

## “Ilie Murgulescu” Institute of Physical Chemistry of the Romanian Academy

### BRIEF HISTORY

The Institute of Physical Chemistry was founded by Academician Ilie Murgulescu in 1963, as a result of splitting of the former Chemical Research Center of the Romanian Academy.

Outstanding personality of the Romanian chemistry, Professor Murgulescu is also the founder of the modern school of physical chemistry at the University of Bucharest. He devised the main research directions in physical chemistry and set up the structural framework of the Institute of Physical Chemistry, developed under his direction (1963 - 1977) and preserved with minor revisions for over 40 years.

For mostly political reasons, especially after the Professor's retirement, the institute was forced into a sinuous administrative trajectory, eventually resulting in the loss of its dedicated building and legal personality. In spite of these shortcomings, its research staff was able to develop professionally and get ready for the major changes of the year 1990. Professor Ilie Murgulescu survived those troubled times and had a decisive contribution to the return of the Institute of Physical Chemistry back to the Romanian Academy. After his passing away in 1991, Academician Ilie Murgulescu made the last and unanimously expected gift to the Institute of Physical Chemistry: his name.



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### Director:

Dr. Ioan Balint ([ibalint@icf.ro](mailto:ibalint@icf.ro))

### Deputy Director:

Dr. Victor Fruth ([vfruth@icf.ro](mailto:vfruth@icf.ro))

### Scientific Secretary:

Dr. Maria Mitu ([maria\\_mitu@icf.ro](mailto:maria_mitu@icf.ro))

### Economic Director:

Ec. Gabriela Constantinescu ([constantinescu@icf.ro](mailto:constantinescu@icf.ro))

### Structure of research activity:

Laboratories: 8

Programs: 7; Projects: 24; Themes: 66

### Laboratories

#### 1. Quantum Chemistry and Molecular Structure

<http://www.icf.ro/Institut/Lab1.html>

Head of laboratory: Dr. Gabriela Ionita  
([ige@icf.ro](mailto:ige@icf.ro))

#### 2. Chemical Thermodynamics

<http://www.icf.ro/Institut/Lab2.html>

Head of laboratory: Dr. Speranta Tanasescu  
([stanasescu@icf.ro](mailto:stanasescu@icf.ro))

#### 3. Chemical Kinetics

<http://www.icf.ro/Institut/Lab3.html>

Head of laboratory: Dr. Adina Magdalena Musuc  
([amusuc@icf.ro](mailto:amusuc@icf.ro))

#### 4. Surface Chemistry and Catalysis

<http://www.icf.ro/Institut/Lab4.html>

Head of laboratory: Dr. Mariuca Gartner  
([mgartner@icf.ro](mailto:mgartner@icf.ro))

#### 5. Electrochemistry and Corrosion

<http://www.icf.ro/Institut/Lab5.html>

Head of laboratory: Dr. Maria Marcu  
([m\\_marcu@icf.ro](mailto:m_marcu@icf.ro))

#### 6. Oxide Compounds and Materials Science

<http://www.icf.ro/Institut/Lab6.html>

Head of laboratory: Dr. Irina Atkinson  
([iatkinson@icf.ro](mailto:iatkinson@icf.ro))

#### 7. Colloid Chemistry

<http://www.icf.ro/Institut/Lab7.html>

Head of laboratory: Dr. Adriana Baran  
([abaran@icf.ro](mailto:abaran@icf.ro))

#### 8. Coordination and Supramolecular Chemistry

<http://www.icf.ro/Institut/Lab8.html>

Head of laboratory: Dr. Gabriela Marinescu  
([gmarinescu@icf.ro](mailto:gmarinescu@icf.ro))

### RESEARCH PROGRAMS

P1. Thermodynamics and Chemical Kinetics. Quantum Chemistry

P2. Catalytic materials and processes

P3. Electrode processes, Corrosion and Materials for Electrochemical Systems

P4. Materials science and advanced characterization methods

P5. Complex Functional Colloids

P6. Biomedical and environmental applications

P7. Science of surfaces and thin layers

### Human resources:

Scientific researchers I: 27

Scientific researchers II: 29

Scientific researchers III: 54

Scientific researchers: 10

Assistant (junior) researchers: 21

Auxiliary staff: 22

Administrative and technical staff: 24

## RESEARCH DIRECTIONS AND INFRASTRUCTURE

### P1. Thermodynamics and Chemical Kinetics. Quantum Chemistry

#### Chemical thermodynamics

**Chemical thermodynamic group** (Dr. Speranta Tanasescu) is a leading laboratory for basic and applied thermodynamic research. The research team is composed of thirteen senior scientists and three junior scientists. The members of the research group have an extensive experience in the research work of physical chemistry and related interdisciplinary fields. They are drawn from *chemistry, biochemistry, materials and engineering backgrounds*; especially the senior researchers have *significant cross-disciplinary practice*.

#### Research fields:

The scientific research is focused on three major fields:

- (1) *Thermodynamics of the condensed systems in the pure phases and at the equilibrium between phases;*
- (2) *Bio-thermodynamics and thermochemical characterization of the biological interest compounds. Bio-Nano interactions;*
- (3) *Fundamental and applied thermal studies.*

#### Members:

- Dr. Speranta TANASESCU ([stanasescu@icf.ro](mailto:stanasescu@icf.ro)), PhD Senior Researcher I, PhD Supervisor in Chemistry, Head of the Chemical Thermodynamics Laboratory - Physical Chemistry, Applied Chemical Thermodynamics (Phase diagrams, Nonstoichiometric compounds, Micro and Nanomaterials, Thermodynamics at bio/nano interface).

- Dr. Florina TEODORESCU ([fteodorescu@icf.ro](mailto:fteodorescu@icf.ro)) - Synthesis and characterization of nanoparticles for biomedical applications, thermodynamics of biomolecule–nanoparticle interactions by means spectroscopic and calorimetric studies.

- Dr. Habil. Andrei ROTARU ([andrei.rotaru@icf.ro](mailto:andrei.rotaru@icf.ro)) - Physical Chemistry, Thermophysical properties of materials, Solid state chemistry, Condensed matter physics, Dynamics of nonlinear systems, Surface science, Processing thin films of soft materials.

- Dr. Dana DRAGOESCU ([ddragoescu@icf.ro](mailto:ddragoescu@icf.ro)) - Thermodynamic and Thermophysical properties of organic compounds and their derivatives.

- Dr. Eng. Florinela SIRBU ([sflorinela@yahoo.com](mailto:sflorinela@yahoo.com)) - Thermodynamics of electrolytes/nonelectrolytes multicomponent liquids mixtures. experimental data, correlation, estimation and prediction.

- Dr. Ana NEACSU ([aneacsu@icf.ro](mailto:aneacsu@icf.ro)) - Thermochemistry of the biological interest compounds.

- Dr. Cornelia-Alina MARINESCU ([aalcorinaa@yahoo.com](mailto:aalcorinaa@yahoo.com)) - Thermodynamics of materials in dynamic/equilibrium regimes.

- Dr. Florentina-Violeta MAXIM ([fmaxim@icf.ro](mailto:fmaxim@icf.ro)) - Metal oxides thermodynamics, Design and development of materials used in the supercritical water technologies for wastewaters treatment and energy harvesting from wet biomass and wastes.

- Dr. Anuța Mihaela SOFRONIA ([amsofronia@yahoo.com](mailto:amsofronia@yahoo.com)) - Thermodynamics of materials in dynamic / equilibrium regimes.

- Dr. Eng. Cristina Silvia MUNTEANU (STOICESCU), ([cristina.silvia.stoicescu@gmail.com](mailto:cristina.silvia.stoicescu@gmail.com)) - Thermodynamics of liquid mixtures and phase equilibria / correlation and prediction of experimental data.

- Dr. Romică SANDU ([rsandu@icf.ro](mailto:rsandu@icf.ro)) - Biochemistry; Thermodynamic study of the intermolecular interactions.

- Dr. Alina BOTEANU-PETCU ([alina.petcu30@yahoo.com](mailto:alina.petcu30@yahoo.com)) - Thermodynamics of micro/nano materials; Bio/nano interaction

- Dr. Mihaela-Daniela GHEORGHE ([chiscan\\_danny@icf.ro](mailto:chiscan_danny@icf.ro)) - Thermochemistry of the biological interest compounds, Bio/nano interactions.

- Dr. Dana Andreea NEACSU ([addneacsu@icf.ro](mailto:addneacsu@icf.ro)) - Thermal analysis and calorimetry, DFT calculations, FT-IR and UV-Vis analysis.

- Ioana GHEORGHE ([igheorghe@icf.ro](mailto:igheorghe@icf.ro)) - Thermochemical study of biological interest compounds.

- Adriana Petruța SERBAN ([aserban@icf.ro](mailto:aserban@icf.ro)) - Studies of the biomolecules / nano-based drugs interaction, PhD student.

#### Research Equipment

<https://eeris.eu/ERIF-2000-000R-0451>

- SetSys DSC-TG/DTA Setaram Equipment (ambient-1650 °C)
- Set-Sys Evolution TMA Setaram (ambient-1550 °C)
- Drop Calorimeter MHTC-96 Setaram (ambient – 1500 °C)
- Calvet calorimeter C80 Setaram (ambient - 300 °C)
- Apparatus for Electromotive force measurements (EMF) & Solid state coulometric titration
- Isothermal titration calorimeter Microcal iTC200 (25-80°C)
- NanoDSC, TA Instruments (-10 °C to 130 °C)
- DSC Perkin Elmer (-100 to 500°C)
- Macro- and microcombustion calorimeters Parr
- SPR Equipment (Surface Plasmon Resonance) Esprit, Autolab
- Frequency response analyzer Solartron, 10 μHz - 20 MHz & Potentiostat-Galvanostat for impedance spectroscopy Solartron Analytical 1255A
- UV-Vis spectrophotometer Varian Cary 300
- FT-IR Spectrometer Nicolet iS10
- Chromatograph with FID si TCD detectors
- Equipment for liquid - vapor equilibrium measurements
- Anton Paar Densimeter DSA 5000M
- Anton Paar AMVn Automated Microviscometer
- Anton Paar Abbemat RXA 170 digital Refractometer
- Precision LCR Meter Model 4285A-AGILENT
- High-speed surface area & pore size analyzer BET-NOVA 2200e
- Nano-Zetasizer Malvern for size and charge determination
- Apparatus for interfacial energy measurement K100MK2Krus
- Thermo Scientific Orion 5-star Plus pH/Conductivity/ Dissolved Oxygen Meter

#### International projects, inter-academic and scientific collaborations (selected the most recent):

→ **Horizon 2020 - Innovation Action (IA):** *Safety testing in the life cycle of nanotechnology-enabled medical technologies for health (SAFE-N-MEDTECH)* 2019 - 2023 Scientific Responsible: Dr. Speranta Tanasescu

→ **Horizon 2020 EuroNanoMed III:** *Targeted multifunctional nanoemulsions to interrupt metastatic progression (METASTARG)* 2019-2022 Scientific Responsible: Dr. Speranta Tanasescu

→ **Horizon 2020 - Research and Innovation Action (RIA):** *Development and implementation of Grouping and Safe-by-Design approaches within regulatory frameworks (NANoRegII)* 2015-2020, Sci. Resp. Dr. Speranta Tanasescu

→ **Horizon 2020 - Coordination and Support Action (CSA):** *Promoting the Implementation of Safe by Design (ProSafe)*, 2015-2017, Scientific Responsible: Dr. Speranta Tanasescu

→ **Joint Research Project Romanian Academy - National Academy of Sciences of Belarus,** *A comparative study of the thermophysical properties for binary mixtures of cycloalkanes and cycloketones with aromatic hydrocarbons, AR-FRBCF*, 2020-2021, Proj. Director: Dr. Dana Dragoescu

→ **Joint Research Project Romanian Academy – Hungarian Academy of Sciences, Structural and thermodynamic studies of aqueous solutions, AR-HAS, 2018-2021, Project Director: Dr. Dana Dragoescu**

→ **Research Collaboration Agreement with Paul Scherrer Institute, Research Division Energy and Environment, Group of Chemical Processes and Materials, Villigen, Switzerland 2019-2025 Scientific Responsible Dr. Florentina Maxim**

**National granted projects (selected the most recent from 14):**

→ **PN-III-P4-ID-PCE-2020-1241: Carbon supported metal oxides produced by supercritical water impregnation method (APASUPER) 2021-2023 Project Director Dr. Florentina Maxim**

→ **PN-II-PT-PCCA-2013-4-2094: Research of the bone substitution with biocomposite materials processed by powder metallurgy specific techniques, (BONY) 2014-2017 Scientific Responsible: Dr. Speranta Tanasescu**

### Selected papers published in 2021:

- Towards FAIR Nanosafety Data, N. Jeliaskova [...], A. Botea-Petcu, D. Gheorghe, R. Sandu, A. Precupas, S. Tanasescu et al, *Nat Nanotechnol*, 16(6), (2021) 644-654.
- Thermodynamics and dynamics of supercritical water pseudo-boiling, F. Maxim *et al. Adv. Sci.*, 8 (2021), 2002312.
- Revising protein Corona Characterization Combining ITC and NanoDSC to Understand the Interaction of Proteins with porous Nanoparticles, A. Balmori, R. Sandu, D. Gheorghe, A. Botea-Petcu, A. Precupas, S. Tanasescu et al., *Front. Bioeng Biotechnol*, 9, (2021) 650281.
- Functional Materials for Waste-to-Energy Processes in Supercritical Water, F. Maxim, I. Poenaru, E. Toma, G. Stoian, F. Teodorescu, C. Hornoiu, S. Tanasescu, *Energies*, 14(2021) 7399
- Microstructural and thermoanalytical characterization of super duplex stainless steel - UNS S32760-F55, F. Khoshnaw, C. Marinescu, A.M. Sofronia, C. Munteanu, M. Marcu, L.E. Barbulescu, C. Ciobota, E.M. Cojocar, S. Tanasescu, A. Paraschiv, *Mater Today Commun*, 28, (2021) 102644.
- Density, speed of sound and derived thermodynamic properties of binary liquid mixtures of 1-chlorohexane with toluene and tetradecane under high pressures, A.P. Shchamialiou, V.S. Samuilov, N.V. Holubeva, D. Dragoescu, F. Sirbu, *J Chem Thermodyn*, 154, (2021) 106329.
- Study of the thermophysical properties for aqueous solutions

of alkanediols binary mixtures, D. Dragoescu, F. Sirbu, L. Almasy, *J Mol Liq*, 335, (2021) 116150.

