatible and has reduced carbon dioxide emissions in the environment. Nanocellulose may be obtained from a cellulosic source by mechanical defibrillation, which is an eco-friendly but energy-consuming method. The application of enzymatic or chemical pretreatments may lead to important energy savings but are more expensive and less environmentally friendly. To meet the requirements of many applications, nanocellulose surface should be modified. Chemical modification with carboxylic acids, acid anhydrides, acyl chlorides or silanes is currently used for the surface functionalization of nanocellulose. Previous studies have shown that the treatment of cellulose with a plasma torch completely immersed into a cellulose water suspension induces both the defibrillation and the surface functionalization of cellulose [1]. Plasma treatment of cellulose may thus be considered an effective eco-friendly approach to obtain surface functionalized nanocellulose.

In this work, the changes induced by the plasma treatment of nanocellulose were compared with those obtained by applying a common surface silylation technique. Nanocellulose obtained from microcrystalline cellulose by microfluidization was plasma treated by immersing the plasma source in the water suspension of nanocellulose. In parallel, the same nanocellulose was treated with a silane. The surface changes were characterized by Fourier transform infrared spectroscopy, X-ray photoelectron spectroscopy, and thermogravimetric analysis. The results showed that both treatments led to the surface functionalization of nanocellulose, plasma treatment being environmentally friendly and more cost effective.

References:
[1] S. Vizireanu et al., SCIENTIFIC REPORTS, 2018, 8, 15473.

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*) Author for Correspondence: panaitescu@icechim.ro

P.21. Albumin nanoparticles' synthesis for biomedical applications

M.-E. Barbinta-Patrascu, S. Iftimie, A. Balan, N. Sandu, Diana L. Stan, C. G. Chilom*,

[1] Faculty of Physics, University of Bucharest, Bucharest, Romania
Emails: marcela.barbinta@unibuc.ro; sorina.iftimie@fizica.unibuc.ro; adriana.balan@unibuc.ro; s.nicoleta59@yahoo.ro; claudia-gabriela.chilom@unibuc.ro

One direction in nanomedicine is the use of protein-based particles as drug delivery systems [1]. Serum proteins such as albumin and transferrin from human and animal blood are water-soluble, biodegradable, biocompatible, nontoxic, and transport many drugs in their native form or as micro-/nano-particles.
This research work had the following main goals: i) the synthesis of albumin nanoparticles by the nanoprecipitation method [2], and ii) spectral and morphological characterization of these nanoparticles. The synthesized nanoparticles were crosslinked with ascorbic acid [3], and the time stability was monitored by UV-Vis absorption spectroscopy. Size and morphological aspects were investigated by Scanning Electron Microscopy (SEM).
These results will be the starting point for the synthesis of rutin-functionalized serum protein nanoparticles, a flavonoid with antioxidant and antitumor properties. These nanohybrids will be subsequently introduced into tumor cells.

References:
[1] E. Kianfar, JOURNAL OF NANOBIOTECHNOLOGY, 19, no.1, 159 (2021). doi:10.1186/s12951-021-00896-3.
[2] M. Tarhini, I. Benlyamani, S. Hamdani, G. Agusti, H. Fessi, H. Greige-Gerges, A. Bentaher, A. Elaissari, MATERIALS, 11, no.3, 394 (2018). doi:10.3390/ma11030394.
[3] F. Amighi, Z. Emam-Djomeh, M. Labbafi-Mazraeh-Shahi, JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, 17, no. 10., pp. 1223-1235 (2020). doi:10.1007/s13738-019-01850-9

*) Author for correspondence: claudia-gabriela.chilom@unibuc.ro

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P.22. Biocomposites based on Chistosan and Hydroxyethyl Cellulose- Elaboration and Characterization

Nassima CHEKROUN[1]*, Houcine ZIANI CHERIF[1]

[1] Macromolecular Research Laboratory, Department of chemistry, Faculty of Sciences,Abou Bekr Belkaid University, Tlemcen, Algeria

chekrounnassima7@gmail.com

Abstract:

