UNIVERSITY POLITEHNICA OF BUCHAREST
Department of Physics

ACADEMY OF ROMANIAN SCIENTISTS
Section of Physical Sciences

THE 7th INTERNATIONAL COLLOQUIUM "PHYSICS OF MATERIALS" (PM 7)

NOVEMBER 10-11, 2022
BUCHAREST, ROMANIA

INVITATION

On behalf of the Organizing Committee you are invited to participate to the seventh edition of the International Colloquium "Physics of Materials" (PM-7), organized by the University "Politehnica" of Bucharest and the Academy of Romanian Scientists.

The 7th International Colloquium on "Physics of Materials" will be held on November 10-11, 2022 in Bucharest, Romania. The aim of the Colloquium is to provide a forum for the presentation of new advances in the physics of materials research and novel applications.

The accepted and presented contributions will be selected by the Scientific Committee for publication in either the ISI-quoted journals Scientific Bulletin of UPB, Series A, B or the Annals of the Academy of the Romanian Scientists.

The conference will be held online.

Chair: Prof. Dr. Habil. Doina Mănăilă-Maximean

PROGRAM

8:45 Test connection

9:00 -- 9:10 OPENING: Doina Manaila-Maximean, Doru Delion

9:10 - 11:00 Section 1. Invited communications

		Chairs : Doru Delion **: Doina Manaila-Maximean**
1	**9.10-9:40**	**I1. Porous semiconductor compounds: obtaining and functionalization with metallic nanostructures for multifunctional applications** Eduard V. Monaico National Center for Materials Study and Testing, Technical University of Moldova, Republic of Moldova Email: eduard.monaico@cnstm.utm.md
2	**9:40-10:10**	**I.2. Continuous change from monoclinic to ferroelectric orthorhombic HfO_2 by a martensitic-like transition – challenge for nonvolatile memories** M L Ciurea[1,3], C Palade[1], A-M Lepadatu[1], A Slav[1], O Cojocaru[1,2], A Iuga[1], V A Maraloiu[1], V S Teodorescu[1,4], T Stoica[1], [1]National Institute of Materials Physics, 077125 Magurele, Romania Email: ciurea@infim.ro [2]University of Bucharest, Faculty of Physics, 077125 Magurele, Romania [3]Academy of Romanian Scientists, 050094 Bucharest, Romania
3	**10:10-10:30**	**I.3. Numerical simulations as a solution to design the desired optical properties of multilayers thin films** Mihaela Girtan[1*] [1] Photonics Laboratory, Angers University, 2, Bd. Lavoisier, 49045, Angers, France, mihaela.girtan@univ-angers.fr
4	**10:30-10 :50**	**I.4. Optical properties of spatially-ordered two-dimensional structures of spherical particles in absorbing matrix** V.A. Loiko, A.A. Miskevich, N.A. Loiko *B.I. Stepanov Institute of Physics of the National Academy of Sciences of Belarus, Minsk, Belarus* *E-mail: loiko@ifanbel.bas-net.by*

10:50 - 11:00 Coffee Break

11:00 - 12:30 Section 2. Invited and oral communications

		Chairs : Magdalena Ciurea **: Teodora Staicu**
5	**11:00 - 11:30**	**I.5. Tandem heterojunction solar cells with Cu_2O/ZnO Si based: optimization and defect analysis** L. FARA[1,2]*, I. CHILIBON[3], D. CRACIUNESCU[1], S. FARA[1] [1]Department of Physics, Faculty of Applied Sciences, Polytechnic University of Bucharest, Romania [2]Academy of Romanian Scientists, Bucharest, Romania [3]National Institute of Research and Development for Optoelectronics (INOE-2000), Bucharest-Magurele, Romania * lfara@renerg.pub.ro

6	**11:30-11:50**	**I.6. DICATIONIC IMIDAZOLIUM AND PYRIDINIUM SALTS: STUDY OF IONIC CONDUCTIVITY, LIQUID CRYSTALLINE AND EMISSION PROPERTIES** M. Iliş[1], M. Micutz[1], T. Staicu[1], Doina Manaila-Maximean[2], and V. Cîrcu[1*] [1] University of Bucharest, Bucharest, Romania Email: viorel.circu@chimie.unibuc.ro [2] University Politehnica of Bucharest, Bucharest, Romania
7	**11:50-12:00**	**O.1. Evaluation of mechanical and dielectric properties of some biodegradable cellulose-based composites** A.I. Barzic[1*], E. Turcu[1], M. Asandulesa[1], C. Tugui[1] and R.M. Albu[1] [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
8	**12:00-12:15**	**O.2. Behaviour of composite materials with polymer matrix / metal powders** D.E.Gavrilă[1], A.Caramitu[2], S.Mitrea[2],V.Stoian[1] [1]*Physics Department, Faculty of Applied Sciences, University POLITEHNICA of Bucharest* [2]*National Institute of Research and Development for Electrical Engineering* ***ICPE-CA*** *Bucharest* doina.gavrila@physics.pub.ro
9	**12:15-12:30**	**O.3. Nanoparticles of cobalt doped magnetite for tumor treatment** Helmina Ardeleanu[1*], Iordana Aşefănoaei [1], Dorina Creanga[1] [1] University Alexandru Ioan Cuza, Iasi, Romania Email: ardeleanu_helmina@yahoo.com

12:30-13:15 LUNCH

13:15-15:15 Session 3: Invited and oral communications

		Chairs: Radu Fierascu **: Doina Manaila-Maximean**
10	**13:15-13:35**	**I.7. PCM simple modelling and energy storage simulation** C. Stanciu[1*], and D. Stanciu[1] [1] University Politehnica of Bucharest, Romania Email: camelia.stanciu@upb.ro
11	**13:35-13:55**	**I.8.** Adsorption of Methylene Blue upon substrates of fabrics and filter paper type L. Frunza*, N.G. Apostol, I. Zgura, C.P. Ganea, V.F. Cotorobai National Institute of Materials Physics, 077125 Magurele, Romania Email: lfrunza@infim.ro
12	**13:55-14:05**	**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
13	**14:05-14:20**	**O.5. Orbital character of two dimensional electron gas at an oxide interface** M. A. Husanu[1*], A. Iancu[1], D. G. Popescu[1], C. Chirila[1], C. M. Teodorescu[1] [1] *National Institute of Materials Physics, Atomistilor 405A, 077125 Magurele, Romania* ahusanu@infim.ro
14	**14:20-14:30**	**O.6. Synthesis and characterization of cellulose acetate-TiO_2 polymeric membrane for water and wastewater treatment** S. Căprărescu[1*], V. Purcar[2], C. Modrogan[3], A. M. Dăncilă[3] and O. D. Orbuleț[3] [1] University Politehnica of Bucharest, Faculty of Chemical Engineering and Biotechnologies, Inorganic Chemistry, Physical Chemistry and Electrochemistry Department, Romania Email: simona.caprarescu@upb.ro [2] National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM, Bucharest, Romania [3] University Politehnica of Bucharest, Faculty of Chemical Engineering and Biotechnologies, Analytical Chemistry and Environmental Engineering Department, Romania

15	**14:30-14:45**	**O.7. FORMAL ACTIVITIES TO LEARN ABOUT NEW MATERIALS AND TECHNOLOGIES USED IN MAKING SENSORS AND ACTUATORS** L.C Farcaş[1,2*], C. Enachescu[1] [1]Alexandru Ioan Cuza University of Iasi, Faculty of Physics, Iasi, Romania [2"]St. John of La Salle" Technological High School, Pildesti, Romania Email: lidycera@yahoo.com
16		

14:45-15:00 Coffee Break

15:10 -17:00 POSTER Session

Chairs: Marian Micutz
Viorel Cîrcu

The authors will be connected online in the order of the posters (see Abstract book _posters) for five minutes and the interested scientists might contact the authors directly. More details will be available.