• Optical and viscometric properties for 1-chlorohexane+ toluene/tetradecane binary mixtures at temperatures from 298.15 K to 318.15 K and atmospheric pressure, F. Sirbu, D. Dragoescu, A. Shchamialiou, *J Mol Liq*, 339, (2021) 116171.

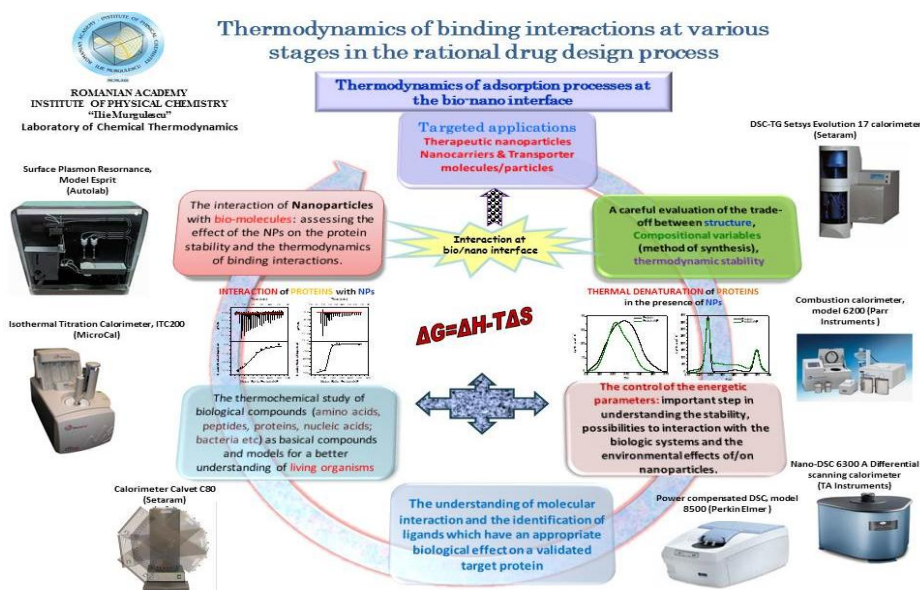
• Characterization of biomass renewable energy resources from some perennial species, A. Neacsu, D. Gheorghe, *Rev Roum Chim*, 66(4), (2021) 2054-2071

• Azorubine: Physical, thermal and bioactive properties of the widely employed food, pharmaceutical and cosmetic red azo-dye material, M. Leulescu, A. Rotaru, A. Moanță, G. Iacobescu, I. Pălărie, N. Cioateră, M. Popescu, M.C. Criveanu, E. Morintale, M. Bojan, P. Rotaru, *J Therm Anal Calorim* 143(6), (2021) 3945-3967.

• The electro-mechanical control of element NiTi shape memory alloy strip while bending, based on thermal analysis evidence, S. Degeratu, G.E. Subțirelu, A. Rotaru, N.G. Bîzdoacă, P. Rotaru, *J Therm Anal Calorim*, 143(6), (2021) 3805-3815.

### Highlights

- A careful evaluation of the trade-off between structures, physical-chemical properties, thermodynamic stability
- The understanding of the thermodynamic properties dependence on compositional variables: the key to enable optimization and full exploitation of multifunctional materials
- Thermodynamic study of metal oxide nanomaterials prepared under supercritical water conditions
- The control of the energetic parameters: important step in understanding the reactivity, the interaction with the biologic systems and the environmental effects of/on micro and nanomaterials
- Thermochemical study of amino acids, peptides, proteins, enzymes etc as basic compounds and models for a better understanding of living organisms.
- Thermodynamics of the interaction at the bio/nano interface. Nano-scale mechanisms
- Thermodynamic study of electrolytes, nonelectrolytes, and organic compounds in liquids mixtures
- Thermodynamic and kinetic modeling of thermally-induced heterogeneous processes; dynamic processes and physico-chemistry of the surfaces of functional solid materials.
- Thermal processing and investigation of advanced materials used in engineering, food safety, eco- and bio-applications.



*Dynamics of rapid oxidation and decomposition reactions in homogeneous system*, coordinated by Dr. Maria Mitu

### Research fields:

Studies of fast gas-phase reactions, as homogeneous hydrocarbon oxidations:

- Fuel-oxidizer ignition: flammability conditions, critical conditions for local explosion initiation by electric sparks or by hot bodies.
- Premixed hydrocarbon-air flames propagation, in deflagration regime: explosion pressures, explosion times, rates of pressure rise, severity factors, and normal burning velocities.
- Numerical modeling of flame propagation, under confined or unconfined conditions.
- Chemical kinetics.

### Members – Senior researchers:

- Dr. Adina Magdalena Musuc, Head of Laboratory; [amusuc@icf.ro](mailto:amusuc@icf.ro)
- Dr. Maria Mitu; [maria\\_mitu@icf.ro](mailto:maria_mitu@icf.ro)
- Dr. Codina Movileanu; [cmovileanu@icf.ro](mailto:cmovileanu@icf.ro)
- Dr. Venera Giurcan; [venerab@icf.ro](mailto:venerab@icf.ro)
- Dr. Domnina Razus (honorary researcher); [drazus@icf.ro](mailto:drazus@icf.ro)

### Research Equipment (<https://eeris.eu/ERIF-2000-000L-0462>):

- Equipment for study of explosive processes of gaseous mixtures at initial pressures 0.2 – 2 bar and 20 – 250° C: vacuum pumps, metallic storage cylinders, digital manometers for various pressure ranges (0 – 1000 mbar abs; 1 bara-10 bara), metallic explosion vessels (spherical or cylindrical with various inner volumes within 0.1 – 2.0 L).
- Electronic devices for controlled ignition of flammable mixtures by means of inductive-capacitive electric sparks, break sparks or heated wires
- Pressure transducers: piezoelectric, Kistler
- Charge Amplifiers, Kistler
- Digital Oscilloscopes, Tektronix
- Acquisition Data System, Tektronix
- Temperature controllers
- Combustion gas analyzer Kane 455

### Experimental methods specific to fast reactions in the gas phase:

- transient measurements of pressure evolution during exothermic processes (explosions)
- transient measurements of the heating current for a filament initiating the explosive combustion
- other measurements specific to gas explosions: quenching distances; explosion limits, minimum (limiting) oxygen concentration, minimum (critical) inerting concentration.



Explosion set-up



**Selected research project:** *Influence of hydrogen addition on the explosivity of LPG-air gaseous mixtures*, PN-III-P4-PCE-2021-0369 (2022-2024).

### International cooperation agreements:

“*Safety Characteristics of Gaseous Mixtures*”, Cooperation with PTB (Physikalische-Technische Bundesanstalt), Braunschweig, Germany;

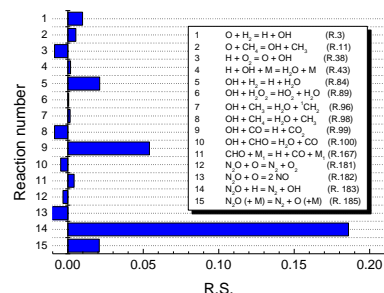
„*Flammability of Fuel/Inert/Oxidant Gaseous Mixtures*”, Cooperation with BAM (Bundesanstalt für Materialforschung und -prüfung), Berlin, Germany.

### Selected papers:

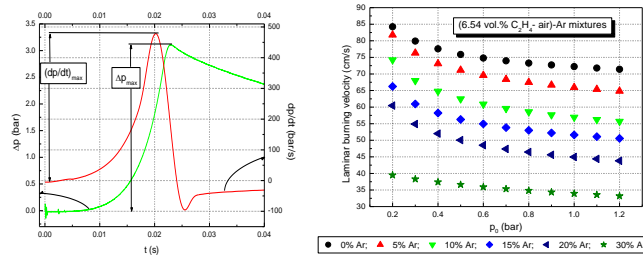
- C. Movileanu, V. Giurcan, M. Mitu, D. Razus, D. Oancea, *Ignition by Low-Voltage Electric Discharges of Diluted and Undiluted C3H8–Air Mixtures*, Ind. Eng. Chem. Res. 60, 12123-12132 (2021).
- M. Mitu, E. Brandes, S. Zakel, W. Hirsch, *Explosion regions and limiting oxygen concentrations of methyl propionate, methyl acetate, dimethyl carbonate with air and inert gas mixtures*, J. Loss Prev. Process Ind. 69, 104384 (2021).
- M. Mitu, D. Razus, V. Schroeder, *Laminar burning velocities of hydrogen-blended methane–air and natural gas–air mixtures, calculated from the early stage of p(t) records in a spherical vessel*, Energies 14(22), 7556 (2021).
- C. Movileanu, M. Mitu, V. Giurcan, D. Razus, D. Oancea, *Quenching distances and minimum ignition energies of propane-air-inert mixtures*, Fuel 274, 117836 (2020).
- D. Razus, M. Mitu, V. Giurcan, C. Movileanu, D. Oancea, *Additive influence on maximum experimental safe gap of ethylene-air mixtures*, Fuel 237, 888-894 (2019).



D. Oancea, D. Razus,  
“*Explozia chimică*”,  
Editura Academiei Române, 2021,  
ISBN 978-973-27-3370-7

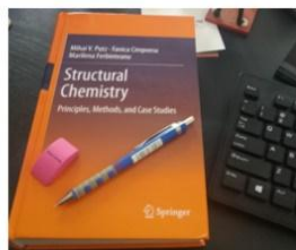


Relative sensitivities of the laminar burning velocity of the stoichiometric CH<sub>4</sub>-N<sub>2</sub>O-N<sub>2</sub> mixture (40% N<sub>2</sub>), with respect to the rates of several elementary reactions. [Process Saf. Environ. Prot., 114, 240-250 (2018)].



Pressure-time evolution in closed vessel explosion

Experimental laminar burning velocities



### Theoretical and Structural Chemistry Group.

As suggested by our logo, we cover a large thematic area. Octahedron stands for inorganic and coordination branches, hexagon represents the organic chemistry, the icosahedron hints the clusters and organometallics; the bi-lobal shape and torus signify the specialized issue of magnetic anisotropy. Such aperture is possible since, in spite of specific differences, the bond mechanisms are unitary. In other words, all compounds and materials show structures and properties determined by quantum chemistry. Theoretical fundamentals form a necessary background for experimental paradigms themselves. The modern chemistry would be impossible without having clearly defined the concepts of atom, molecule, electron, spectral states, transitions, and so on, all assets from the perennial vaults of theoretical treasures.

### Group Members:

- Dr. Fanica Cimpoesu,

Mentor; elaborates models and algorithms. ([fcimpoesu@icf.ro](mailto:fcimpoesu@icf.ro))

- Dr. Ana Maria Toader, quantum calculations, applies and validates models, magneto-structural correlations. ([atoader@icf.ro](mailto:atoader@icf.ro))

- Dr. Maria Cristina Buta, does quantum calculations and draws relations to experiment, spin chemistry. ([cbuta@icf.ro](mailto:cbuta@icf.ro))

- Dr. Bogdan Frecus - part-time, quantum calculations. ([bfrecus@icf.ro](mailto:bfrecus@icf.ro))

- Dr. Alice Mischie (part. involv.), statistic correlations. ([amischie@icf.ro](mailto:amischie@icf.ro))

**Bond. Chemical Bond!** The group was constituted in 2016, having as goal to spy the secrets of the chemical bond. We do computation with state-of-the-art methods (DFT, CASSCF, PW-bands), mastering also less used procedures, such as Valence Bond (VB). We deny ourselves facile works, inserting non-routine steps, in the quest for physical and chemical heuristic meaning. Aside computers, we use pencil, paper and gum-erasers.