Blood loss during surgery and combat trauma remain major complications leading to patient death. Local hemostasis of diffuse bleeding has resulted in low mortality and morbidity over the past two decades, but relatively high costs limit their application in low- and middle-income countries, stimulating the search for effective and inexpensive materials. Accordingly, the use of biomaterials known for their coagulating effects such as gelatin, rice starch, oxidized cellulose and chitosan is well known. These biomaterials have been used for their natural origin, their abundance as well as their biodegradability. The aim of this work is to develop an effective chitosan-based hemostatic material used as a wound dressing, using chitosan a bioactive material which has hemostatic properties, as well as hydroxyethyl cellulose, a water-soluble polymer which aims to improve the mechanical properties of chitosan. Thus, films containing chitosan and hydroxyethyl cellulose were prepared by the solution casting method, and their characterization by FTIR and UV-VISIBLE was carried out.

Keywords: Biomaterials, Chitosan, Hydroxyethyl cellulose, Hemostasis, Coagulation.

References:

[1] P. Hangge, J. Stone, H. Albadawi, Y.S. Zhang, A. Khademhosseini, R. Oklu**.** Hemostasis and nanotechnology. *Cardiovasc Diagn Ther*. 2017. (**Publication**)

[2] Xiaohui Wei, Sheng Ding, Shisheng Liu, Kun Yang a, Junjie Cai, Fan Li, Chunlai Wang, Song Lin, Feng Tian. Polysaccharides-modified chitosan as improved and rapid hemostasis foam sponges. *Carbohydrate Polymers.* 2021. (**Publication**)

[3] N. Chekroun, Elaboration d'un biocomposite à potentiel pharmacologique. Master en Chimie des Matériaux. Université Abou Bekr Belkaid-TLEMCEN, 2019/2020. (**Thesis**)

*) Author for Correspondence: Nassima Chekroun

7. Methods for material characterization

P.23. Estimation of Cutting Edge Width in the case of Electrical Steels

G. Paltanea[1], V. Manescu[1]* (Paltanea), C. Paun[1,2], H. Gavrila[1]

[1]University Politehnica of Bucharest, Bucharest, Romania

Email: gheorghe.paltanea@upb.ro, veronica.paltanea@upb.ro, pauncostel1986@yahoo.com, horia.gavrila@upb.ro

[2] National Institute for Research and Development in Microtechnologies, Romania

Electrical steels (Fe-Si) have the property to concentrate the magnetic flux in different parts of the magnetic circuits, and due to the easiness of reversing their magnetization, the most important industrial applications of these materials are the conversion of electromagnetic energy into mechanic energy (electrical machines) and the modification of parameters characterizing the use of electrical energy (electrical transformers). These materials have excellent magnetic properties obtained by cold-rolling intermediate manufacturing steps, but their energy loss and magnetic permeability are strongly influenced by the strip-cutting technology and the magnetic core forming procedure. The most used cutting procedure is the mechanical one. It is based on a shearing process that appears along the material when it is plastically deformed. A negative effect, which consists of a strain-hardening phenomenon, is put in evidence near the cutting edge [1].

In this work, which provides an extensive set of experimental results on different types of Fe-Si sheets, we aim at a simple phenomenological assessment of the degradation of the magnetization curve and magnetic losses enforced by cutting. Different types of commercial Fe-Si sheets were cut as strips of different widths (5 mm $\leq w \leq$ 60 mm), using both guillotine punching, water-jet method, laser cutting, and electrical discharge method and magnetically characterized using a single strip tester.

The method for estimating of the cutting edge width consists of a simple scheme, where the work-hardened region of the strip is identified with two bands of width L_c running along the cutting line at the edges. By measuring the complete normal magnetization curves at two different widths, one can estimate the width of the damaged bands L_c and, for any magnetic field value, the associated magnetization [2]. The entire evolution of the curves with w is then obtained and found to agree with the experimental curves, despite of the somewhat crude scheme involved.

References:

[1] G. Paltanea, V. Manescu (Paltanea), R. Stefanoiu, I.V. Nemoianu, H. Gavrila, MATERIALS, 13, 1455, 2020

[2] V. Manescu (Paltanea), G. Paltanea, E. Ferrara, I.V. Nemoianu, F. Fiorillo, H. Gavrila, JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, 499, 166257, 2020.