FRIDAY, November 11

9:45 Test connection

10:00-11:00 Session 4 Invited communications

		Chairs : Camelia Stanciu **: Andrei Dragulinescu** **: Viorel Circu**
16	**10:00-10-30**	**I.9. At the Frontier Between Materials Science and Biotechnology: Nanomaterials Phytosynthesis** I. Fierascu[1,2], R.C. Fierascu[1,3*], A.M. Baroi[1,2], R.I. Matei (Brazdis)[1,3], T. Fistos[1,3], I.C. Fierascu[1,2], I. Chican[1], and I.S. Hosu[1] [1]National Institute for Research & Development in Chemistry and Petrochemistry - ICECHIM Bucharest, Romania Email: irina.fierascu@icechim.ro, fierascu.radu@icechim.ro, anda.baroi@icechim.ro, roxanda.brazdis@icechim.ro, toma.fistos@icechim.ro, irina-elena.chican@icechim.ro, ioana.hosu@icechim.ro [2] University "Politehnica" of Bucharest, Romania [3] University of Agronomic Sciences and Veterinary Medicine of Bucharest, Romania [4] University of Medicine and Pharmacy "Carol Davila", Romania Email: ioana.fierascu@drd.umfcd.ro
17	**10:30-11**	**I.10. Pincer Complexes of Gold(III): Organometallic Chemistry, Liquid Crystals, Photophysics and OLEDs** Alice J. McEllin[1], Rachel R. Parker[1], Rachel F. Stracey[1], Denghui Liu[2], Xiankang Yu[2], Xinrui Chen[2], Xinagbing Zhen[3], Adrian C. Whitwood[1], J. A. Gareth Williams[4], Yafei Wang[2], Jason M. Lynam[1] and Duncan W. Bruce[1*] [1] Department of Chemistry, University of York, YORK YO10 5DD UK; E-mail: duncan.bruce@york.ac.uk; [2] School of Materials Science & Engineering, Changzhou University, CHANGZHOU 213164, PR CHINA; [3] Department of Materials Science and Engineering, University of Sheffield, Sheffield, UK; [4] Department of Chemistry, Durham University, South Road, DURHAM, DH1 3LE UK.

11:00-13:15 Session 5: Oral communications

		Chairs : Camelia Stanciu **: Andrei Dragulinescu**
18	**11:00 - 11:15**	**O.9. Structure–property relationships in photopolymerizable systems : Effect of composition and resulting physical properties of acrylates based copolymers** D. Bendeddouche[1*], G F-Z. HAKEM[1], U. MASCHKE [2], L. BEDJAOUI-ALACHAHER[1] [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
19	**11:15-11:30**	**O.10. Corrosion protection of metallic substrates by silane-based coatings** D. Bala[1,*], A. Sfetcu[1], M.A. Tănase[1,2], L.O. Cinteză[1] [1]University of Bucharest, Faculty of Chemistry, Department of Physical Chemistry, 4-12 Regina Elisabeta, 030018 Bucharest, Romania *[2]INCDCP-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
20	**11:30-11:45**	**O.11. Physical and chemical properties of cyano-containing polyimide/azo-chromophore systems designed for flexible electronic products** I. Stoica[1*], E.-L. Epure[2], A. I. Barzic[1], M. Asandulesa[1], C. Ursu[1], I. Mihaila[3], A.-D. Diaconu[1], I. Sava[1] [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, e-mail: stoica_iuliana@icmpp.ro
21	**11:45-12:00**	**O.12. Technology for obtaining the amorphous luminophore composition As_2S_3:Eu(DBM)$_3$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;*
22	**12:00-12:15**	**O.13. Light-emitting materials based on nematic liquid crystals doped with double cyclopalladated complexes** Daiana G. Mitrea[1], Monica Iliș[1], Doina Mănăilă-Maximean[2], Viorel Cîrcu[1*] [1]Department of Inorganic Chemistry, University of Bucharest, Bucharest, Romania Email: daiana.mitrea@drd.unibuc.ro, [*]viorel.circu@chimie.unibuc.ro [2]Department of Physics, University Politehnica of Bucharest, Bucharest, Romania
23	**12:15-12:30**	**O.14. 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
24	**12:30-12:45**	**O.15. Design and Simulations of Perovskite-Based Solar Cells with Efficiencies Over 30%** S. H. M. A. Hussein[1,2], A. Drăgulinescu[3*] [1] Faculty of Engineering in Foreign Languages, Politehnica University of Bucharest, 1-3 Iuliu Maniu Blvd., Spl. Independenţei 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. Independenţei 313, sector 6, RO-060032, Bucharest, Romania Email: dragulinescu@yahoo.com
25	**12:45-13:00**	**O.16. Nanoscale Imaging of Polymer Coated Gold Nanoparticles with Scattering-type Scanning Near-Field Optical Microscopy** Stefan G. Stanciu[1], Denis E. Tranca[1], Giulia Zampini[2], Radu Hristu[1], George A. Stanciu[1], Xinzhong Chen[3,4], Mengkun Liu[3,4], Harald A. Stenmark[5], and Loredana Latterini[2] [1]Center for Microscopy-Microanalysis and Information Processing, Politehnica University of Bucharest, Romania., [2]Department of Chemistry, Biology and Biotechnology, Perugia University, Italy. [3]Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA. [4]National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York, USA. [5]Department of Molecular Cell Biology, Institute for Cancer Research, Oslo University Hospital, Oslo Norway sgstanciu@gmail.com
26	**13:-13:15**	**O.17. Rheological aspects on some hydrogels e-beam crosslinked** T. Staicu[1], M. Demeter[2], M. Ilis[3], V. Circu[3], 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), Atomiştilor 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

VIRTUAL ABSTRACT BOOK – INVITED PAPERS

I.1. Porous semiconductor compounds: obtaining and functionalization with metallic nanostructures for multifunctional applications

Eduard V. Monaico

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

The report will focus on different aspects of pore growth during electrochemical etching in a controlled fashion [1], transition from the porous semiconductor structures to the formation of semiconductor nanowires [2,3], as well as technologies for controlled electrochemical deposition of metal nanostructures into porous semiconductor templates [4].

The obtained metal-semiconductor structures were exploited in a variable capacitance device elaboration with a record capacitance density variation of about 6×10^{-3} pF/V per 1 μm^2 of surface [5]. An IR photodetector based on a single GaAs nanowire with good sensitivity and dynamic characteristics was demonstrated [3]. The fabricated core-shell GaAs/Fe nanowire arrays, along with possibilities to tune the orientation to the substrate surface, showed magnetic anisotropy with respect to the coercivity and the remanence ratio [6,7].

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.; Tiginyanu, I.; Volciuc, O.; Mehrtens, T.; Rosenauer, A.; Gutowski, J.; Nielsch, K. Formation of InP Nanomembranes and Nanowires under Fast Anodic Etching of Bulk Substrates. *Electrochemistry Communications* **2014**, *47*, pp. 29–32, doi:10.1016/j.elecom.2014.07.015.
[3] 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.
[4] Monaico, E.I.; Monaico, E.V.; Ursaki, V.V.; Tiginyanu, I.M. Controlled Electroplating of Noble Metals on III-V Semiconductor Nanotemplates Fabricated by Anodic Etching of Bulk Substrates. *Coatings* **2022**, *12*, 1521, doi:10.3390/coatings12101521.
[5] Tiginyanu, I.; Monaico, E.; Sergentu, V.; Tiron, A.; Ursaki, V. Metallized Porous GaP Templates for Electronic and Photonic Applications. *ECS J. Solid State Sci. Technol.* **2015**, *4*, P57, doi:10.1149/2.0011503jss.
[6] Monaico, E.V.; Morari, V.; Ursaki, V.V.; Nielsch, K.; Tiginyanu, I.M. Core–Shell GaAs-Fe Nanowire Arrays: Fabrication Using Electrochemical Etching and Deposition and Study of Their Magnetic Properties. *Nanomaterials* **2022**, *12*, 1506, doi:10.3390/nano12091506.
[7] Monaico, E.V.; Morari, V.; Kutuzau, M.; Ursaki, V.V.; Nielsch, K.; Tiginyanu, I.M. Magnetic Properties of GaAs/NiFe Coaxial Core-Shell Structures. *Materials* **2022**, *15*, 6262, doi:10.3390/ma15186262.