**New keys for old keywords.** Combining concrete applications with method development ideas, we revisit important paradigms: aromaticity, hybridization, ligand field theory. We employ phenomenological (effective) Hamiltonians as post-computational tools, to illuminate the black-box of big calculations and establish a common language with the experiment. We conceive new algorithms, coded in *Matlab*, *Mathematica*, *Fortran*.

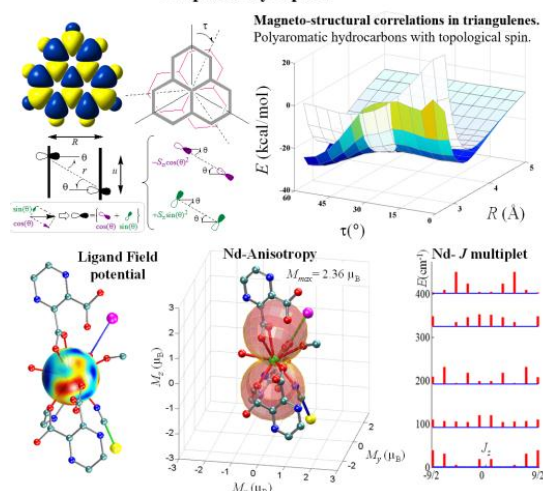
**Breakthroughs: Lanthanide quantum chemistry and magnetic anisotropy.** We have a strong-hold in the quantum chemistry of lanthanide compounds. Not many groups can do this, since it

implies a good chemical intuition and advanced handling in the calculation setting and in the post-computational analysis. The lanthanide compounds can be characterized as non-*aufbau* structures, namely situations not implemented in current quantum chemistry codes. We deal with the magnetism, spectroscopy and luminescence properties of lanthanide compounds. Transition metal coordination complexes are also in our focus, dealing with structure-property relationships in terms of exchange coupling, magnetic anisotropy, ligand field theory and spectroscopy.

**Organic spin chemistry.** Besides of magneto-structural correlations in metal-ion systems, we innovatively applied this paradigm to non-metal spin carriers, working systematic analyses on stable nitroxide-based organic radicals and the special class of triangulenes (aromatic hydrocarbons with regular triangular shapes and topologically-driven spin). Since the spin interactions are essential in life-chemistry, in respiratory systems and anti-oxidant activity, we are currently initiating a front of work in this domain too.

**Plans and future quests: Back to the basis!** The most audacious activity of the group, still remained hidden in the background of a rather tedious technical preparative, is the revisiting of the actual Gaussian Type Orbitals (GTO) infrastructure, having deeper flaws than commonly acknowledged by most users.

### Graphical Synopsis.



**Book:** M. V. Putz, F. Cimpoesu, M. Ferbinteanu, *Structural Chemistry, Principles, Methods, and Case Studies*; Springer: Cham, Switzerland, 2018.

### Articles:

- Coord. Chem. Rev.* **2021**, 441, 213981 IF=22.315;
- Chem.-Eur. J.* **2018**, 24, 61, 16276, IF=5.24;
- J. Phys. Chem. A* **2021**, 125, 32, 6893, IF=2.6;
- Chemistry* **2021**, 3, 1, 411;
- Curr. Med. Chem.* **2020**, 27, 99, IF=4.18;
- Int. J. Mol. Sci.* **2019**, 20, 23, IF=5.92;
- Int. J. Mol. Sci.* **2019**, 20, 19, IF=5.92;
- J. Phys. Chem. C* **2019**, 123, 11, 6869, IF=4.19;
- Inorg. Chem. Front.* **2018**, 5, 1967, IF=6.57;
- Eur. J. Inorg. Chem.* **2018**, 12, 1409, IF=2.53;
- Inorg. Chem.* **2017**, 56, 16, 9474, IF=5.16;
- Curr. Org. Chem.* **2017**, 21, 27, 2768, IF=1.93;
- RSC Adv.* **2017**, 7, 35, 21375, IF=3.36;
- Theor. Chem. Acc.* **2016**, 135, 5, IF=1.70.

## P2. Catalytic materials and processes

*Catalytic materials for the energy and environmental fields*, coordinated by **Dr. Ioan Balint**  
*Non-polluting catalytic processes developed as applications of nanomaterials*, coordinated by **Dr. Viorica Parvulescu**

*Catalytic materials for the energy and environmental fields*, coordinated by **Dr. Ioan Balint**

### Research interests:

- Material synthesis: mesoporous nano oxides; mono/bimetallic metal nanoparticles;
- Catalysis: catalytic combustion of hydrocarbons; oxidative coupling of methane; hydrogenation and oxidative conversion of conversion hydrocarbons; deNO<sub>x</sub> reaction; structure-sensitive reactions; nitrate and nitrite abatement;
- Photocatalysis / light harvesting for water and air depollution; water splitting; light-induced reactive oxygen species generation; dye sensitized solar cells;
- Fractal characterization of catalysis.

### Key team members:

**Dr. Balint Ioan**, (coordinator) is a senior researcher. The main research directions are: material chemistry, catalysis and photocatalysis, defect chemistry.

**Dr. Papa Florica**, is a senior researcher. The most significant research directions are material chemistry, heterogeneous catalysis, photocatalysis.

**Dr. Crina Anastasescu**, is a senior researcher with expertise in the synthesis of oxide materials with photocatalytic properties.

**Dr. Razvan State**, is a young scientific researcher. The most significant research directions are focusing on the synthesis, characterization and photocatalytic properties of nanomaterials.

**Dr Anca Vasile**, is a senior researcher with expertise in the field of environmental protection, nanoparticle synthesis with thermosensitive polymers.

**Dr. Dobrescu Gianina**, is a senior researcher. She is a known specialist in fractal analysis, computer chemical modeling of chemical processes, and image analysis.

**Dr. Monica Pavel**, is a senior researcher focused on the synthesis of inorganic materials applied to photocatalytic field.

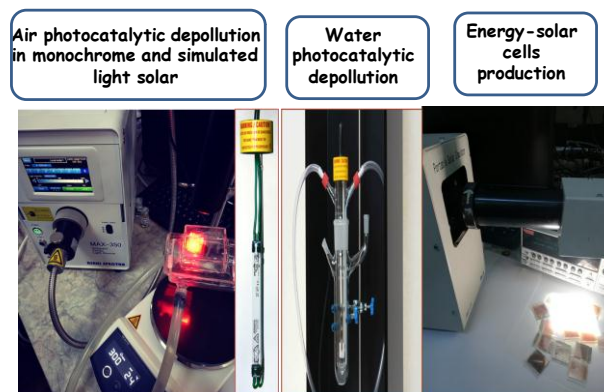
### Research Projects:

- *Advanced materials and laser / plasma technologies for energy and depollution: increasing the potential application and scientific interconnection in the field of ecnanotechnologies* (Project leader: Ioan Balint)
- *Water treatment from contaminated sources (with nitrates and chlorinated organic compounds) using integrated catalytic reduction / oxidation processes and biofiltration* (Project leader: Florica Papa)

### Research Equipment:

- Gas chromatograph (Agilent 7890A) equipped with a flame ionization detector (FID)
- HP-PlotQ capillary column (30 m × 0.53 mm)
- Ion chromatography (Dionex ICS 900)
- Fluorescence Spectrophotometer Agilent Technologies, apparatus
- Solar light simulator Peccell-L01, equipped with a 150 W xenon short-arc lamp
- ChemBet-3000 Quantachrome Instrument equipped with a thermal conductivity detector (TCD) apparatus

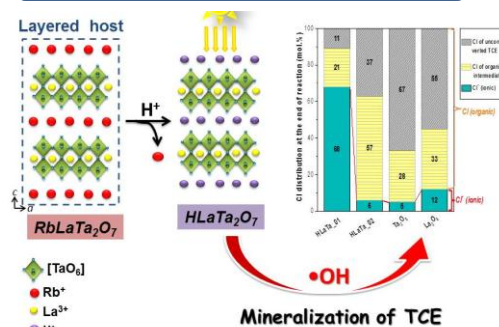
- Gas chromatograph Buck Scientific, equipped with TCD detectors. The H<sub>2</sub> and O<sub>2</sub>
- High performance liquid chromatograph (HPLC), equipped with UV-Vis detector (Waters, model 2489)



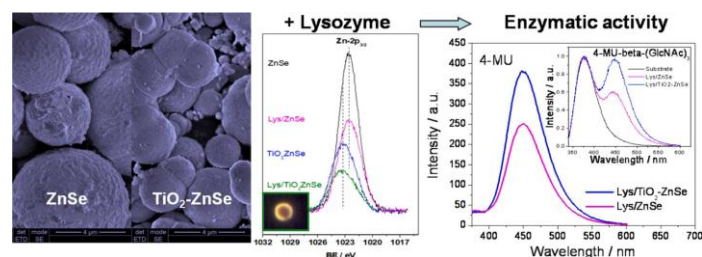
### Selected paper:

- C. Anastasescu, I.C. Gifu, C. Negrila, R. Socoteanu, I. Atkinson, J. M. Calderon-Moreno, C. Munteanu, G. Plavan, S. A. Strungaru, B. Cheatham, A. V. Maraloiu, V. S. Teodorescu, M. Anastasescu, M. Zaharescu, I. Balint, V. Lazarescu, *Morpho-structural properties of ZnSe, TiO<sub>2</sub>-ZnSe materials and enzymatic activity of their bioinorganic hybrids with lysozyme*, Materials Science and Engineering: B, 272, 115350 (2021).
- A. Vasile, F. Papa, V. Bratan, C. Munteanu, M. Teodorescu, I. Atkinson, M. Anastasescu, D. Kawamoto, I. Balint, C. Negrila, C.D. Ene, T. Spataru, *Water denitration over titania-supported Pt and Cu by combined photocatalytic and catalytic processes: Implications for hydrogen generation properties in a photocatalytic system*, Journal of Environmental Chemical Engineering, 10(2), 107129 (2022).
- G. Dobrescu, F. Papa, R. State, M. Raciulete, D. Berger, I. Balint, N.I. Ionescu, *Modified Catalysts and Their Fractal Properties*; Catalysts 11, 1518 (2021).

### The photocatalytic performance of protonated HLaTa<sub>2</sub>O<sub>7</sub> for TCE mineralization



### The hydrolytic activity of Lys/ZnSe and Lys/TiO<sub>2</sub>-ZnSe is twofold higher than for free lysozyme.



*Non-polluting catalytic processes developed as applications of nanomaterials*, coordinated by **Dr. Viorica Parvulescu** ([vpirvulescu@icf.ro](mailto:vpirvulescu@icf.ro))

#### Research fields:

- Nanomaterials developed as mesostructured catalysts with transition metals as adsorbents, active catalysts and photocatalysts for air and water depollution;
- Nanoarchitectures as support for biocomponents extracted from plants and hybrid catalysts with organometallic complexes with oxidative catalytic properties, antimicrobial and cytotoxic properties;
- Correlation of the structural, textural, electrical, magnetic and optical properties of nanomaterials, as a result of their synthesis conditions, with catalytic and photocatalytic activity.

#### Members:

Dr. Veronica Bratan ([vbratan@icf.ro](mailto:vbratan@icf.ro))

Dr. Elena Madalina Ciobanu ([mciobanu@icf.ro](mailto:mciobanu@icf.ro))

Dr. Cristian Hornoiu ([chornoiu@icf.ro](mailto:chornoiu@icf.ro))

Dr. Viorel Chihaiia ([vchihaiia@icf.ro](mailto:vchihaiia@icf.ro))

Dr. Gabriela Petcu ([gpetcu@icf.ro](mailto:gpetcu@icf.ro))

Dr. Daniela Negoescu ([danielan@icf.ro](mailto:danielan@icf.ro))

#### Research Equipment:

<https://eeris.eu/ERIF-2000-000J-0827>

- Scanning Electron Microscope (SEM) – EVO LS 10
- UV-Vis- NIR Spectrophotometer, JASCO V-570 equipped with Integrating Sphere
- Steroglass Strike 202 Rotary Evaporator, Furnaces: DENKAL 6B and tubulars
- Viscosimeter (Temperature Sensing Range: -100 °C to 300 °C)
- Gas Chromatographs, catalytic and photocatalytic reactors

#### Bilateral collaboration projects:

Interacademic projects (Institute of Catalysis Sofia, Institute of Nanotechnology, Lecce, Italy), Collaboration project (Université de Lorraine, Nancy, France)

#### Books:

- V. Parvulescu, Chapter title: *Catalytic behavior of metal active sites from modified mesoporous silicas in oxidation of organic compounds*, Book title: Redox (ISBN 978-1-78984-887-8) Ed. IntechOpen, Ed. Rozina Khattak 2019.
- V. Parvulescu, M. Ciobanu, G. Petcu, chapter 10: *Immobilization of Semiconductor Photocatalysts Section IV: Plasmonics and hybrids photocatalytic materials* from: Handbook of Smart Photocatalytic Materials: Editor(s): Chaudhery Mustansar Hussain, Ajay Kumar Mishra, Handbook of Smart Photocatalytic Materials, Elsevier, 2020, Pages 103-140, ISBN 9780128190517.