*) Author for Correspondence: veronica.paltanea@upb.ro

P.24. Evaluation of Intermolecular Interactions in Organic Cocrystal of 2-Nitroterephthalic Acid and 1,2-Bis(4-pyridyl)ethane Using Hirshfeld Surface Analysis

D.Tapu[1]*, E. Melnic[2], M. Fonari[2] and D. Chisca[1,2]

[1]Ion Creangă State Pedagogical University, Faculty of Biology and Chemistry, Ion Creangă str. 1, MD-2069, Chisinau, Moldova,
Email: ms.dumi@inbox.ru
[2]Institute of Applied Physics, Academiei str. 5 MD-2028, Chisinau, Moldova

1,2-Bis(4-pyridyl)ethane is a versatile spacer used in the building of supramolecular architectures both by protonation at the pyridinic nitrogen and by the formation of cocrystals involving N···H–O hydrogen bonds [1, 2]. Here we report the crystal structure of 2-nitroterephthalic acid (H_2ntp) and 1,2-bis(4-pyridyl)ethane (bpe) adduct with 1:1 molar ratio. The compound crystallizes in the triclinic system, space group *P*-1 with unit cell dimensions a = 9.5957(8), b = 9.7846(8), c = 10.6757(10) Å, α = 96.628(7), β = 94.893(7), γ = 111.821(8)°, V = 915.329 Å^3.

In the cocrystal, the supramolecular linear hydrogen-bonded polymer is formed through the alternating strong O–H···N hydrogen bond (2.546(3) Å) and heteromeric supramolecular synthon, $R_2^2(7)$ based on O–H···N and C–H···N hydrogen bonds between the bpe and H_2ntp molecules. The 3D supramolecular architecture is stabilised by the C–H···O hydrogen bonds and π···π interactions between pyridine fragments of bpe molecules with Cg1···Cg2 distance of 3.702 Å. The reliability of supramolecular synthons as well as the distribution of intermolecular interactions in the cocrystal was estimated using Hirshfeld surface (HS) analysis. This analysis and 2D fingerprint plots show that a maximum contribution in HS (Fig. 1) is attributed to O···H (35.5%), H···H (27.5%), H···C (20.0%) and H···N (7.0%)contacts, which confirm the dominance of hydrogen bonds.

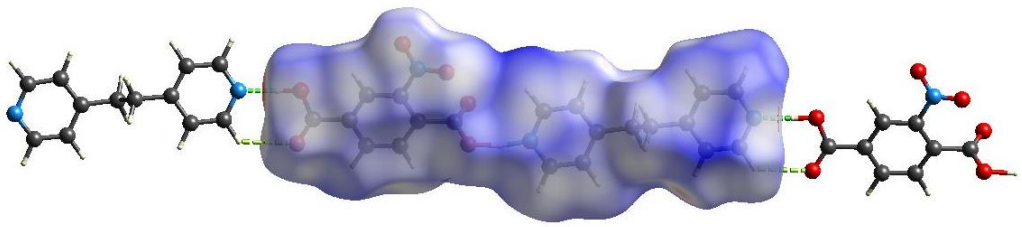

Figure 1. A view of the three-dimensional Hirshfeld surface of the title compound.

[1] S. F. Lush. JOURNAL OF STRUCTURAL CHEMISTRY. **55**, no. 8, pp. 1527-1532.
[2] S. Ebenezr. JOURNAL OF MOLECULAR STRUCTURE. 990, pp. 281-289.