I.2. Continuous change from monoclinic to ferroelectric orthorhombic HfO_2 by a martensitic-like transition – challenge for nonvolatile memories

M L Ciurea[1,3], C Palade[1], A-M Lepadatu[1], A Slav[1], O Cojocaru[1,2], A Iuga[1], V A Maraloiu[1], V S Teodorescu[1,4], T Stoica[1],

[1]National Institute of Materials Physics, 077125 Magurele, Romania
Email: ciurea@infim.ro
[2]University of Bucharest, Faculty of Physics, 077125 Magurele, Romania
[3]Academy of Romanian Scientists, 050094 Bucharest, Romania

In the last decades a lot of effort has been spent for obtaining lead-free ferroelectric materials at nanoscale for micro- and nano - electronic devices, the ferroelectric orthorhombic HfO_2 (o-HfO_2) being one of the most important. The formation of orthorhombic phase and controlling ferroelectricity in HfO_2 are reported in literature to be strongly dependent on factors as size effect, surface and interface energy, oxygen vacancies, dopant concentration and stress [1,2].

We obtain ferroelectric o-HfO_2 in HfO_2/Ge-HfO_2/HfO_2 3-layer structure deposited by magnetron sputtering and then nanostructured by rapid thermal annealing (RTA) [3]. The o-HfO_2 is formed in Ge NCs-HfO_2 intermediate layer, HfO_2 crystallization and ferroelectric phase formation being significantly influenced by Ge doping and the stress field present in the 3-layer. Therefore, o-HfO_2 is also formed inside the adjacent layers, in the 5 nm regions near the interface in which Ge has diffused. At the surface of cap layer/structure surface, HfO_2 is monoclinic.

A continuous spatial transition (over few atomic layers) from monoclinic to orthorhombic phase was revealed inside single HfO_2 nanocrystals. In our opinion, the crystallization mechanism consists in a martensitic-like transformation of the initially grown tetragonal phase that during RTA transforms in orthorhombic (in regions with remaining stress and in those with Ge dopping), and in monoclinic phase where HfO_2 is relaxed, as at 3-layer surface. These leads to the continuous spatial transition from monoclinic to orthorhombic phase under the influence of Ge-doping and remaining stress. Atomistic calculations support our model.
The ferroelectric behavior is revealed by remanent polarization – voltage hysteresis loops and the total remanent polarization is of 6.5 $\mu C/cm^2$, being comparable to
the values reported for thick HfO_2 and large ferroelectric domains.

This work was supported by the Romanian Ministry of Research, Innovation & Digitization and CNCS – UEFISCDI, project no. PN-III-P4-ID-PCCF-2016-0033, PN-III-P2-2.1-PED-2019-0205, PN-III-P1-1.1-PD-2019-1038, and Research and Innovation (NIMP Core Program PN19-03 Contract no. 21N/2019).

References:
[1] *J. Mater. Chem.* C **9**, 12353 (2021); [2] *Nanotechnology* **30**, 445501 (2019);
[3] *Nanomaterials* **12**, 279 (2022).

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

I.3.
Numerical simulations as a solution to design the desired optical properties of multilayers thin films

Mihaela Girtan[1*]

[1] Photonics Laboratory, Angers University, 2, Bd. Lavoisier, 49045, Angers, France,

mihaela.girtan@univ-angers.fr

Ellipsometry is a non-destructive, non-invasive non-contact, very precise, reproducible and very sensitive technique for study the ultra-thin films. Spectroscopic ellipsometry (SE) provides a widely applicable method for determining accurate characterization of optical and electrical transport properties of thin films multilayers structures, in particularly when the multilayer of device structure, is of critical importance to their effective implementation. The difficulty consist to discern between two or more ellipsometric models which both fits well the same data. In the most reported data in literature, the ellispometric models studied are considered enough good if the experimental data of the global refractive index (n) and extinction coefficient (k) fits well with the dispersion curves. Improved models can be constructed however by also comparing the calculated the transmission coefficient from ellipsometry with the experimental values obtained from direct spectrophotometry measurements. This procedure allows to establish in a more accurate way the best dispersion model for each sample. The good correlations obtained between the electrical and optical properties determined experimentally by different techniques and the electrical and optical characteristics obtained by theoretical ellipsometric simulations, indicate that high accurate ellipsometric modelling approach, can give the possibility in the future to predict the appropriate device architecture in function of the desired optical and electrical properties and to reduce hence the experimental tests and the waste of materials in the optimization of multilayers thin films fabrication process.

This paper provide a comprehensive study of the spectroscopic ellipsometric measurements of single oxide films and multi layers thin-film coupled with other direct measurements techniques in order to present a possible method for designing, by numerical simulations, new multilayers architectures with the desired properties.

I.4. Optical properties of spatially-ordered two-dimensional structures of spherical particles in absorbing matrix

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

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

The developed by us statistical method to solve the problem of light scattering and absorption by a short- and long-range ordered monolayer of spherical particles in an unbounded nonabsorbing host medium [1-7] is generalized to a host medium with light absorption. It takes into account multiple scattering of waves, is based on the quasicrystalline approximation (QCA), mean field approximation and the expansion of fields and tensor Green's function in terms of the vector spherical wave functions and has no restrictions on the distance between particles. The method allows one to describe optical properties of a "monolayer of spherical particles in light absorbing matrix" system.

The data for coefficients of coherent transmission and reflection, incoherent scattering, and absorption are presented. Comparison with the data for inverse system (the matrix is made from the material of the particles, and the particles are made from the matrix material) is fulfilled.

The influence of particle and matrix complex refractive indices, particle diameters, their spatial order, and monolayer filling factors on the optical properties of the system is considered. The effect of "extraordinary transmittance" is illustrated for monolayer of spherical nanovoids in the silver matrix.

The results obtained can serve as a basis for solving the inverse problem of light scattering. They can be used to solve the wide range of problems of photonics, optoelectronics, and chemistry: to develop the solar cells, photonic crystals, optical coatings, photodetectors, chemical photoreactors, and other devices based on particulate two-dimensional structures.

- V. A. Loiko, A. A. Miskevich, "Multiple Scattering of Light in Ordered Particulate Media" pp. 101-231. **"**Springer Series in Light Scattering". A. Kokhanovsky (Ed.). Springer. 2018.
- N. A. Loiko, A. A. Miskevich, and V. A. Loiko, "Incoherent component of light scattered by a monolayer of spherical particles: analysis of angular distribution and absorption of light," J. Opt. Soc. Am. A. 35, No 1,108-118 (2018).
- N. A. Loiko, A. A. Miskevich, and V. A. Loiko, "Scattering of Polarized and Natural Light by a Monolayer of Spherical Homogeneous Spatially Ordered Particles under Normal Illumination," Opt. Spectr. 125, 655-666 (2018).
- A. A. Miskevich, N. A. Loiko, and V.A. Loiko, "Absorption of light by a particulate monolayer: Effect of ordering, concentration, and size of particles," J. Quant. Spectr. Rad. Transf. 229, 50–59 (2019).
- N. A. Loiko, A. A. Miskevich, and V. A. Loiko, "Scattering and Absorption of Light by a Monolayer of Spherical Particles under Oblique Illumination," J. Exp. Theor. Phys. 131(2), 227-243 (2020).
- N. A. Loiko, A. A. Miskevich, and V. A. Loiko, "Polarization of light scattered by a two-dimensional array of dielectric spherical particles," J. Opt. Soc. Am. B 38(9), C22-C32 (2021).
- N. A. Loiko, A. A. Miskevich, and V. A. Loiko, "Absorption of diffuse light by 2D arrays of spherical particles," J. Quant. Spectr. Rad. Transf. 289, 108291-1-9 (2022).