#### Selected papers:

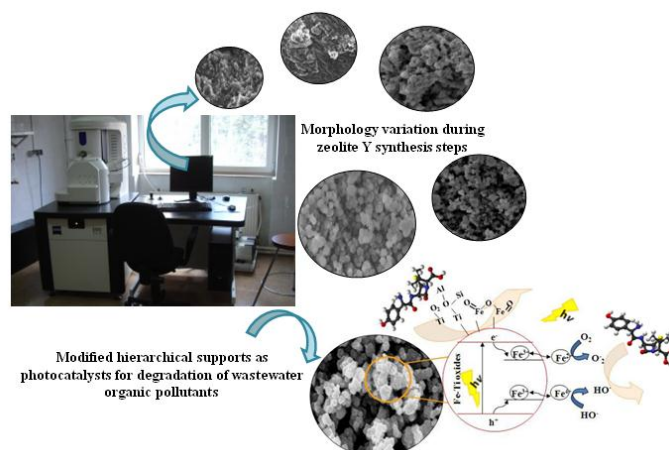
- M. Filip, G. Petcu, E.M. Anghel, S. Petrescu, B. Trica, P. Osiceanu, N. Stanica, I. Atkinson, C. Munteanu, M. Muresanu, V. Parvulescu, *FeTi- SBA-15 magnetic nanocomposites with photocatalytic properties*, Catalysis Today 366, 10-19 (2021) (IF = 6.766)
- M. Ciobanu, G. Petcu, E.M. Anghel, F. Papa, N.G. Apostol, D.C. Culita, I. Atkinson, S. Todorova, M. Shopka, A.

Naydenov, R. Velinova, V. Parvulescu, *Influence of Ce addition and Pt loading upon the catalytic properties of modified mesoporous PtTi-SBA-15 in total oxidation reactions*, Applied Catalysis A: General, 118123 (2021) (IF = 5.706)

- V. Bratan, P. Chesler, C. Hornoiu, M. Scurtu, G. Postole, P. Pietrzyk, A. Gervasini, A. Auroux, N.I. Ionescu, *In situ electrical conductivity study of Pt-impregnated VO<sub>x</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalysts in propene deep oxidation*, J. Mater. Sci. 55, 10466–10481 (2020) (IF = 4.220)
- M. Ciobanu, L. Pirvu, G. Paun, S. Savin, B.-G. Albu, C. Munteanu, J. Pandeale Cusu, I. Atkinson, D. Culita, G. Petcu, V. Parvulescu, *Development of a new (bio)hybrid matrix based on Althaea officinalis and Betonica officinalis extracts loaded into mesoporous silica nanoparticles for bioactive compounds with therapeutic applications*, Journal of Drug Delivery Science and Technology 51, 605-613 (2020) (IF = 2.606)
- G. Petcu, E. M. Anghel, S. Somacescu, S. Preda, D.C. Culita, S. Mocanu, M. Ciobanu, V. Parvulescu, *Hierarchical Zeolite Y Containing Ti and Fe Oxides as Photocatalysts for Degradation of Amoxicillin*, J. Nanosci. Nanotechnol. 20, 1158–1169 (2020) (IF = 1.354)

#### Highlights

- Activated Pt catalysts by strong interaction with high dispersed TiO<sub>2</sub>, TiO<sub>2</sub>-CeO<sub>2</sub> supports on mesoporous silica
- Active mesoporous catalysts for methane and CO total oxidation
- Ce-modified mesoporous TiO<sub>2</sub> for simultaneous wastewater treatment and electric power generation.
- Effect of synthesis method on magnetic and photocatalytic properties of FeTi-SBA-15 nanocomposites.
- Synthesis mechanism of hierarchical zeolite Y modified with Ti
- Plasmonic resonance effect on photocatalytic properties of Au or Ag/C/N/TiO<sub>2</sub> nanocomposites
- Composite Membranes with functionalized KIT-6 and polymeric matrix
- Supported AuNPs obtained by green synthesis with photocatalytic and anti antibacterial properties
- New photocatalysts for dyes and antibiotics degradation in water
- New (bio)hybrid matrix based on plant extracts loaded into mesoporous silica nanoparticles with therapeutic applications



### P3. Electrode processes, Corrosion and Materials for Electrochemical Systems

*Electrochemical preparation and characterization of active materials with predetermined features*, coordinated by **Dr. Nicolae Spataru**

*Characterization of some innovative alloys, protective films and biodegradable inhibitors in corrosive media*, coordinated by **Dr. Florina Branzoi**

*Ionic liquids: electrochemical properties and applications*, coordinated by **Dr. Ana Maria Popescu**

#### Research fields:

- Synthesis and electrochemical characterization of new semiconducting materials with possible application in electroanalysis.
- Electrosynthesis and electrochemical characterization of some hybrid materials with electrocatalytic and photoelectrocatalytic properties.
- Nanostructured composite materials: functional interfaces for biomedical and energy storage applications.
- Assessment, modeling, characterization and stability monitoring of some bioalloys for implant applications and of some multilayer, multifunctional, coatings.
- Study of the adsorption of some organic compounds and of their corrosion inhibition efficiency in various aggressive media.
- High and low temperature ionic liquids applicable for electrochemically obtaining metals and metallic compounds and for corrosion prevention.

#### Members:

**Dr. Spataru Nicolae**, CSI. The main research interests include electrocatalysis, electroanalysis and diamond electrochemistry. ([nspataru@icf.ro](mailto:nspataru@icf.ro))

**Dr. Eng. Maria Marcu**, CSIII. Dr. Marcu's research interests include application of nanostructured materials with oxide matrix in energy and study of metallic biomaterials. ([m\\_marcu@icf.ro](mailto:m_marcu@icf.ro))

**Dr. Ana Maria Popescu**, CSII. She has expertise in ionic liquids, molten salts and aqua media. She spent an year (2002) as a NATO postdoctoral fellowship in Marseille, France, at IUSTI Marseille University. ([ampop@icf.ro](mailto:ampop@icf.ro))

**Dr. Tanta Spataru**, CSII. Her research interests include electrocatalysis, synthesis of electrodic materials for fuel cells; photoassisted electrochemical processes; electrochemistry of diamond and bioelectrochemistry. ([tspataru@icf.ro](mailto:tspataru@icf.ro))

**Dr. Florina Branzoi**, CSII. She has expertise in synthesis of composite materials and corrosion inhibitors. ([fbranzoi@icf.ro](mailto:fbranzoi@icf.ro))

**Dr. Cecilia Lete**, CSII. She has expertise in synthesis and electrochemical characterization of polymeric composite materials with application in electroanalysis. ([clete@icf.ro](mailto:clete@icf.ro))

**Dr. Virgil Constantin**, CSII. His expertise includes electrochemistry of molten salts/ ionic liquids and corrosion of all media. ([vconstan@icf.ro](mailto:vconstan@icf.ro))

**Dr. Cora Vasilescu**, CSII. She has expertise in corrosion of metallic biomaterials. ([cvasilescu@icf.ro](mailto:cvasilescu@icf.ro))

**Dr. Mariana Marin**, CSIII. She has expertise in synthesis and electrochemical characterization of polymeric composite materials with application in electroanalysis. ([mmaria@icf.ro](mailto:mmaria@icf.ro))

**Dr. Preda Loredana**, CSIII. Her research includes electrochemical characterization of nanostructured materials

with application in electrocatalysis, photo-electrochemistry and storage energy. ([predalore@yahoo.com](mailto:predalore@yahoo.com))

**Dr. Silviu Iulian Drob**, CS III. His expertise includes corrosion of metals and metallic biomaterials. ([sidrob@icf.ro](mailto:sidrob@icf.ro))

**Dr. Cristina Donath**, CS III. Her expertise includes ionic liquids and molten salts. ([cristidonath@yahoo.com](mailto:cristidonath@yahoo.com))

**Dr. Ionela Neacsu**, CS III. Her expertise includes corrosion in aqua and ionic liquids. ([neac\\_elena@yahoo.com](mailto:neac_elena@yahoo.com))

**Mihai Marian Radu, Alexandru Marius Mihai and Sorina Alexandra Leau**, Ph.D. students.

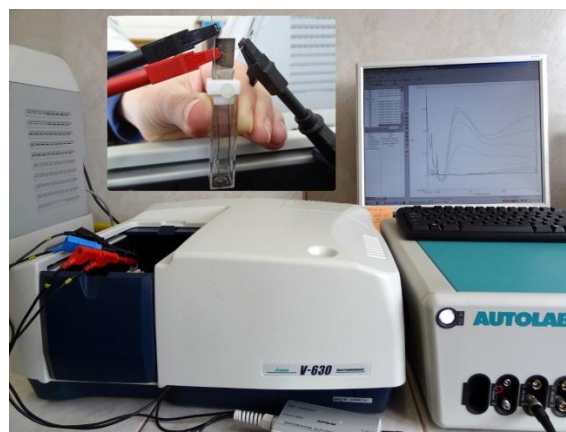
#### Research Equipment:

<https://eeris.eu/ERIF-2000-000L-0428>

- Potentiostat/galvanostat PAR 273A with PAR Frequency Response Detector
- Keithley 2425 SourceMeter
- Potentiostat/Galvanostat VoltaLab 40
- FT-IR Spectrometer
- Corrosion test cabinet
- Potentiostat/Galvanostat PARSTAT 2273
- 100x-1000x Magnification Trinocular Metallurgical-Metallographic Microscope



Potentiostat/galvanostat PARSTAT 4000 with Rotating Disk Electrode



Potentiostat/Galvanostat AUTOLAB 302N with Electrochemical Quartz Crystal Microbalance

#### Research Projects:

1. *Electrochemical synthesis of high entropy alloys with superior tribological and corrosion resistance* (HEASYNTCORR), PN-III-P2-2.1-PED-2019-0022, Ctr.nr. 330PED/2020-2022; Project manager: dr. A.M.Popescu

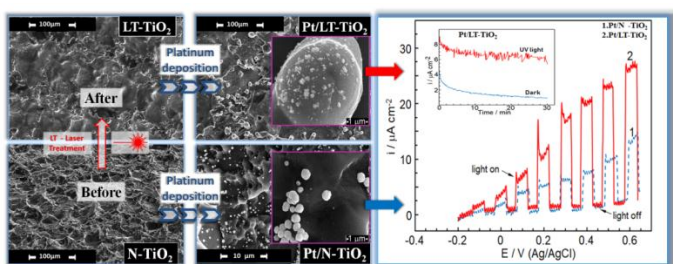


2. Tertiary alloy with antibacterial properties and non-toxic alloying elements for implants. / (ZIRTAAG), PN-III-P1-1.1-TE-2019, Ctr. Nr. 86/2020; Project manager: dr. S.I. Drob.
3. Corrosion resistance of new composite materials based on encapsulated iron powders for electronic industry, Bilateral project AR 445/12.05.2020: Institute of Physical Chemistry of Romanian Academy and National Foundation for Scientific Research, Belarus, 2020-2021. Project manager: dr. A.M.Popescu
4. Investigations of ionic liquids and different sea waters corrosive action on surface characteristics and magnetic properties of some functional alloys, Bilateral project AR 1855/8.05.2019: Institute of Physical Chemistry of Romanian Academy and National Foundation for Scientific Research, Belarus, 2018-2019. Project manager: dr. A.M.Popescu
5. Electrosynthesis and electroanalytical applications of nanocomposites materials based on conducting polymers, Bilateral Project: Institute of Physical Chemistry of Romanian Academy, University Politehnica from Bucharest and Institute of Physical Chemistry "Rostislav Kaischew" Sofia, Bulgaria, University Politehnica from Bucharest, 2017-2019. Project manager: dr. Cecilia Lete

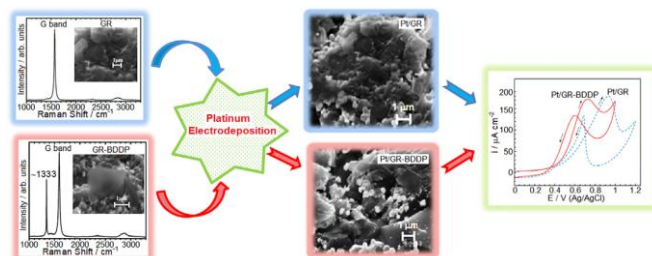
### Representative research results

- J. J. García-Guzmán, D. López-Iglesias, M. Marin, C. Lete, S. Lupu, J. M. Palacios Santander, L. Cubillana-Aguilera, *Electrochemical Biosensors for antioxidants, Advanced Biosensors for Health Care: Materials and Applications, Elsevier 2019, 105-146 (Book Chapter).*

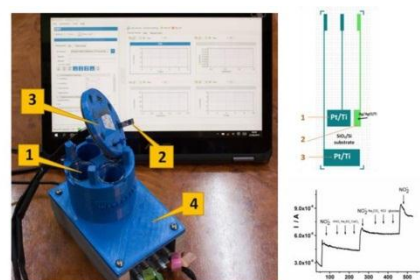
- The new concept of Pt/TiO<sub>2</sub> multilayer electrode for photo-assisted methanol oxidation, with improved electrocatalytic activity by the laser treatment of native TiO<sub>2</sub> films has been developed. Upon UV irradiation, platinum deposited on laser treated TiO<sub>2</sub> electrodes exhibits a strong enhancement of the methanol oxidation current and, importantly, a much better resistance to poisoning. The results have been published in 2019 in Q1 ISI journal (M.M. Radu, N. Becherescu, T. Spătaru,\* P. Osiceanu, M.A. Mihai, A.M. Mihai, J.M. Calderon-Moreno, N. Spataru, A. Fujishima, *Improved suitability as catalyst support and more efficient charge carrier separation of native air-formed TiO<sub>2</sub> films by mild laser treatment*, Journal of Power Sources 437, 226921 (2019), IF = 8.247.