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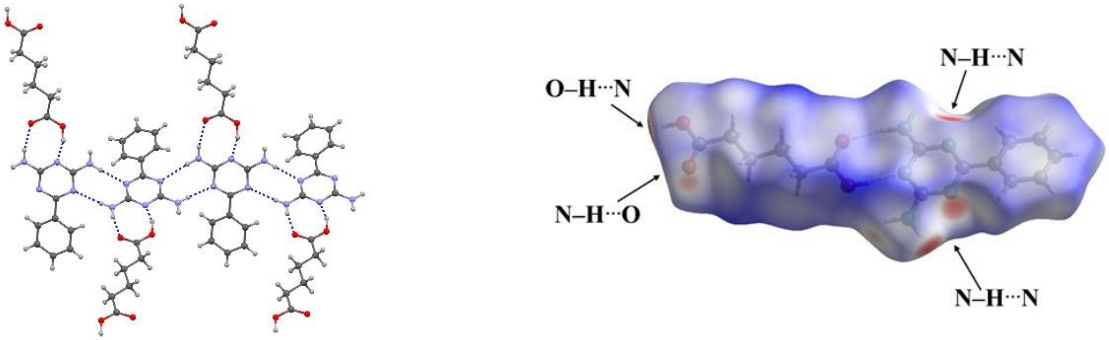
P.25. Hirshfeld Surface Analysis of Supramolecular Synthons in Cocrystal of 2,4-Diamino-6-Phenyl-1,3,5-Triazine with Adipic Acid

N. Craciun[1,2*], D. Chisca[1,2], E. Melnic[2], and M. S. Fonari[2]

[1]Ion Creangă State Pedagogical University, Faculty of Biology and Chemistry, Ion Creangă str. 1, MD-2069, Chisinau, Moldova
Email: nicoleta.craciun@ifa.md
[2]Institute of Applied Physics, Academiei str. 5 MD-2028, Chisinau, Moldova

Triazine and its derivatives are considered to be a favourite choice and valuable building blocks for design of cocrystals with desired physicochemical properties based on the supramolecular synthons formation. The cocrystal of 2,4-diamino-6-phenyl-1,3,5-triazine (dpt) with adipic acid (H_2adip) [1] was repeatedly grown to analyse the intermolecular interactions by Hirshfeld surface analysis using Crystal Explorer 17.5 software [2].

In co-crystal, molecules of dpt are self-assembled into homomeric chain through N-H···N hydrogen bonds (N···N distances are 2.987(2) and 3.152(2) Å) in the form of cyclic eight-membered $R_2^2(8)$ supramolecular homosynthon, while molecules of adipic acid are paired with dpt by N-H···O hydrogen bonds *via* supramolecular heterosynthon resulting in a cyclic eight-membered $R_2^2(8)$ motif (N···O distances are 2.917(2) and 3.351(2) Å. These interactions lead to the formation of the 3D H-bonded supramolecular network, and play a dominant role in stabilizing the crystal structure. Hirshfeld surface analysis and 2D fingerprint plots clearly indicate the maximum contribution attributed to H···H (46.8%), O···H (15.5%), and N···H (15.1%) contacts, which confirm the dominance of hydrogen bonds.



a **b**

Figure1. a) Supramolecular chain and b) Hirshfeld surface for supramolecular synthons of the title compound

[1] B. R. Jali. JOURNAL OF CHEMICAL CRYSTALLOGRAPHY. **43**, pp. 531–537.
[2] M. J. TURNER. CRYSTALEXPLORER 17.5, UNIVERSITY OF WESTERN AUSTRALIA, AUSTRALIA, 2017.

Acknowledgements. Authors thank the projects ANCD 20.80009.5007.15 (R. Moldova) and ANCD 20.80009.5007.28 (R. Moldova) for support.

P.26.
Study of the effect of composition and the resulting physical properties of acrylic terpolymers

G F-Z. HAKEM[1]*, D. BENDEDOUCHE[1], A. BOURICHE[1] ,
L. BEDJAOUI-ALACHAHER[1]

[1]Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou Bekr Belkaid, 13000, Tlemcen, Algeria
Email[1]* : ghizlenefatimazahra.hakem@univ-tlemcen.dz

Photoinitiated linear polymers were formed by polymerization of isobornyl acrylate (IBoA) with 2-ethylhexyl acrylate (2-EHA) and hydroxyethyl acrylate (HEA). The terpolymers were developed by varying the weight proportion of monomers. The developed terpolymer was characterized by Fourier transform infrared – attenuated total reflection (FTIR-ATR). Their physical properties have been evaluated by Differential Scanning Calorimetry (DSC). The effect of the composition on the structure of the terpolymer and the resulting physical properties such as stiffness decreased by the decrease in the amount in (IBoA) [1-2].