I.5.
Tandem heterojunction solar cells with Cu_2O/ZnO Si based: optimization and defect analysis

L. FARA[1,2]*, I. CHILIBON[3], D. CRACIUNESCU[1], S. FARA[1]

[1]Department of Physics, Faculty of Applied Sciences, Polytechnic University of Bucharest, Romania
[2]Academy of Romanian Scientists, Bucharest, Romania
[3]National Institute of Research and Development for Optoelectronics (INOE-2000), Bucharest-Magurele, Romania
* lfara@renerg.pub.ro

A four-terminal Cu_2O/ c-Si tandem heterojunction solar cell was investigated. The electrical and optical characteristics for aluminium doped ZnO (AZO) and undoped Cu_2O thin film layers were determined.
The modeling of solar device was based on two main simulation softwares: 1) Silvaco used for the top Cu_2O/Zn O subcell, and 2) PC1D/Quokka 2 for the bottom c-Si subcell[1]. Numerical modelling allowed to analyse the main electrical parameters of the two sub cells, in order to optimize the performance of the solar device. A power conversion efficiency of 24.7 % for the four-terminal Cu_2O/c-Si tandem heterojunction solar cell was obtained. The effect of interface defects on the electrical characteristics of the AZO/Cu_2O heterojunction was evaluated. The analysis suggested that the incorporation of a buffer layer could improve the performance of the heterojunction solar cell.

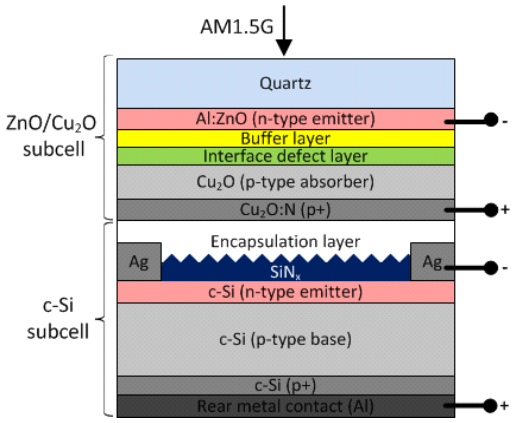


Figure 1. The heterojunction solar cell based on sputtering deposition of metal oxides

References:

[1]. L. Fara, I. Chilibon, Ø. Nordseth, D. Craciunescu, D. Savastru, C. Vasiliu, L. Baschir, S. Fara, R. Kumar, E. Monakhov and J. P. Connolly, Complex Investigation of High Efficiency and Reliable Heterojunction Solar Cell based on an Improved Cu_2O Absorber Layer, ENERGIES **, 13**, Issue 18, 4667; doi:10.3390/en13184667 (2020)

I.6.
DICATIONIC IMIDAZOLIUM AND PYRIDINIUM SALTS: STUDY OF IONIC CONDUCTIVITY, LIQUID CRYSTALLINE AND EMISSION PROPERTIES

M. Iliş[1], M. Micutz[1], T. Staicu[1], Doina Manaila-Maximean[2], and V. Cîrcu[1*]

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

Ionic liquid crystals (ILCs) are a distinct class of materials with unique properties resulting from the combination of liquid crystals and ionic liquids behaviour. ILCs based on imidazolium or pyridinium salts are very well documented; in fact, these salts are the most common ILCs studied for their exceptional characteristics such as low volatility, nonflammability, tunable polarity, high-ionic conductivity related to their ionic liquid nature in connection with their liquid crystalline properties.[1-3] Some recent applications were added: battery materials, solar cells, electrochemical sensors, organic reaction media or electroluminescent switches.

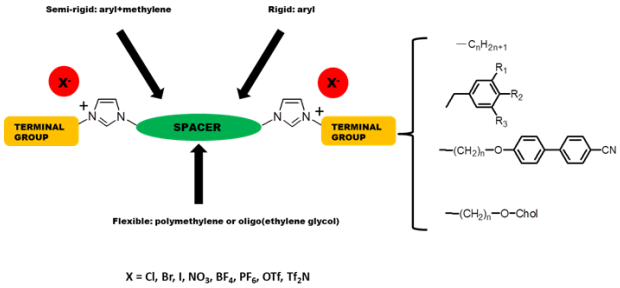


Figure 1. ILCs based on bisimidazolium salts.

This presentation will focus on the design and characterization of various dicationic ionic liquid crystals based on imidazolium or pyiridinium salts with various counterions, which have been reported recently by our group. The type of mesogenic group, spacer length and the nature of counterion will be related to the liquid crystals properties. Also, the emission properties of the simple organic salt or coupled with emissive units (polyoxometalates) will be discussed.

References:

[1]. N. Kapernaum, A. Lange, M. Ebert, M. A. Grunwald, C. Haege, S. Marino, A. Zens, A. Taubert, F. Giesselmann, S. Laschat (2022). CHEMPLUSCHEM, 87, e202100397.
[2]. K. V. Axenov, S. Laschat (2011), MATERIALS, 4, 206–259.
[3]. V. Cîrcu, Ionic liquid crystals based on pyridinium salts, in PROGRESS AND DEVELOPMENTS IN IONIC LIQUIDS (Ed.: S. Handy), IntechOpen, 2017, pp. 285–311.

*) Author for Correspondence

I.7. PCM simple modelling and energy storage simulation

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

[1] University Politehnica of Bucharest, Romania
Email: camelia.stanciu@upb.ro

Nowadays efforts are made to develop more efficient techniques for producing electric energy from renewable energy sources. In this context, a special attention is directed towards the solar to electric energy conversion. This can be obtained either directly by employing photovoltaic panels, or indirectly by using thermodynamic cycles. One main advantage of the last methods consists in the possibility of extending the system operation over periods of solar energy unavailability, by integrating a thermal energy storage subsystem. Phase change materials (PCM) turn out to be good candidates for such purposes.

The proposed paper provides a simple mathematical modelling, based on energy conservation law, to simulate the melting process of a PCM driven a commercial parabolic through collector (PTC). The considered system is presented in Figure 1.

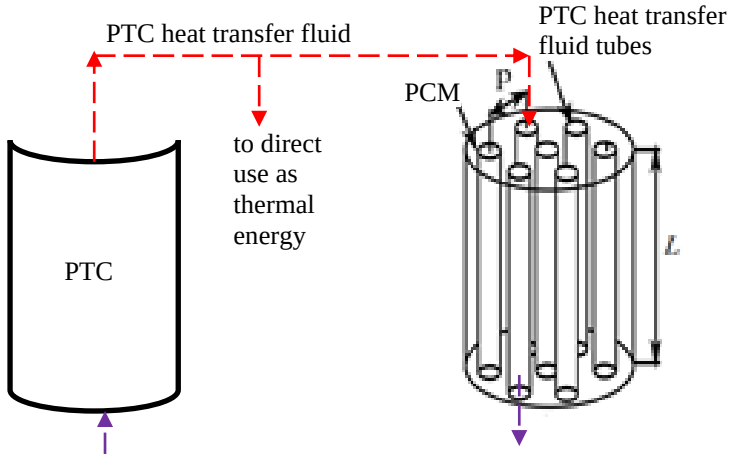


Figure 1. PTC-PCM studied system.