- A new composite carbon hybrid as a substrate for the electrocatalyst was obtained by boron-doped diamond powder (BDDP) embedment in a drop-casted graphene (GR) layer with higher porosity and better electrochemical activity for fuel cell methanol oxidation (Spătaru, N., Calderon-Moreno, J.M., Osiceanu, P., Kondo, T., Terashima, C., Popa, M., Radu, M.M., Culita, D., Preda, L., Mihai, M.A., Spătaru, T.\*, *Conductive diamond powder inclusion in drop-casted graphene for enhanced effectiveness as electrocatalyst substrate*. Chemical Engineering Journal, (2020) 402, 126258. IF = 13.273).



- A new nitrite sensing platform based on SnO<sub>2</sub>/Pt/Ti/SiO<sub>2</sub>/Si was designed, fabricated and tested. SnO<sub>2</sub> coatings were prepared by classic sol-gel and microwave assisted sol-gel technique. The sensing platform demonstrated high sensitivity, selectivity and good stability for nitrite detection being a proper tool in nitrite sensing in real samples (C. Lete, M. Chelu, M. Marin, S. Mihaiu, S. Preda, M. Anastasescu, J.M. Calderón-Moreno, S. Dinulescu, C. Moldovan, M. Gartner, *Nitrite electrochemical sensing platform based on tin oxide films*, Sensors and Actuators B: Chemical 316,12810 (2020) IF = 7.340).



A novel electrochemical sensing platform based on SnO<sub>2</sub>/Pt/Ti/SiO<sub>2</sub>/Si for selective nitrite detection

### Other significant papers:

- J.J. García-Guzmán, D. López-Iglesias, L. Cubillana-Aguilera, D. Bellido-Milla, J.M. Palacios-Santander, M. Marin, S.D. Grigorescu, C. Lete, S. Lupu, *Silver nanostructures - poly(3,4-ethylenedioxythiophene) sensing material prepared by sinusoidal voltage procedure for detection of antioxidants*, Electrochimica Acta 393,139082 (2021) IF = 6.9
- A. Banu, M. Marcu, C. Juganaru, P. Osiceanu, M. Anastasescu, L. Capra, *Corrosion behavior of CoCrMoW cast alloy in lactic acid environment*, Arabian Journal of Chemistry 12 (8), 2007-2016 (2019) IF = 4.76
- M. Marcu, L. Preda, T. Spataru, J. Calderon Moreno, P.Osiceanu, and N. Spataru. *Anodic Voltammetry of Epinephrine at Graphene-Modified Conductive Diamond Electrodes and Its Analytical Application*, J. Electrochem. Soc. 165(11); B 515-522 (2018) IF = 3.66
- C. Vasilescu, P. Osiceanu, J.M. Calderon Moreno, S.I. Drob, S. Preda, M. Popa, I. Dan, M. Marcu, M. Prodana, I.A. Popovici, D. Ionita, E. Vasilescu, *Microstructure, surface characterization and long-term stability of new quaternary Ti-Zr-Ta-Ag alloy for implant use*, Materials Science and Engineering: C 71, 322-334 (2017) IF = 5.08
- F. Branzoi, A. Băran, S. Petrescu, *Evaluation of Corrosion Protection Performance of New Polymer Composite Coatings on Carbon Steel in Acid Medium by Electrodeposition Methods*, Coatings 11(8), 903 (2021) IF = 2.86
- A.M. Popescu, F. Branzoi, I. Constantin, M. Anastasescu, M. Burada, D. Mitrică, I. Anisei, M.T. Olaru, V. Constantin, *Electrodeposition, characterization and corrosion behaviour of CoCrFeMnNi high entropy alloy thin films*, Coatings 11, 1367(2021) IF = 2.86

## P4. Materials science and advanced characterization methods

*Crystallized, vitreous and glass-ceramic oxide systems with special applications*, coordinated by **Dr. Victor Fruth**

*Oxide systems obtained by chemical methods in solution*, coordinated by **Dr. Monica Popa**

*Advanced materials for production and storage of energy under safe environment*, coordinated by **Dr. Elena Maria Anghel**

### Research fields:

- Reaction mechanisms in oxide systems with electrical and magnetic properties;
- Physicochemical phenomena in porous materials and their applications;
- Correlation between structure and properties of vitreous/crystallized systems and their applications;
- Oxide systems obtained by sol-gel/wet chemical methods devoted to studying the chemistry of the processes, structural characterization and preparation of mono and poly-component powders and films, oxide and hybrid nanocomposites, oxide nanotubes;
- Thermo-structural studies of the materials designed for energy and environmental applications.

### Members:

The research team is composed of senior and early career researchers committed to developing high-quality research and enabling the transition from fundamental research to applied. Our scientists have an established history of successful collaboration with universities and industry partners.

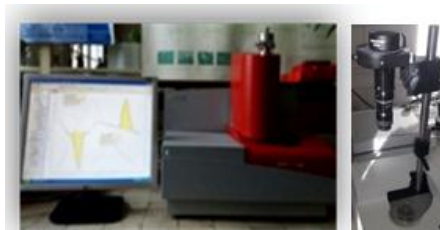
### Research Equipment:

<https://eeris.eu/ERIF-2000-000A-1294>

- Microscop SEM Quanta 3D FEG D9399-Morphology investigation of materials by SEM and elemental analysis by EDS. Contact persons: Dr. S. Petrescu ([simon\\_pet@icf.ro](mailto:simon_pet@icf.ro)); Dr. J.C. Moreno ([calderon@icf.ro](mailto:calderon@icf.ro)); Dr. F. Maxim ([fmaxim@icf.ro](mailto:fmaxim@icf.ro))
- Microscop TEM Tecnai G2 F30 S-Twin-Contact persons: Dr. J.C. Moreno ([calderon@icf.ro](mailto:calderon@icf.ro)); Dr. C. Munteanu ([cmunteanu@icf.ro](mailto:cmunteanu@icf.ro)).



- Thermogravimetric and thermal differential analysis apparatus Mettler Toledo TGA/SDTA851e and the possibility of coupling DSC823e. Contact persons: Dr. Jeanina Pandeale Cusu ([jeanina@icf.ro](mailto:jeanina@icf.ro)); Dr. Raul Augustin Mitran ([raul.mitran@gmail.com](mailto:raul.mitran@gmail.com)); ([daniel.lincu1113a@gmail.com](mailto:daniel.lincu1113a@gmail.com))
- Differential scanning calorimetry (Mettler Toledo DSC3+): Temperature range: -80 - +700°C
- Optical Microscope module (Olympus SC50) for DSC3+ provides complementary data on the physico-chemical processes during heating/cooling. Contact persons: Dr. Jeanina Pandeale Cusu ([jeanina@icf.ro](mailto:jeanina@icf.ro)); Dr. Raul Augustin Mitran ([raul.mitran@gmail.com](mailto:raul.mitran@gmail.com)); ([daniel.lincu1113a@gmail.com](mailto:daniel.lincu1113a@gmail.com))



- LABSYS evo TG/DTA/DSC 1600-TG/DTA/DSC 1600 system can be used for measurements up to 1600 °C. Contact persons: Dr. E.M. Anghel ([manghel@icf.ro](mailto:manghel@icf.ro)); Dr. S. Petrescu ([simon\\_pet@icf.ro](mailto:simon_pet@icf.ro))

Thermal Conductivity Analyzer C-THERM TCi. Contact persons: Dr. E.M. Anghel ([manghel@icf.ro](mailto:manghel@icf.ro)) and Dr. S. Petrescu ([simon\\_pet@icf.ro](mailto:simon_pet@icf.ro))

- LABRAM HR 800 SYSTEM (HORIBA JOBIN YVON)-The non-destructive and efficient Raman technique provides information about chemical composition, molecular structure, crystallographic orientation, temperature, phase transition and mechanical stress. Contact persons: Dr. M. Popa ([pmonica@icf.ro](mailto:pmonica@icf.ro)), Dr. E.M. Anghel ([manghel@icf.ro](mailto:manghel@icf.ro)), Dr. S. Petrescu ([simon\\_pet@icf.ro](mailto:simon_pet@icf.ro)); Dr. J. Caldereon Moreno ([calderon@icf.ro](mailto:calderon@icf.ro))



- Rigaku Ultima IV X-Ray Diffractometer- Ultima IV X-ray diffractometer can perform micro-crystalline diffraction, thin-film diffraction, small angle scattering, and *in-situ* X-ray diffraction measurements (up to 1500°C). Contact persons: Dr. S. Preda ([predas@icf.ro](mailto:predas@icf.ro)); Dr. I. Atkinson ([iatkinson@icf.ro](mailto:iatkinson@icf.ro))

- Rigaku ZSX Primus II tube-above wavelength dispersive X-ray fluorescence (WDXRF) spectrometer delivers rapid quantitative determination of major and minor atomic elements, from beryllium (Be) through uranium (U). Contact persons: Dr. I. Atkinson ([iatkinson@icf.ro](mailto:iatkinson@icf.ro)); Dr. S. Preda ([predas01@yahoo.co.uk](mailto:predas01@yahoo.co.uk), [predas@icf.ro](mailto:predas@icf.ro)); Dr. J. Pandeale Cusu ([jeanina@icf.ro](mailto:jeanina@icf.ro))

- FT-IR Spectrometer NICOLET 6700- Contact persons: Dr. O.C. Mocioiu ([omocioiu@icf.ro](mailto:omocioiu@icf.ro)); Dr. A. Rusu ([arusu@icf.ro](mailto:arusu@icf.ro))

- SHIMADZU Dynamic Ultra-Micro Hardness Tester DUH-211 determines dynamic hardness through the indentation process. Can evaluate hardness corresponding to ISO14577-1. Contact persons: Dr. L. Predoana ([lpredoana@icf.ro](mailto:lpredoana@icf.ro)); C. Codrea ([codrea.cosmin@yahoo.com](mailto:codrea.cosmin@yahoo.com))

- SOLARTRON 1260A, 1260A Impedance Analyzer measurement cell with controlled temperature and atmosphere - ProboSTAT, vertical furnace 1200 °C, controller temperature Eurotherm 2216e. Contact persons: Dr. O.C. Mocioiu ([omocioiu@icf.ro](mailto:omocioiu@icf.ro)); Dr. C. Hornoiu ([chornoiu@icf.ro](mailto:chornoiu@icf.ro))

- UV-Vis spectrometer with in-situ optic fiber probe (Agilent Cary 60)-Spectral range 200 – 1100 nm. Absorbance 0-3. Contact persons: Dr. Raul Augustin Mitran ([raul.mitran@gmail.com](mailto:raul.mitran@gmail.com)); ([daniel.lincu1113a@gmail.com](mailto:daniel.lincu1113a@gmail.com))

- Filmetrics Profilim 3D uses White-Light Interferometry (WLI) and Phase-Shift Interference (PSI) imaging through microscope objectives, to produce a 3D image of the sample. Contact

persons: Dr. L. Predoana ([lpredoana@icf.ro](mailto:lpredoana@icf.ro)); C. Codrea ([codrea.cosmin@yahoo.com](mailto:codrea.cosmin@yahoo.com))  
 - Micromeritics BET Surface Area and Porosity Analyzer-  
 Contact persons: Dr. D.C. Culita ([daniela.culita@gmail.com](mailto:daniela.culita@gmail.com))

### Selected research projects:

- COST Action** - Network for research, innovation and product development on porous semiconductors and oxides-2021-2025-Dr.V. Fruth (ICF)
- PNCD III- Proiecte complexe CDI (PCCDI) 51PCCDI/2018, PN-III-P1-1.2-PCCDI-2017-0476**, Materiale traditionale si avansate utilizate pentru protejarea componentelor arhitecturale ale patrimoniului cultural (2018-2021) Dr. L. Predoana
- TE no. 95/2018 project** "Nanoconfinement in mesoporous Silica: Towards next generation Energy Storage Materials" (2018-2020)- Dr. R.A. Mitran
- TE no. 166/2020 project** "Metal-ceramic nanocomposites: next-generation thermal energy storage materials" (2020-2022) Dr. R.A. Mitran
- PCCDI no. 85/2018 project** "Complex valorisation of Black sea region bioresources by developing and applying innovative and emerging biotechnologies" (2018-2021) Dr. R.A. Mitran
- PED no. 258/2020 PN-III-P2-2.1-PED-2019-0598**, Functionalized mesoporous bioglass based 3D scaffolds for hard tissue regeneration (2020-2022), Dr. I. Atkinson
- Joint Research Project** between National Research Council of Italy, the Institute for the Structure of Matter of National Research Council (CNR-ISM) and Institute of Physical Chemistry of the Romanian Academy, Piezoelectric and Multiferroic Molecular Perovskites for Flexible and Wearable Devices, Responsible Dr. V. Fruth
- Joint Research Project** between Institute of Physical Chemistry of the Romanian Academy, Romania and Centre of Natural Sciences, Hungarian Academy of Sciences, Hungary, "Reduced semiconductor oxides for TCO, photocatalysis and gas sensing applications". Acad. Dr. M. Zaharescu
- Joint Research Project** between Institute of Physical Chemistry of the Romanian Academy, Romania and Institute of Photonics and Electronics of the Czech Academy of Sciences, Czech Republic, Transparent ceramic luminophores for high-power lasers operating in short infrared range, Dr. L. Predoana
- Mobility Project AR-17-02** "Structure-thermal properties correlation of the composite materials for energy fields" Dr. E.M. Anghel