References :
[1] Seok, W.C, J. T. Change of characterization and film morphology based on acrylic pressure sensitive adhesives by hydrophilic derivative ration. Polymers, 12, 1504, 2020.
[2] Luo Z, Liu C, Quan P, Yang D, Zhao H, Wan X, Fang L. Mechanistic insights of the controlled release capacity of polar functional group in transdermal drug delivery system: the relationship of hydrogen bonding strength and controlled release capacity. 2020.

P.27. Elaboration and characterization of PDLC films containing acrylic polymers

G F-Z. HAKEM[1]*, D. BENDEDOUCHE[1], A. BOURICHE[1], L. BEDJAOUI-ALACHAHER[1]

[1]Laboratory of Research on Macromolecules (LRM), Faculty of Sciences, University of Abou Bekr Belkaid, 13000, Tlemcen, Algeria
Email[1]* : ghizlenefatimazahra.hakem@univ-tlemcen.dz

Polymer-Dispersed Liquid Crystals, PDLCs, are formed by liquid crystal droplets embedded in a polymer matrix, which can assume different liquid crystal director configuration [1]. The content of this work is the development and characterization of PDLC films composed of monomer Isobornyl acrylate (IBoA) and a mixture of IBoA and 2-Ethylhexyl acrylate (2-EHA) monomers, with a liquid crystal E7. Their unique optical and electro-optical properties make them suitable for applications in various technological fields [2,3]. These systems are developed by UV light curing of two different mixtures, the first one is made of IBoA, the liquid crystal E7 in the presence of the photoinitiator Darocur 1173 and the crosslinking agent 1,6 hexanedioldiacrylate (HDDA). The second mixture contains the same components as the first except the addition of monomer 2-Ethylhexyl acrylate (2-EHA).
An electro-optical characterization of the polymerized mixtures xas carried out in order to understand the behavior under the effect of an electric field.
Keywords : liquid crystal E7, composite materials PDLC, electro-optical characterization.

References

[1] M Baratta, Gi. De Filpo, A. Tursi, A. I. Mashin and F.P.Nicoletta ; Polymer Dispersed Liquid Crystals with elongated droplets as novel pressure sensor. Liquid crystals. 2021,49 :5,657-665.
[2] M H Saeed, Y Gao, L Zhou, T Zhong, and al. Effects of multifunctional acrylates and thiols on the morphology and elctro-optical properties of polymer-dispersed liquid crystal films. Liquid Crystals. 2021, 48 :15,2188-2199.
[3] Gao H, Zhang S, Saeed MH, and al. Study on the motphologies and electro-optical properties of cyano-phenyl-ester liquid crystals/polymer composite films prepared by a setepwise polymerisation. Liquid Crystals. 2020 ;47 :1497-1506.

P.28. Electro-optic properties of liquid crystal dispersed nanodiamonds

C. Cirtoaje*[1] and E. Petrescu[1]

[1] University Politehnica of Bucharest, Romania
Email: cristina.cirtoaje@upb.ro

Nanodiamonds, also known as diamond nanoparticles, are diamonds with the size less than 100 nm. Due to their potential for surface functionalization and biocompatibility, they present great interest not only in optoelectronics [1] but also for biological applications as drug delivery system or in imagistic techniques [2]. Just like other nanoparticles dispersed in nematic liquid crystal, nanodiamonds affect the host electro-optic properties by their influence on the Freedericksz transition threshold and their behavior to the applied field. A 5CB dispersion of 65 nm nanodiamons powder, dodecane functionalized, was analyzed at different temperatures. The results indicated a high temperature dependence of the transition threshold of nanodiamond containing samples similar to those of single carbon layer nanoparticles such as SWCNTs and graphene[3].