Analytical development, as well as numerical and graphical results are presented for several days operation. Sensitivity studies with respect to system dimension (number of coupled PTC and PCM modules) are included.

*) Author for Correspondence

I.8. Adsorption of Methylene Blue upon substrates of fabrics and filter paper type

L. Frunza*, N.G. Apostol, I. Zgura, C.P. Ganea, V.F. Cotorobai

National Institute of Materials Physics, 077125 Magurele, Romania
Email: lfrunza@infim.ro

We have recently investigated the photocatalytic behavior of some fabrics deposited with semiconductor oxide (TiO2, ZnO) nanoparticles in pure or doped state; methylene blue (MB) and its degradation was chosen as a well known dye and test reaction (see e.g. [1,2] and the long list of reference cited herein). Closely related to these, is the radial liquid spreading from an infinite reservoir containing a dye solution onto a horizontal fabric or a common filter paper (which are playing as the catalyst supports): The topic is discussed in this presentation.
The images of the wet spot during the radial wicking were collected with a webcam; then these were processed with routines giving the area of the wet spot as function of time. One can thus speak about the wicking kinetics and further, about the possible mechanism. The experiments were performed using polyester (PES) and wool (WO) samples differing not only by the yarn composition but also by the roughness of the surfaces. White or colored fabrics were considered The data were compared with the results obtained for the common filter paper (CFP) for laboratory use.
MB was commercially purchased and used as such. Aqueous MB solutions were either diluted (0.1 mM) or more concentrated (1 mM). Sample notation keeps the material label for the 'substrate' while MB appears with the dye concentration; thus MB(0.1)/CFP means a filter paper sample imbibed with diluted MB solution.
The samples were routinely characterized both in the original and the MB deposited form as well to consider the structure, the surface morphology and the deposition changes. by applying several techniques [1,2].
MB wicking in textiles was followed by an optical method. The analysis of the images of the wet spots allows to conclude that the procedure developed is useful in comparing the behavior of the fabrics against the MB imbibition and further in the tests of MB degradation. Moreover, the kinetics of wetting can be discussed as well. There are elliptical wet spots. Water (the solvent) has a higher wicking rate than the dye. The dye is concentrated in a small region due to adsorption upon supports. The evolution of the elliptical wet spot conserves the ratio of the main ellipse axes.
Acknowledgements. The authors gratefully thank the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI) for the financial support under the project PN19-030101 of the CORE Program.
References:
[1] L. Frunza, et al., CATALYSIS TODAY 306, 2018, pp. 251-259.
[2] I. Zgura, et al., JOAM 17, No. 7-8, 2015, pp. 1055-1063
*) Author for Correspondence:

I.9.
At the Frontier Between Materials Science and Biotechnology: Nanomaterials Phytosynthesis

I. Fierascu[1,2], R.C. Fierascu[1,3*], A.M. Baroi[1,2], R.I. Matei (Brazdis)[1,3], T. Fistos[1,3], I.C. Fierascu[1,2], I. Chican[1], and I.S. Hosu[1]

[1]National Institute for Research & Development in Chemistry and Petrochemistry - ICECHIM Bucharest, Romania Email: irina.fierascu@icechim.ro, fierascu.radu@icechim.ro, anda.baroi@icechim.ro, roxanda.brazdis@icechim.ro, toma.fistos@icechim.ro, irina-elena.chican@icechim.ro, ioana.hosu@icechim.ro

[2] University "Politehnica" of Bucharest, Romania

[3] University of Agronomic Sciences and Veterinary Medicine of Bucharest, Romania

[4] University of Medicine and Pharmacy "Carol Davila", Romania Email: ioana.fierascu@drd.umfcd.ro

Nanotechnology represents one of the most important advances in materials science, as it provided important break-throughs in many different aspects of every day life. Among different methods for nanomaterials development, phytosynthesis of materials is of part importance due to its several advantages of other methods.

For over a decade now, our research group evaluated the possibilities of phytosynthesis of different types of nanoparticles, gaining insights on the advantages of this method, as well as on its limitations. A successful approach for the development of phytosynthesized nanomaterials with enhanced applications requires an application-correlated strategy, involving knowledge of biotechnology, nanotechnology, materials science and others.

Through selected examples from our published works [1-3], the high potential of the phytosynthesized nanomaterials for practical applications will be clearly demonstrated.

Acknowledgements: This work was supported by the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P4-PCE-2021-0292, contract 92PCE/2022, and project number PN-III-P2-2.1-PED-2021-0273, contract 644PED/2022, within PNCDI III. The support provided by the Ministry of Research, Innovation and Digitization through Program 1 - Development of the national research and development system, Subprogram 1.2 -Institutional performance - Projects to finance excellence in RDI, Contract no. 15PFE / 2021 is also gratefully acknowledged.

References: (12pt)

[1] C. Ungureanu et al., MATERIALS, 15(15), 5374

[2] I. Fierascu et al., MATERIALS, 10(5), 748

[3] R.C. Fierascu et al., JOURNAL OF MATERIALS SCIENCE, 55(5), 1915-1932

*) Author for Correspondence: fierascu.radu@icechim.ro

I.10. Pincer Complexes of Gold(III): Organometallic Chemistry, Liquid Crystals, Photophysics and OLEDs

Alice J. McEllin[1], Rachel R. Parker[1], Rachel F. Stracey[1], Denghui Liu[2], Xiankang Yu[2], Xinrui Chen[2], Xinagbing Zhen[3], Adrian C. Whitwood[1], J. A. Gareth Williams[4], Yafei Wang[2], Jason M. Lynam[1] and Duncan W. Bruce[1*]

[1] Department of Chemistry, University of York, YORK YO10 5DD UK;
E-mail: duncan.bruce@york.ac.uk;
[2] School of Materials Science & Engineering, Changzhou University, CHANGZHOU 213164, PR CHINA;
[3] Department of Materials Science and Engineering, University of Sheffield, Sheffield, UK;
[4] Department of Chemistry, Durham University, South Road, DURHAM, DH1 3LE UK.

Gold(III) complexes of *C^N^C* pincer ligand are promising emissive materials for OLED devices owing to the accessibility of triplet excited states. It is likely that there is also merit in further functionalising the emissive component of OLEDs by conferring liquid crystal properties and, to that end, we undertook the preparation of several series of materials with the general structure shown in the Figure.

The complexes vary through: (i) the number/position(s) of chains on the pincer backbone (*n* = 1 or 2) and (ii) the number and nature of the chains (hydrocarbon and semiperfluorocarbon) on the phenyl-acetylene (*m* = 0-3).

Among the properties are: (i) good photoluminescence quantum yields and OLED external quantum efficiencies; [1] (ii) wide-range liquid crystal mesophases

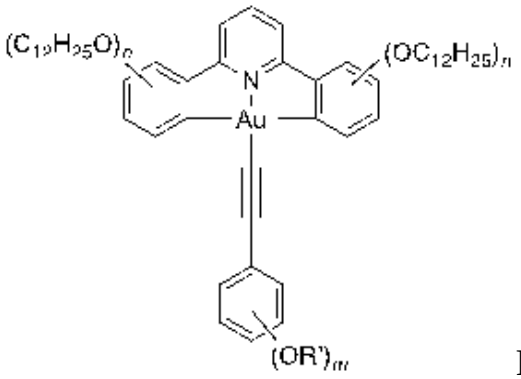


Figure: General structure of the complexes investigated in this study.