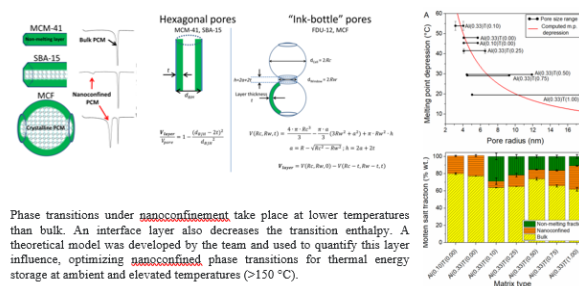
### Selected papers:

- V. Fruth, L. Todan, C.I. Codrea, I. Poenaru, S. Petrescu, L. Aricov, M. Ciobanu, L. Jecu, R. Mariana Ion, L. Predoana, *Multifunctional Composite Coatings Based on Photoactive Metal Oxide Nanopowders (MgO/TiO<sub>2</sub>) in Hydrophobic Polymer Matrix for Stone Heritage Conservation*, *Nanomaterials* 11 (10), 2586 (2021).
- M. Gabrovskaa, I. Ivanov, D. Nikolova, J. Krstic, A.M. Venezia, D. Crişan, M. Crişan, K. Tenchev, V. Idakiev, T. Tabakova, *Improved water-gas shift performance of Au/NiAl LDHs nanostructured catalysts via CeO<sub>2</sub> addition*, *Nanomaterials* 11, 366 (2021).
- O. C. Mocioiu, I. Atkinson, A-M. Mocioiu, S. Neagu, R. Ruginescu, R. A. Mitran, M. Enache, *Effect of ZnO on properties of gels for heritage objects conservation*, *Gels* 7, 251 (2021).
- L. Predoana, I. Atkinson, D. A. Karaj, V. O. Odhiambo, L. P. Bakos, T.N. Kovács, J. Pandelescu, S. Petrescu, A. Rusu, I.

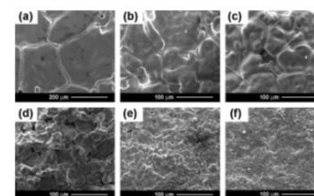
M. Szilágyi, G. Pokol, M. Zaharescu, *Comparative study of the thermal behavior of Sr-Cu-O gels obtained by sol-gel and microwave-assisted sol-gel method*, *J. Therm. Anal. Calorim.* 143, 2893-2900 (2021).

- R.A. Mitran, D. Lincu, L. Buhălţeanu, D. Berger, C. Matei, *Shape-stabilized phase change materials using molten NaNO<sub>3</sub>-KNO<sub>3</sub> eutectic and mesoporous silica matrices*, *Sol. Energy Mater. Sol. Cells* 215, 110644 (2020).
- S. Petrescu, S. M. Avramescu, A. M. Musuc, F. Neatu, M. Florea, P. Ionita, *Crown-ether functionalized graphene oxide for metal ions sequestration*, *Mat. Res. Bull.* 122, 110643 (2020).
- I. Bunoiu, M. Mindroiu, C.C. Manole, M. Andrei, A. Nicoara, E. Vasilescu, M. Popa, A.C. Didilescu, *Electrochemical testing of a novel alloy in natural and artificial body fluids*, *Ann. Anat.* 217, 54-59 (2018).
- M. Zaharescu, L. Predoana, J. Pandelescu, *Relevance of thermal analysis for sol-gel-derived nanomaterials*, *J Sol Gel Sci. Technol.* 86,7-23 (2018).
- E. M. Anghel, P. M. Pavel, M. Constantinescu, S. Petrescu, I. Atkinson, E. Buixaderas, *Thermal transfer performance of a spherical encapsulated PEG 6000-based composite for thermal energy storage*, *Applied Energy* 208, 1222-1231 (2017).

### Highlights



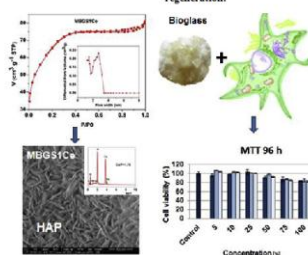
### Microstructure and dielectric properties of sol-gel BaTi<sub>1-x</sub>Hf<sub>x</sub>O<sub>3</sub> ceramics



FE-SEM images showing the microstructure of the conventionally sintered sol-gel BTH ceramics, (1400°C/4 h): (a) x = 0; (b) x = 0.03; (c) x = 0.05; (d) x = 0.10; (e) x = 0.20; (f) x = 0.30.

[E.M. Soare et al.14th ECerS Conference for Young Scientists in Ceramics ,Novi Sad, Serbia, 20-23 October, 2021]

### Ce-containing mesoporous bioactive glasses synthesized by sol-gel method with enhanced surface area and no cell cytotoxic activity for bone regeneration.



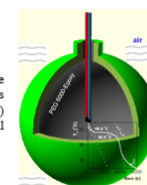
[I. Atkinson et al., *Micropor. Mesopor. Mater.*, 76, 2019, 76-88.]

### Latent heat storage materials

Polymeric phase change materials, PCMs, (PEG-epoxy resin-aluminium) were developed, characterized and thermally tested in laboratory modules with various geometries in order to be used subsequently in thermal energy storage (TES) systems. Using a two-front solids model is a new approach for modelling thermal transfer in *semicrystalline* solids.

### Spherical laboratory module for thermal energy storage

[E.M. Anghel et al., *Appl. Energy* 208 (2017) 1222.]



*From coordination compounds to advanced materials by soft chemistry methods. Nanomaterials and organic compounds with specific reactivity*, coordinated by **Dr. Daniela C. Culita**  
*Green syntheses of materials*, coordinated by **Dr. Diana Visinescu**

Research fields:

- Coordination compounds as precursors of new advanced materials with special magnetic, optic, and electric properties.
- Inorganic and hybrid organic-inorganic systems with biological applications and for depollution processes.
- Nanomaterials and organic compounds with specific reactivity.
- Eco-friendly synthesis approaches of nanomaterials and composites.

*Metallosupramolecular chemistry: crystal engineering of (multi)functional molecular materials*, coordinated by **Dr. Gabriela Marinescu**

Research fields:

- Polynuclear metal complexes and coordination polymers.
- A metallosupramolecular approach toward functional magnetic materials.
- Design of (multi)functional molecular materials: magneto-structural/optical investigations.
- Luminescent molecular materials.
- Coordination compounds with biological properties.

#### Team members

**Dr. Gabriela MARINESCU**, CS I. Research interests: Rational design and synthesis of homo- and heterometallic compounds and coordination polymers using different organic ligands/complex as ligand; Strategies to generate nanomaterials with optical, magnetic and biological properties. Group coordinator, e-mail: [gmarinescu@icf.ro](mailto:gmarinescu@icf.ro)

**Dr. Diana Beatrice VISINESCU**, CS I. Research interests: Coordination chemistry; Polynuclear complexes; Magneto-chemistry; Crystal engineering; Supramolecular Chemistry; Chemistry of materials. e-mail: [dianavisinescu@icf.ro](mailto:dianavisinescu@icf.ro)

**Dr. Daniela Cristina CULITA**, CS II. Research interests: Development of novel materials for biomedical applications and environmental remediation; Characterization techniques (N<sub>2</sub> physisorption, nano/microparticles analysis by DLS/ELS, spectroscopic techniques). e-mail: [dculita@icf.ro](mailto:dculita@icf.ro)

**Dr. Greta Mihaela SOCOTEANU (Patrinoiu)**, CS II. Research interests: Carbon-based nanomaterials; Hydrothermal carbonization; Green chemistry; Environmental remediation. e-mail: [gretamihaela@icf.ro](mailto:gretamihaela@icf.ro)

**Dr. Dana Mihaela GINGASU**, CS II. Research interests: Synthesis of polynuclear coordination compounds that can be used as precursors for oxide nanomaterials; Green approaches of synthesis pathways which involves plant resources. e-mail: [dgingasu@icf.ro](mailto:dgingasu@icf.ro)

**Dr. Madalina TUDOSE**, CS III. Research interests: Organic and materials chemistry; Synthesis, characterization and applications of hybrid nanomaterials. e-mail: [mtudose@icf.ro](mailto:mtudose@icf.ro)

**Dr. Cristian-Dumitru ENE**, CS III. Research interests: Polymorphism in supramolecular and coordination chemistry; Chirality; Synthesis of organic ligands and coordination compounds; Phase transition; Single crystal to single crystal transformation; Optical properties of complexes. Thermogravimetric analysis. e-mail: [cene@icf.ro](mailto:cene@icf.ro)

**Dr. Elena Nusa HRISTEA**, CS. Research interests: Synthesis and characterization of molecules that can be involved in supramolecular assemblies. e-mail: [enhristea04@gmail.com](mailto:enhristea04@gmail.com)

**Dr. Rodica Daniela CARPEN**, CS. Research interests: Synthesis of organic compounds with predetermined physico-chemical properties; Noncovalent interactions with dual molecular probes. e-mail: [rodicad2003@yahoo.com](mailto:rodicad2003@yahoo.com)

**Dr. Teodora MOCANU**, AC. Research interests: Crystal engineering; Metallosupramolecular chemistry; Molecular magnetism. e-mail: [tmocanu@icf.ro](mailto:tmocanu@icf.ro)

**Dr. Adela Maria SPINCIU**, AC. Research interests: Coordination chemistry; Chemistry of materials: synthesis of metal oxide and metal oxide/C-based composites for sensing applications. e-mail: [aspinciu@icf.ro](mailto:aspinciu@icf.ro)

#### Research Equipment

- JASCO FT/IR – 4700 Spectrometer
- JASCO V-750 UV-Visible Spectrophotometer
- JASCO UV-Visible-NIR Spectrophotometer
- JASCO FP-8300 Fluorescence Spectrometer
- Simultaneous Thermal Analyzer – Netzsch STA 449 F1 Jupiter
- Vibrating sample magnetometer Lake Shore VSM 7404
- Nabertherm R 120/500/13 Compact Tube Furnaces (1300°C, 500 mm)
- Vacuum Oven BMT Vacucell 22

#### Selected research projects

- **Research Project PN-III-P1-1.1-TE-2021-0288**, Biomedical applications of hybrid materials based on graphene oxide and fluorescent structures

- **Exploratory Research Project PN-III-P4-ID-PCE-2020-2324**, (Poly)saccharides-derived hydrothermal carbonaceous materials - a platform for developing a new generation of copper-based green electrochemical sensors

- **Exploratory Research Project PN-III-P4-ID-PCE-2016-0321**, New versatile dicyanidometallate precursors [M<sup>III</sup>(L)(CN)<sub>2</sub>]<sup>-</sup> for designing heterometallic molecular magnetic materials

- **Demonstration Experimental Project PN-III-P2-2.1-PED-2016-3-0240**, Sustainable materials based on zinc oxide for antimicrobial applications

- **Partnerships in priority domains PN-II-PT-PCCA-2013-4-0418 Project**, Innovative materials and processes for the selective removal of heavy metals from wastewater

- **Interacademic exchange** between the Romanian Academy and the Bulgarian Academy of Sciences, Application of 3D cell cultures to study antitumor activity of metal compounds

#### Selected publications

1. M.-G. Alexandru, D. Visinescu, B. Braun-Cula, S. Shova, F. Lloret, J. Cano, M. Julve, *A rare isostructural series of 3d–4f cyanido-bridged heterometallic squares obtained by assembling [Fe<sup>III</sup>{HB(pz)<sub>3</sub>}(CN)<sub>3</sub>]<sup>-</sup> and Ln<sup>III</sup> ions: synthesis, X-ray structure and cryomagnetic study*, *Dalton Trans.* 50, 14640-14652 (2021).

2. D. Visinescu, M.-G. Alexandru, D.G. Dumitrescu, S. Shova, F. Lloret, M. Julve, *Cyanido-bridged {Fe<sup>III</sup>Ln<sup>III</sup>} heterobimetallic chains assembled through the [Fe<sup>III</sup>{HB(pz)<sub>3</sub>}(CN)<sub>3</sub>]<sup>-</sup> complex as metalloligand: synthesis, crystal structure and magnetic properties*, *CrystEngComm* 23, 4615-4626 (2021).