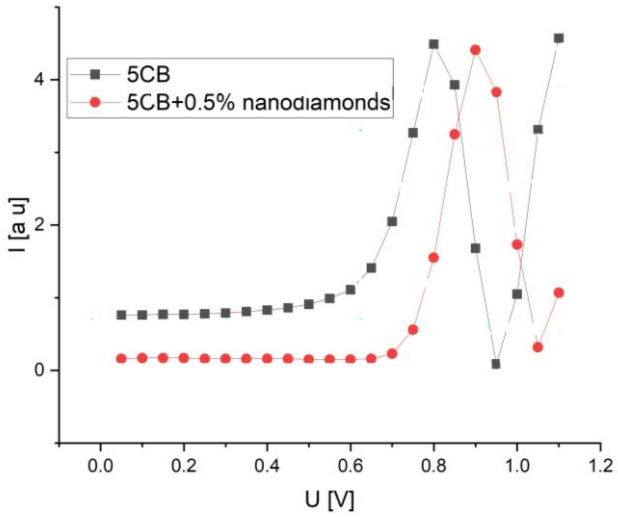


Figure 1. Intensity versus applied voltage plot for 5CB and 5CB +0.5% nanodiamonds

References:

[1]. Shenderova, O., Hens, S., Vlasov, I., Borjanovic, V., & McGuire, G. (2009). Nanodiamond Particles in Electronic and Optical Applications. MRS Proceedings, 1203, 1203-J08-01. doi:10.1557/PROC-1203-J08-01

[2]. Jin-Xu Qin, Xi-Gui Yang, Chao-Fan Lv, Yi-Zhe Li, Kai-Kai Liu, Jin-Hao Zang, Xun Yang, Lin Dong, Chong-Xin Shan, Nanodiamonds: synthesis, properties, and applications in nanomedicine, Materials & Design, Volume 210, 2021, 110091, ISSN 0264-1275, DOI: https://doi.org/10.1016/j.matdes.2021.110091.

[3]. Emil Petrescu, Cristina Cirtoaje, Ștefan Postelnicu Freedericksz transition in nematic liquid crystals with carbon nanomaterials U.P.B. Sci. Bull., Series A, Vol. 84, Iss. 1, 2022 ISSN 1223-7027

P.29. ZrO_2 for photocatalytic applications

M. Frenti[1], C. Mita[2], N. Cornei[2], V. Tiron[3], G. Bulai[4], M. Dobromir[3], A.S. Doroshkevich[5], D. Mardare[1*],

[1] PhD student, "Alexandru Ioan Cuza" University of Iasi, Faculty of Physics, 11 Carol I Blvd., 700506 Iasi Romania,
Email: mariana.amarinei@student.uaic.ro, marianafrenti2009@gmail.com
[2]"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, 11 Carol I Blvd., 700506 Iasi Romania,
Email: cmita@uaic.ro, ncornei@uaic.ro
[3]"Alexandru Ioan Cuza" University of Iasi, Research Center on Advanced Materials and Technologies, Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, 700506 Iasi, Romania,
Email: vasile.tiron@uaic.ro, marius.dobromir@uaic.ro
[4]Alexandru Ioan Cuza University of Iasi, Integrated Centre for Environmental Science Studies in the North-East Development Region – CERNESIM, 11 Carol I Blvd., 700506, Iasi, Romania
Email: georgiana.bulai@uaic.ro
[5]Joint Institute for Nuclear Research, Str. Joliot-Curie, 6, Dubna, 141980, Russia,
Email: doroh@jinr.ru

ZrO_2 is a transition metal oxide which is nontoxic, chemical and mechanical stable being a good material for photocatalytic applications [1]. The aim of this work was to investigate the influence of nitrogen doping on the photocatalytic activity of ZrO_2 thin films deposited by HiPIMS sputtering method, on Si substrates. The as-deposited films are polycrystalline, N doping inducing a phase transformation from monoclinic to tetragonal structure. Information on the elemental composition of the atomic species at the films surface was obtained by X-ray photoelectron spectroscopy. The undoped films are absorbent in the red zone of visible spectrum while the incorporation of nitrogen determines the shift of the fundamental absorption edge to the green one, as revealed by diffuse reflectance spectroscopy. We have investigated the decomposition of Rhodamine B under the same irradiation conditions, in the presence and in the absence of H_2O_2. Particularly, it was obtained a 60 % degradation rate, in 180 min, for N-doped ZrO_2, in the presence of H_2O_2.

References

[1] A. Areeb, T. Yousaf, M. Murtaza, M. Zahra, M. I. Zafar, A. Waseem, MATERIALS TODAY COMMUNICATIONS 28 (2021) 102678, pp.1-15

*) Author for Correspondence: Diana Mardare, dianam@uaic.ro