[1,2] and (iii) almost unprecedented observation of a frustrated nematic liquid crystal phase in a disc-like material.[3] Furthermore, such complexes cannot be synthesised directly from the ligand, rather through a toxic intermediate organomercury(II). Importantly we have recently shown how they can now be accessed either through palladium(II) intermediates or directly using Rh catalysis. [4]

References

1. R. R. Parker, D. Liu, X. Yu, A. C. Whitwood, W. Zhu, J. A. G. Williams, Y. Wang, J. M. Lynam and D. W. Bruce, *J. Mater. Chem. C*, 2021, **9**, 12871302.
2. R. R. Parker, R. F. Stracey, A. J. McEllin, X. Chen, Y. Wang, J. A. G. Williams, J. M. Lynam and D. W. Bruce, *ACS Omega*, 2022, **7**, 24903-24917.
3. R. R. Parker, A. J. McEllin, X. Zeng, J. M. Lynam and D. W. Bruce, *Liq. Cryst.*, 2022, **49**, 1162-1173.
4. A. J. McEllin, A. C. Whitwood, J. M. Lynam and D. W. Bruce, *ChemRxiv*, https://chemrxiv.org/engage/chemrxiv/article-details/62fa41022135016c2d39e943.

Abstract book
ORAL COMMUNICATIONS

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

A.I. Barzic[1*], E. Turcu[1], M. Asandulesa[1], C. Tugui[1] and R.M. Albu[1]

[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

This is a template for your preparation of abstracts to be submitted to the 7th International Colloquium "Physics of Materials" to be held in Bucharest, Romania, November 10-11, 2022.

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.

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.Gavrilă[1], A.Caramitu[2], S.Mitrea[2],V.Stoian[1]

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

[2]*National 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 Aşefănoaei [1], Dorina Creanga[1]

[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, $Co_xFe_{3-x}O_4$ 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. Offen 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

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

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

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

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. Iancu[1], D. G. Popescu[1], C. Chirila[1], C. M. Teodorescu[1]
[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 appers at the interface between $SrTiO_3$ and $LaAlO_3$ by direct visualization of the electronic band structure [2-4]. The soft X-ray photoemssion experiments performed with synchrotron radiation reveal in additon to the intrinsic electronic structure of the interface 2DEG, derived from the Ti t_{2g} orbitals, the occurrence of oxygen vacancies (OV) states manisfested as defect-like non dispersive bands at ~1.5 eV below the Fermi energy. Their dimensionality is explored in angle resolved photoemssion 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 rhe 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-TiO_2 polymeric membrane for water and wastewater treatment

S. Căprărescu[1*], V. Purcar[2], C. Modrogan[3], A. M. Dăncilă[3] and O. D. Orbuleţ[3]

[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-TiO_2 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 TiO_2 nanoparticles into the polymer matrix chains lead to the modification of the absorption band intensities. The microscopy analysis of the polymeric membrane containing TiO_2 nanoparticles showed that the nanoparticles were uniformly distributed in the polymer matrix. The impedance results indicated that the TiO_2 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. Modrogan, A.-L. Chiriac, C. A. Nicolae, POLYMERS, 12, no. 8, 2020, 1792.
[6] S. Căprărescu, C. Modrogan, 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 Farcaș[1,2*], C. Enachescu[1]

[1]Alexandru Ioan Cuza University of Iasi, Faculty of Physics, Iasi, Romania
[2]"St. John of La Salle" Technological High School, Pildesti, 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 involvment 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 Conducticity 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. HAKEM[1], U. MASCHKE [2], L. BEDJAOUI-ALACHAHER[1]

[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 (^{1}H 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 (Tg) 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].

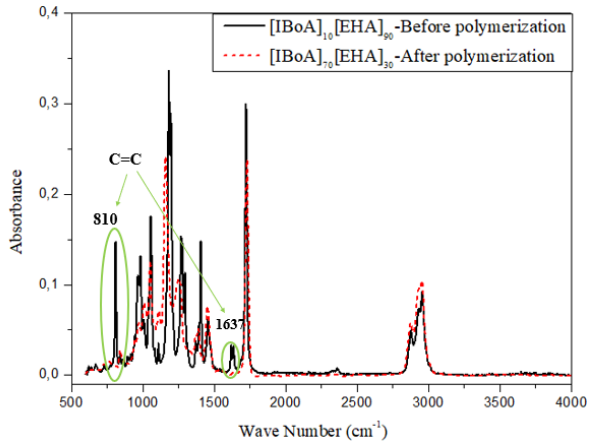


Figure 1. FTIR spectra of Cop[IBoA]$_{70}$[EHA]$_{30}$, Before and After polymerization.

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. Sfetcu[1], M.A. Tănase[1,2], L.O. Cinteză[1]
[1]University of Bucharest, Faculty of Chemistry, Department of Physical Chemistry, 4-12 Regina Elisabeta, 030018 Bucharest, Romania
[2]*INCDCP-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. Ghebaur, 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. Epure[2], A. I. Barzic[1], M. Asandulesa[1], C. Ursu[1], I. Mihaila[3], A.-D. Diaconu[1], I. Sava[1]

[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 comportment, 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 As_2S_3:Eu(DBM)$_3$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 Eu(DBM)$_3$Phen with enhanced luminescence properties.

Thin films of the amorphous composition As_2S_3: Eu(DBM)$_3$Phen were obtained on optical glass substrate by the method of simultaneous thermal co-evaporation in vacuum ($2\cdot10^{-5}$ mm. Hg) from two tantalum evaporators: "quasi-closed" for As_2S_3 [1] and cross-shaped for Eu(DBM)$_3$Phen. Transparent amorphous films were obtained with thicknesses in the range of 125 ÷ 1000 nm.

On Fig.1. is shown the sample of the amorphous composition As_2S_3:Eu(DBM)$_3$Phen with two different thicknesses: 0.9 μm on the left and 3 μm 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.

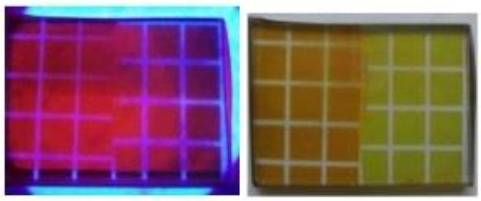


Fig. 1. Thin film network (left) and Red luminescence (write).

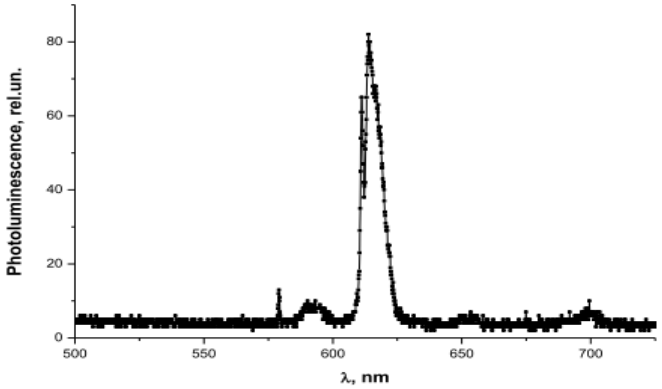


Fig. 2. PL spectrum of the material: λex=405nm, T=300 K.

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

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

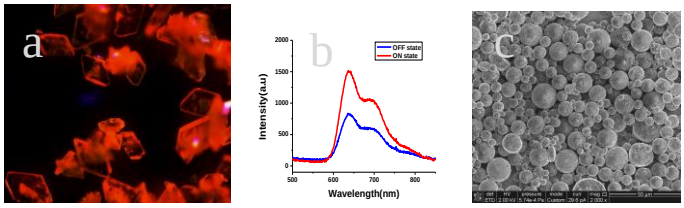


Figure 1. a) Solid state emission of the Pd(II) complex upon UV irradiation; b) Effect of the applied voltage on the PL intensity for the E7+5% Pd (II) complex mixture filled in a planar ITO cell; c) SEM picture of spherical microcapsules.