3. G. Marinescu, A.M. Madalan, C. Maxim, S. Sova, R. Clerac, M. Andruh, *Heterometallic 3d-4d coordination polymers*

assembled from *trans*- [Ru<sup>III</sup>(L)(CN)<sub>2</sub>]<sup>-</sup> tectons and 3d cations, *Dalton Trans.* 48, 15455-15464 (2019).

4. G. Marinescu, D.C. Culita, C. Romanitan, S. Somacescu, C.D. Ene, V. Marinescu, D.G. Negreanu, C. Maxim, M. Popa, L. Marutescu, M. Stan, C. Chifiriuc, *Novel hybrid materials based on heteroleptic Ru(III) complexes immobilized on SBA-15 mesoporous silica as highly potent antimicrobial and cytotoxic agents*, *Appl. Surf. Sci.* 520, 146379 (2020).

5. G. Patrinoiu, J.M. Calderon-Moreno, S. Somacescu, A.M. Musuc, T. Spataru, P. Ionita, O. Carp, *Rational Functionalization Towards Redox-Active TEMPO Stable Free-Radical-Hydrochar Composites*, *ChemSusChem* 14, 2042-2049 (2021).

6. M. Tudose, E.M. Anghel, E.N. Hristea, M. Voicescu, S. Somacescu, D.C. Culita, A.M. Musuc, F.D. Dumitrascu, A.M. Hanganu, A. Kuncser, F.L. Zorila, M. Alexandru, M.A. Acasandrei, D.I. Savu, *Benzofurazan derivatives modified graphene oxide nanocomposite: physico-chemical characterization and interaction with bacterial and tumoral cells*, *Mater. Sci. Eng. C.* 123, 112028 (2021).

7. D. Gingasu, I. Mindru, D.C. Culita, G. Marinescu, S. Somacescu, A. Ianculescu, V.-A. Surdu, S. Preda, O. Oprea, B.S. Vasile, *Mentha piperita-mediated synthesis of cobalt aluminate nanoparticles and their photocatalytic activity*, *J. Mat. Sci.-Mat. Electron* 32, 11220–11231 (2021).

8. C.D. Ene, P. Cucos, A. Ianculescu, D.C. Culita, E.M. Anghel, A. Cucos, I. Atkinson, M.C. Chifiriuc, J.M. Calderón-Moreno, O. Carp, *Benign by design: porous spherical ZnO-alginate family via a dual-template synthesis*, *Appl. Surf. Sci.* 580, 152231 (2022).

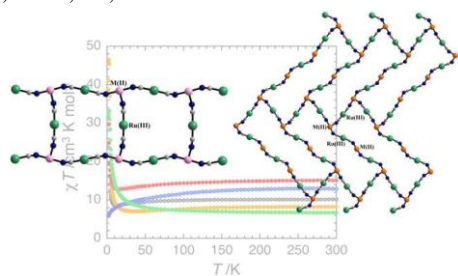
## Highlights

### Heterometallic coordination polymers

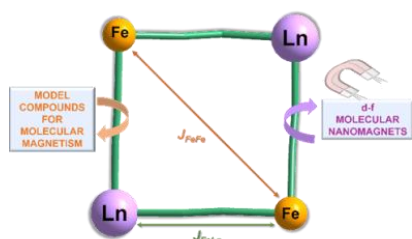
*Building Blocks to design 3d-4d and 4d-4f heterometallic complexes*

Heterometallic 3d-4d coordination polymers (1-D and 2-D) assembled from *trans*-[Ru<sup>III</sup>(L)(CN)<sub>2</sub>]<sup>-</sup> building blocks.

*Dalton Trans.*, 2019, 48, 15455-15464.



### Design of d-f square-like heterometallic complexes



A rare isostructural series of 3d-4f cyanido-bridged heterometallic squares obtained by assembling [Fe<sup>III</sup>{HB(pz)<sub>3</sub>}(CN)<sub>3</sub>]<sup>-</sup> and Ln<sup>III</sup> ions. New model compounds for molecular magnetism; new and rare examples of cyanido-

bridged d-f showing slow relaxation of the magnetization (single-molecule magnets).

*Dalton Trans.*, 2021, 50, 14640-14652.



### Hybrid materials based on coordination compounds immobilized on mesoporous silica

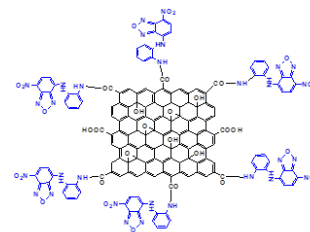
A series of novel hybrid materials based on Ru(III) complexes immobilized on SBA-15 mesoporous silica with high antibacterial and anti-biofilm activity. In vitro tests regarding the cytotoxic effect on adenocarcinoma (HeLa) cells showed that all hybrid materials decreased the cell viability in a dose-dependent manner, being very promising for medical applications.

*Appl. Surf. Sci.*, 2020, 520, 146379.

### Bioactive materials based on functionalized graphene oxide

Novel graphene oxide-based composites obtained through covalent immobilization of benzofurazan derivatives on graphene oxide. The bio-evaluation results suggest that the obtained materials have potential in combating biofilm formation and antitumor activity on human colon cancer cells HCT116.

*Mater. Sci. Eng. C.*, 2021, 123, 112028.

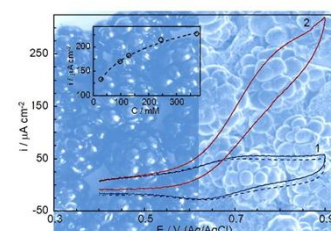


### Eco-friendly synthesis of materials

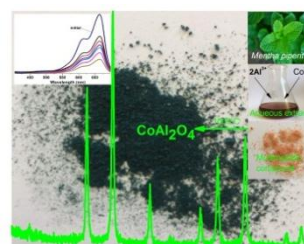
*Radical-biohydrochar composites*

Composites with electrocatalytic activity and capacitive characteristics from the association of carbonaceous materials obtained from biomass with stable organic radicals.

*ChemSusChem.*, 2021, 14, 2042-2049.



### Synthesis of materials using plant extract



A new “green” method for synthesis of cobalt aluminate nanoparticles (CoAl<sub>2</sub>O<sub>4</sub>) using mentha leaves aqueous extract.

*J. Mat. Sci.-Mat. Electron*, 2021, 32, 11220–11231.

## P5. Complex Functional Colloids

Coordinator: **Dr. Adriana Baran**

### Research fields

Associative colloids for advanced, composite and multifunctional nanomaterials with industrial applications, in biotechnology and medicine (colloids; surfactants; polymers; surfactant-polymer interaction, air-water interfaces; spread and thin liquid films; soft nanoparticles; gels and microgels; surfactant-protein interaction; protein-polysaccharide systems; functional colloids in drug delivery).

### Members

**Dr. Adriana Baran**, CS III. Research interests: synthesis of nanoparticles using surfactant-polyelectrolyte and/or associative polymer-surfactant mixtures, and in characterization of advanced nanomaterials.

e-mail: [abaran@icf.ro](mailto:abaran@icf.ro)

**Dr. Gabriela Stinga**, CS III. Research interests: physico-chemical properties of surfactants, fluorescent probes/fluorescently/hydrophobically labeled polymers or surfactant/polymer mixture in micellar heterogeneous microenvironments as well as micellar catalysis.

e-mail: [gbaluta@icf.ro](mailto:gbaluta@icf.ro)

**Dr. Alina Iovescu**, CS III. Research interests: polymer-surfactant and protein-surfactant interaction, hydrophobically modified polymers, fluorescently labelled polymers and fluorescent probes, micellar aggregates, amphiphilic nanostructures at interfaces.

e-mail: [aiovescu@icf.ro](mailto:aiovescu@icf.ro)

**Dr. Monica Elisabeta Maxim**, CS III. Research interests: polymer-surfactant nanostructures deposited on solid surfaces, physico-chemical properties of surfactants, fluorescent probes/fluorescently labeled polymers in micellar aqueous and non-aqueous media.

e-mail: [mmaxim@icf.ro](mailto:mmaxim@icf.ro)

**Dr. Anca Ruxandra Leonties**, CS III. Research interests: physico-chemical properties of proteins and polymers, proteins (including enzymes), colloidal suspensions (aqueous and non-aqueous) and polymer gels (aqueous and non-aqueous).

e-mail: [aleonties@icf.ro](mailto:aleonties@icf.ro)

**Dr. Ludmila Aricov**, CS. Research interests: synthesis of water-soluble hydrophobically modified polymers, investigation of physicochemical properties of polymers, enzyme immobilization procedures, enzyme catalysis.

e-mail: [laricov@icf.ro](mailto:laricov@icf.ro)

**Raluca-Marieta Visan**, Scientific Research Assistant. Research interests: biophysics, cellular biotechnology, biocompatible nanoparticles and investigation of *Candida rugosa* lipase on non-specific.

e-mail: [rvisan@icf.ro](mailto:rvisan@icf.ro)

### Publications

1. A. Iovescu, G. Stîngă, M. Elisabeta Maxim, M. Gosecka, T. Basinska, S. Slomkowski, D. Angelescu, S. Petrescu, N. Stănică, A. Băran, D.F. Anghel, *Chitosan-polyglycidol complexes to coating iron oxide particles for dye adsorption*, Carbohydrate Polymers 246, 116571 (2020) (I.F. = 9.381)

2. G. Stîngă, A. Băran, A. Iovescu, F. Brânzoi, D.F. Anghel, *Impact of cationic surfactant on fluorescent complex of pyrene labeled poly(acrylic acid) and methylene blue*, Journal of Molecular Liquids 322, 114545 (2021) (I.F. = 6.165).

3. R.M. Vișan, A.R. Leonties, L. Aricov, V. Chihaiia, D.G. Angelescu, *Polymorphism of chitosan-based networks stabilized by phytate investigated by molecular dynamics simulations*,

Physical Chemistry Chemical Physics 23, 22601–22612 (2021) (I.F. = 3.676).

4. A. Băran, L. Aricov, G. Stîngă, A. Iovescu, A.R. Leonties, V.V. Jerca, *The effect of C<sub>12</sub>E<sub>6</sub> nonionic surfactant on the solubilization of Eosin Y in unmodified- and hydrophobically modified poly(acrylic acid) solutions*, Journal of Molecular Liquids 346, 117103 (2022) (I.F. = 6.165).

### Research Equipment

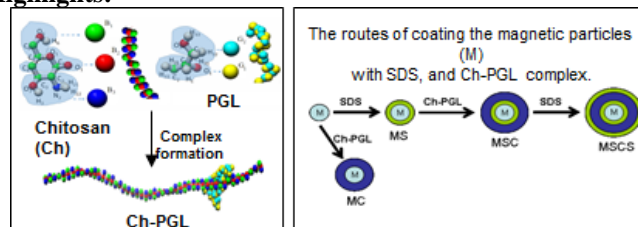
<https://eeri.eu/ERIF-2000-000F-0392>

- K11 Surface Tension Tensiometer (Krüss)
- Contact angle apparatus Easy Drop (Krüss)
- Vibro Viscometer SV (A&D Company)
- Rheometer Kinexus Pro (Malvern Instruments)
- UV-Vis spectrometer Cary 100 (Varian)
- FluoroMax®-4 spectrofluorometer (Horiba Jobin Yvon)
- Dynamic and steady-state fluorimeter FLSP 920 (Edinburgh Instruments)
- Nicolet iZ10 FTIR module (Thermo Scientific)
- Circular dichroism spectrometer Jasco J815 (Jasco)
- Zetasizer NanoZS (Malvern Instruments)



**Interacademic Project:** *Studies on films formed by amphiphilic copolymers by fluorescent methods*, Polish Academy of Science, Center of Molecular and Macromolecular Studies, Lodz, Polonia (Dr. Teresa Basinska).

### Highlights:



Chitosan - polyglycidol - surfactant complexes for coating magnetic particles, for dye adsorption from wastewater



Supramolecular nanomaterials with controlled optical properties for chemical detection and fluorescent imaging

### Research projects:

- *Laccase immobilization onto CS-PAA microspheres and its application for textile dyes biodegradation*, PN-III-P1-1.1-TE-2021-0418 (2022-2024), Anca Leonties;
- *Multi-stimuli responsive PAA decorated with host and guest units*, PN-III-P1-1.1-PD-2021-0169 (2022-2024), Ludmila Aricov.