References:
[1] M. Micutz, M. Iliş, T. Staicu, F. Dumitraşcu , 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.

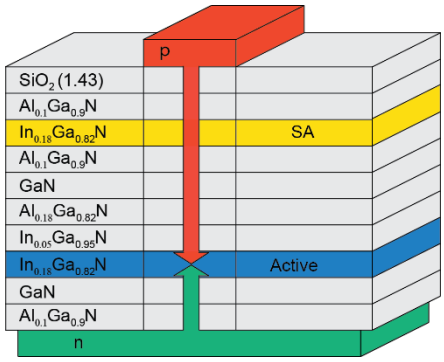


Figure 1. Schematic of the InGaN laser.

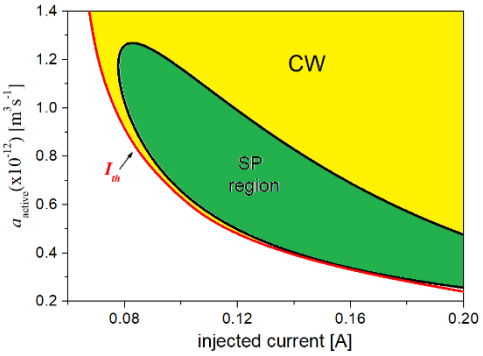


Figure 2 Self-pulsation region.

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 Shiying 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. Drăgulinescu[3*]

[1] Faculty of Engineering in Foreign Languages, Politehnica University of Bucharest, 1-3 Iuliu Maniu Blvd., Spl. Independenţei 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. Independenţei 313, sector 6, RO-060032, Bucharest, Romania
Email: dragulinescu@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. Stanciu[1], Denis E. Tranca[1], Giulia Zampini[2], Radu Hristu[1], George A. Stanciu[1], Xinzhong Chen[3,4], Mengkun Liu[3,4], Harald A. Stenmark[5], and Loredana Latterini[2]

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

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

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

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

[5]Department 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 purposes[1]. 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 efficiency[2], 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 resolution[3]. 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 mapping[4]. 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

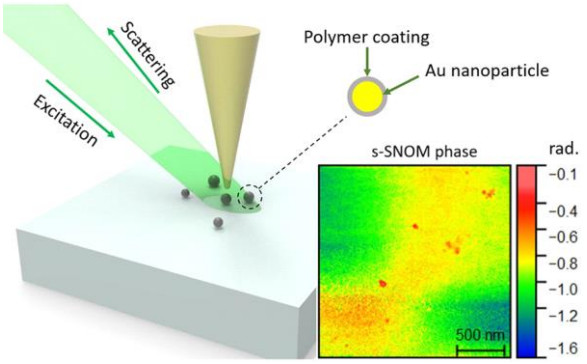


Figure 1: s-SNOM phase imaging of PSS/PDDA coated Au NPs[5].

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.

Hydrogels obtained via gamma irradiation

M. Micutz[1], R.M. Lungu[2], V. Cîrcu[3], M. Iliş[3], and T. Staicu[1*]

[1] Department of Physical Chemistry, University of Bucharest, Bucharest, Romania
Email: micutz@gw-chimie.math.unibuc.ro; teos@gw-chimie.math.unibuc.ro
[2] Scientific Research Center for CBRN Defense and Ecology, Bucharest, Romania
Email: rodi_lm@yahoo.com
[3] Department of Inorganic Chemistry, University of Bucharest, Bucharest, Romania
Email: viorel_carcu@yahoo.com, monica_ilis@yahoo.com

Hydrogels of poly(acrylic acid) and its copolymers with 2-hydroxyethyl-methacrylate were prepared via gamma irradiation of aqueous solutions of either the polymers or the corresponding monomers. When polymer solutions were used, previous solution polymerizations were performed in order to obtain the polymers. For polymers solutions viscometric data show that the overlapping concentrations are below 1 wt.% at pH = 3. Consequently at higher concentrations intermolecular entanglements and hydrogen bonds are favored.

Irradiation was carried out in air at room temperature using a GAMMATOR irradiator containing a ^{137}Cs source, and a dose rate of 0.4 kGy/h. When monomers solutions were irradiated, higher gelation doses were needed for obtaining hydrogels compared with irradiation of polymers solutions.

The obtained hydrogels were characterized by the equilibrium degree of swelling, crosslinking degree, and the average mass between crosslinks. At absorbed doses below 40 kGy the degree of swelling at equilibrium is higher than 100 g/g for all samples, the higher value (547 g/g) being obtained for the poly(acrylic acid) hydrogel prepared by absorption of 30 kGy.

Chemical transformations induced by radiation were investigated by means of FTIR spectroscopy and thermal analysis of polymers before and after irradiation.

*) Author for Correspondence: teos@gw-chimie.math.unibuc.ro

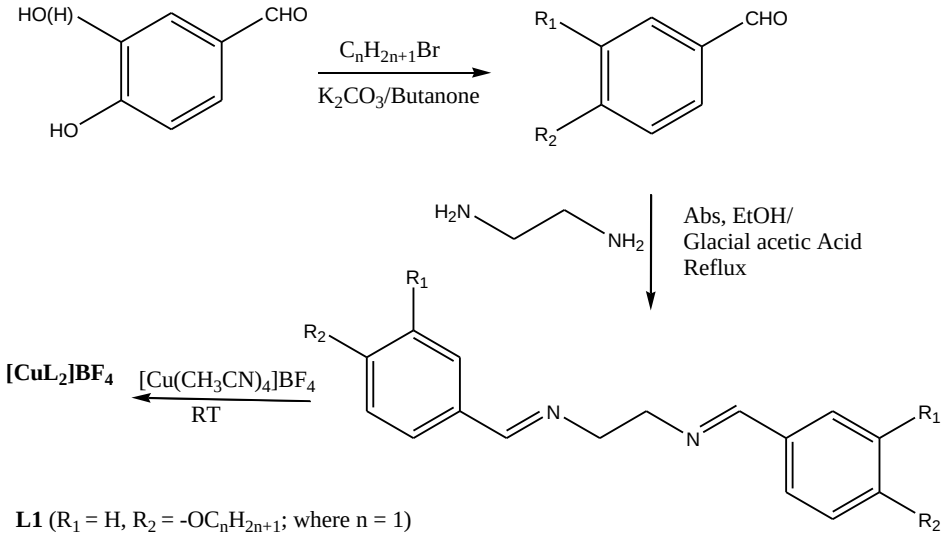
VIRTUAL ABSTRACT BOOK – POSTER SESSION PAPERS

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, **$[Cu(CH_3CN)_4]BF_4$** 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 ^1H & ^{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.

P2. 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.

P3.
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

P4. 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.

P5. 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

P6. 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

4. Electronic, photonic and optoelectronic materials

P7. 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.

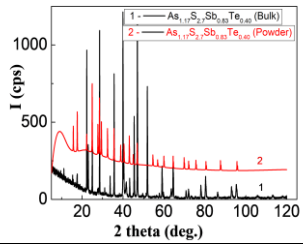


Figure 1. X-Ray Diffraction patterns bulk and powder samples.

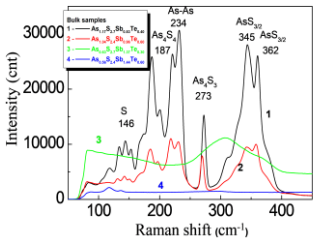


Figure 2. Micro-Raman spectra of bulk samples.

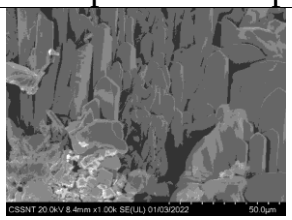


Figure 3. SEM analysis mapping of the polycrystalline bulk samples.

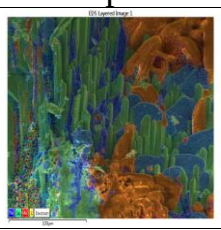


Figure 4. EDX mapping of the polycrystalline bulk samples.

[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

P8. 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

This work was financed by the Romanian UEFISCDI Agency under Contracts TE 50/2022 (DG Popescu) and by the national fellowship program L'Oreal – Unesco "For Women in Science".

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

P9. 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.

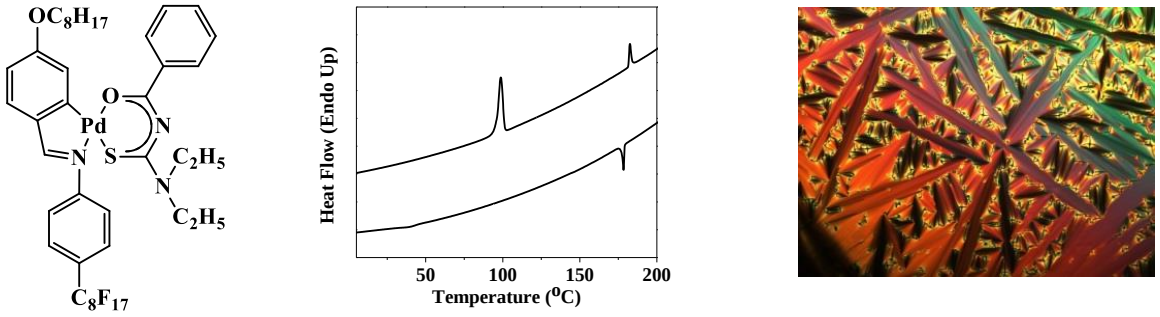


Figure 1. Structure, DSC traces and POM picture showing SmA texture at 170°C for a palladium(II) complex.

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

P10. 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.

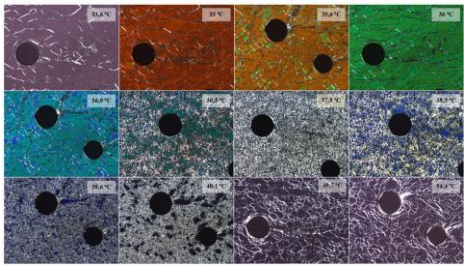


Figure 1 – Variation of color and texture with temperature for one of the mixtures

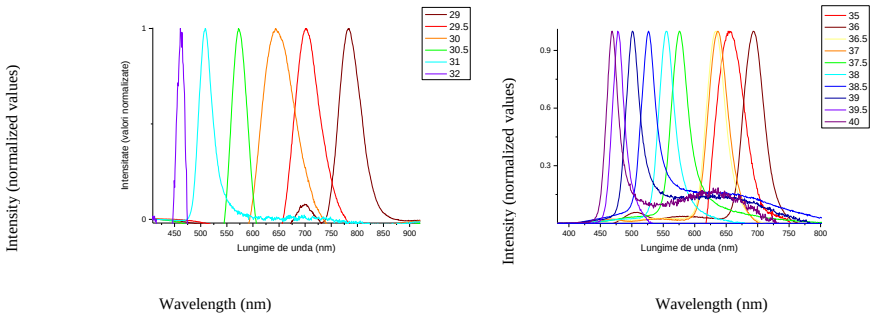


Figure 2 – Selective reflection for both mixtures analyzed

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

P11. 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

P12. 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].

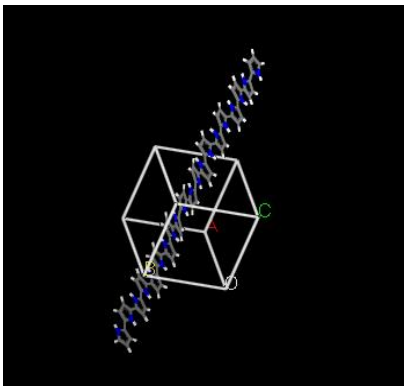


Figure 1. Molecular model of PPY

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.

P13. 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

P14. 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.

6. Biomaterials and organic materials

P15. 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.

Acknowledgements: This work was funded by FEDER funds through the COMPETE 2020 Program and National Funds through the FCT-Portuguese Foundation for Science and Technology under project numbers POCI-01-0145-FEDER-007688 (Reference UID/CTM/50025), UID/Multi/04378/2019 (Unidade de Ciências Biomoleculares Aplicadas-UCIBIO) and PTDC/EEI-EEE/0415/2021 (DigiAqua) granted to C. Marques.

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).

P16. 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.
Acknowledgments: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PTE-2021-0339 (HOLTERM), within PNCDI III.

*) Author for Correspondence: panaitescu@icechim.ro

P17. 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.

Acknowledgments: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2021-2559 (BIOPLASM), within PNCDI III
*) Author for Correspondence: panaitescu@icechim.ro

P18. 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

Founding: This work was supported by the Project No. 582PED/2022, New hybrid protein nanostructures for targeting specific in colon tumor cells (Prot-Col-Target), PN-III-P2-2.1-PED-2021-1323/01.08.2022.

7. Methods for material characterization

P19. Estimation of Cutting Edge Width in the case of Electrical Steels

G. Paltanea[1], V. Manescu (Paltanea)[1*], C. Paun[1,2], and 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.20. 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.

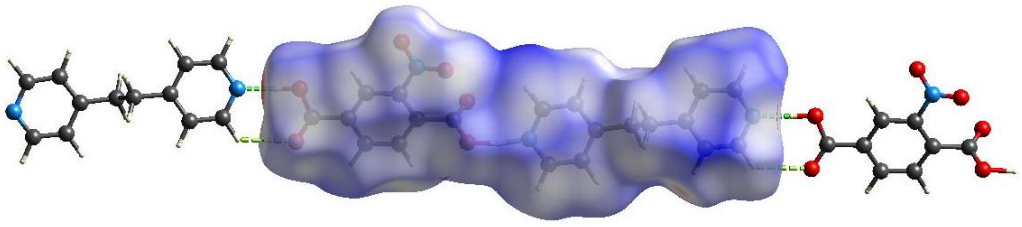


Figure 1. A view of the three-dimensional Hirshfeld surface of the title compound.

[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.

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

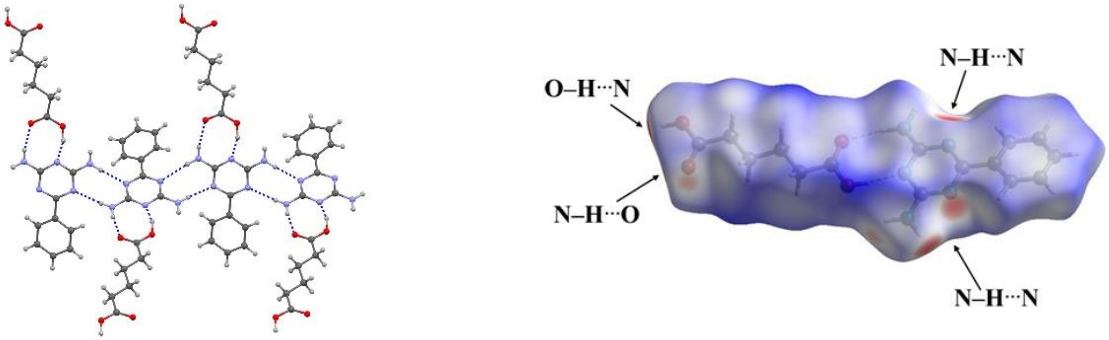
P.21. Hirshfeld Surface Analysis of Supramolecular Synthons in Cocrystal of 2,4-Diamino-6-Phenyl-1,3,5-Triazine with Adipic Acid

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.