## P6. Biomedical and environmental applications

*Molecular and structural studies on biologically relevant systems*, coordinated by **Dr. Gabriela Ionita**

*Non-uniform bio-binding processes*, coordinated by **Dr. Vlad Tudor Popa**

*Molecular and structural studies on biologically relevant systems*, coordinated by **Dr. Gabriela Ionita**

### Research fields

- Electron paramagnetic resonance studies on supramolecular systems, gels, proteins; spin labelling and synthesis of new molecular probes
- Fluorescence spectroscopy and chemiluminescence; biomedical and environmental applications
- Soft matter spectroscopy and computing simulations; nanomaterials synthesis and characterization
- Non-covalent interactions responsible for chirality induction - assessment of structural changes by an induced circular dichroism/molecular modeling approach
- Calorimetric analysis of phase transitions in polymeric micelles and gels; protein thermal denaturation in various interacting systems: natural and synthetic ligands/drugs, nanoparticles
- Tetrapyrrole compounds configured as markers and therapeutic agents in interaction with biological structures at the cellular level

### Members:

**Dr. Gabriela IONITA**, CS I - Head of laboratory ([ige@icf.ro](mailto:ige@icf.ro))  
2001 – Ph.D. in Chemistry, University of Bucharest, Ph.D. supervisor Acad. Prof. Dr. Victor Em. Sahini

2014 – Habilitation, School of Advanced Studies of the Romanian Academy

Research interests: EPR spectroscopy applied to supramolecular chemistry, protein interactions, gels; spin labelling and synthesis of new molecular probes

**Dr. Daniel George ANGELESCU**, CS I  
([dangelescu@hotmail.com](mailto:dangelescu@hotmail.com))

2004 – Ph.D. in Chemistry, University of Bucharest

2013 – Habilitation, School of Advanced Studies of the Romanian Academy

Research interests: Monte Carlo and molecular dynamics simulations of self-assembled macromolecular systems; coarse-grained simulations of polymer containing systems; nanomaterial synthesis; soft matter characterization; surface science

**Dr. Mariana VOICESCU**, CS II ([voicescu@icf.ro](mailto:voicescu@icf.ro))

2004 – Ph.D. in Chemistry, University POLITEHNICA of Bucharest

Research interests: molecular spectroscopy and chemiluminescence on systems of biological interest, with emphasis on fluorescence spectroscopy in protein analysis

**Dr. Iulia MATEI**, CS II ([iuliamatei@icf.ro](mailto:iuliamatei@icf.ro))

2011 – Ph.D. in Chemistry, University of Bucharest, Ph.D. supervisor Prof. Dr. Mihaela Hillebrand

Research interests: photophysical properties of molecular probes; non-covalent interactions in supramolecular host-guest systems; molecular spectroscopy; quantum chemical calculations

**Dr. Radu Petre SOCOTEANU**, CS III ([psradu@yahoo.com](mailto:psradu@yahoo.com))

2003 – Ph.D. in Chemistry, University of Bucharest, Ph.D. supervisor Prof. Dr. Constantin Patroescu

Research interests: markers and therapeutic agents in interaction with biological structures at cellular level

**Dr. Aurica PRECUPAS**, CS III ([aprecupas@icf.ro](mailto:aprecupas@icf.ro))

2011 – Ph.D. in Chemistry, University of Bucharest, Ph.D. supervisor Prof. Dr. Mihaela Hillebrand

Research interests: calorimetric analysis applied to protein interactions with natural and synthetic ligands; nanoparticles; molecular docking

**Dr. Florenta Daniella SAVONEA**, CS III

2006 – Ph.D. in Chemistry, University of Bucharest, Ph. D. supervisor Prof. Dr. Elena Volanschi

Research interests: EPR spectroscopy applied to colloidal systems and mesoporous materials

**Dr. Sorin MOCANU**, CS ([smocanu@icf.ro](mailto:smocanu@icf.ro))

2019 – Ph.D. in Chemistry, School of Advanced Studies of the Romanian Academy, Ph.D. supervisor Dr. Gabriela Ionita

Research interests: synthesis of dual (paramagnetic and fluorescent) molecular probes; interactions in supramolecular host-guest systems

**Alexandru Vincentiu Florian NECULAE**, ACS, Ph.D. student ([aniculae@icf.ro](mailto:aniculae@icf.ro))

Ph.D. student, Ph.D. thesis “Thermo-responsive systems investigated by electron paramagnetic resonance spectroscopy and calorimetric methods”, under the supervision of Dr. Gabriela Ionita

### Research Equipment

<http://erris.gov.ro/EPR-group>

ESR spectrometer (JEOL FA-100 X-band) equipped with a variable temperature controller and an irradiation lamp

Spectrofluorometer (JASCO-6500 equipped with an epifluorescence accessory)

UV-Vis spectrophotometers (JASCO V-630, PERKIN ELMER Lambda 35 equipped with an integrating sphere)

Luminometer (Promega GloMax 20/20)

Pedestal SuperServer Systems (Supermicro)

Workstation/PLATFORM Intel Server System 5U Pedestal

### Selected research projects

- Exploratory research project, UEFISCDI, PN-III-P4-ID-PCE-2016-0734/2017-2019: “Soft interactions in polymer and hybrid hydrogels investigated by electron paramagnetic resonance spectroscopy” (Dr. G. Ionita)

- Experimental demonstrative project, UEFISCDI, PN-III-P2-2.1-PED-2016-0187/2017-2019: “An experimental approach using electron paramagnetic resonance spectroscopy on tears analyses for optimal treatment of dry eye syndrome associated with keratoconus disease” (Dr. G. Ionita)

- Research project for young research teams, UEFISCDI, PN-II-RU-TE-2012-3-0036/2013-2016: “Structure, association and phase stability of complexes containing (bio)macromolecules investigated by Monte Carlo simulations” (Dr. D. Angelescu)

- Research project for young research teams, UEFISCDI, PN-II-RU-TE-2012-3-0055/2013-2016: “Flavone - Protein Systems Involved in Oxidative Stress Probed by Advanced Spectroscopic Methods” (Dr. M. Voicescu)

### Publications

1. M. M. Constantin, C. G. Corbu, S. Mocanu, E. I. Popescu, M. Micutz, T. Staicu, R. Șomoghi, B. Trica, V. T. Popa, A.

Precupas, I. Matei, G. Ionita, *Model systems for evidencing the mediator role of riboflavin in the UVA cross-linking treatment of keratoconus*, *Molecules* 27, 190 (2022) IF 4.412.

2. E. I. Popescu, L. Aricov, S. Mocanu, I. Matei, E. Hristea, R. Baratoiu, A. Leonties, C. Petcu, E. Alexandrescu, G. Ionita, *Subtle influence on alginate gel properties through host-guest interactions between covalently appended cyclodextrin and adamantane units*, *New Journal of Chemistry* 45, 8083-8091 (2021) (IF 3.591).

3. R. M. Visan, A. R. Leonties, L. Aricov, V. Chihai, D. G. Angelescu, *Polymorphism of chitosan-based networks stabilized by phytate investigated by molecular dynamics simulations*, *Physical Chemistry Chemical Physics* 23, 22601-22612 (2021) (IF 3.676).

4. M. Voicescu, O. Craciunescu, D. G. Angelescu, R. Tatia, L. Moldovan, *Spectroscopic, molecular dynamics simulation and biological studies of Flavin MonoNucleotide and Flavin Adenine Dinucleotide in biomimetic systems*, *Spectrochimica Acta A* 246, 118997 (2021) (IF 4.098).

5. A. Precupas, R. Sandu, A. V. F. Neculae, A. Neacsu, V. T. Popa, *Calorimetric, spectroscopic and computational investigation of morin binding effect on bovine serum albumin stability*, *Journal of Molecular Liquids* 333, 115953 (2021) (IF 6.165).

6. R. P. Socoteanu, R. Boscencu, G. Manda, M. Anastasescu, I. V. Neagoe, I. Ferreira Machado, O. Dinca, A. Bucur, L. F. Vieira Ferreira, *Morphologic evaluation of some promising A3B porphyrinic type compounds designed for theranostic applications in cancer*, *Chemical Physics* 544, 111115 (2021) (IF 2.348).

7. L. F. Vieira Ferreira, I. Ferreira Machado, A. Gama, F. Lochte, R. P. Socoteanu, R. Boscencu, *Surface photochemical studies of nano-hybrids of A3B porphyrins and Fe3O4 silica-coated nanoparticles*, *Journal of Photochemistry and Photobiology A: Chemistry* 387, 112152 (2021) (IF 4.291).

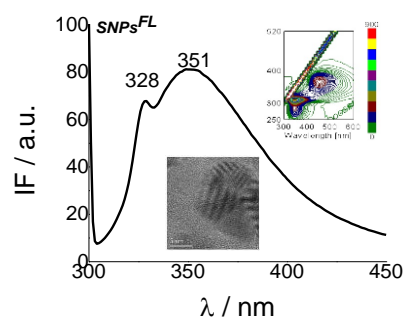
8. G. Ionita, S. Mocanu, I. Matei, *Conformational preferences of TEMPO type radicals in complexes with cyclodextrins revealed by a combination of EPR spectroscopy, induced circular dichroism and molecular modeling*, *Physical Chemistry Chemical Physics* 22, 12154-12165 (2020) (IF 3.676).

9. D.G. Angelescu, *Structural behavior of amphiphilic polyion complexes interacting with saturated lipid membranes investigated by coarse-grained molecular dynamic simulations*, *RSC Advances* 10, 39204 (2020) (IF 3.361).

10. S. Mocanu, G. Ionita, I. Matei, *Solvatochromic characteristics of dansyl molecular probes bearing alkyl diamine chains*, *Spectrochimica Acta A* 237, 118413 (2020) (IF 4.098).

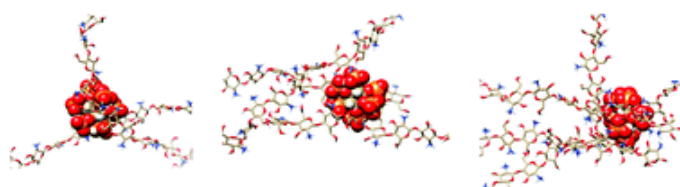
## Highlights

- A fluorescent silver nano-structured system developed by chemical reduction of aqueous AgNO<sub>3</sub> solution by Tryptophan, using Dextran 70 as stabilizing agent (SNPs<sup>FL</sup>).
- Multi-twined nanoparticle, with the size within 15-40 nm,  $\lambda_{em} = 346$  nm, fluorescence quantum yield  $\Phi = 0.034$  and the integrated fluorescence lifetime,  $\tau = 1.82$  ns.
- The results are relevant in using SNPs<sup>FL</sup> as a potential marker/emissive system to solve various biological barriers in humans, like drug release and protein structure.



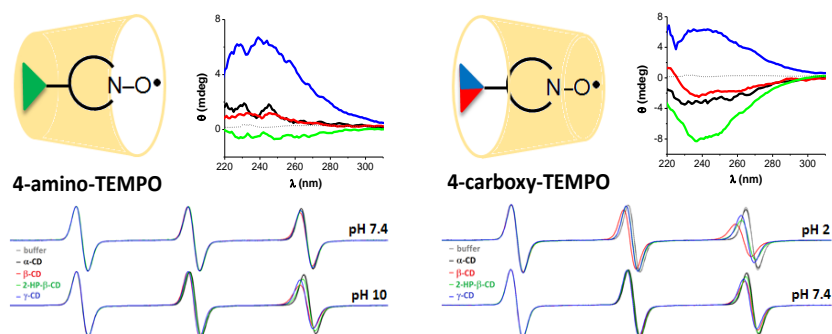
M. Voicescu et al., *J. Fluoresc.*, DOI: 10.1007/s10895-019-02411-2, 2019.

Chitosan hydrogels were synthesized using the phytate anion as crosslinking agent. The physical crosslinking pattern and the dynamics of the system were investigated by molecular dynamics. The circular distribution of cross-linkable phosphates regulates the nearly isotropic orientation of chitosan chains and phytate at the junction. The variety of topological crosslinking demonstrates the phytate ion's potential for developing chitosan-based hydrogels with improved structural attributes.



R.M. Visan, et al., *Phys. Chem. Chem. Phys.* DOI: 10.1039/D1CP02961D, 2021.

- Inclusion complexation of TEMPO-type EPR spin probes with cyclodextrins determines the appearance of induced chirality. The type and protonation state of the substituent linked to the TEMPO structure influence the affinity of the paramagnetic group for the cyclodextrin cavity.



G. Ionita, et al., *Phys. Chem. Chem. Phys.*, DOI: 10.1039/D0CP01937B, 2020.



## Nonuniform bio-binding processes

Coordinator: **Dr. Vlad Tudor Popa**

### Outline:

The project is devoted to various manifestations of the general phenomenon of nonuniformity in chemical, biochemical and biological processes. The contribution of binding, as a crucial step (component) of bio-reactivity, is specially studied.

### Key research fields:

- 1) Microcalorimetric, spectroscopic (CD, DLS, UV-Vis) and computational (docking, MD) investigation of serum proteins thermal denaturation / aggregation in interaction with natural and synthetic ligands / drugs, nanoparticles and polymeric varieties (micelles, gels)
- 2) Thermodynamic estimation (binding constant, partition coefficient, Gibbs free energy, enthalpy, entropy) of various anticancer drugs - surfactant micelles binding: a prerequisite stage for a comprehensive understanding of anticancer drug - biomembranes interaction.
- 3) Enhancing drugs bioavailability via inclusion complexation with pharmaceutical application. Solid state complexes characterization by thermal analysis, FTIR, XRD. Binding - release processes evaluation via pharmacokinetics.
- 4) Microcalorimetric evaluation of bacterial and fungal growth in interaction with various natural and synthetic antibiotics and nanoparticles. Mechanistic contribution of the binding step to the overall growth kinetics.

### Key Members (according with the above research fields):

- 1) Dr. Aurica Precupas, CSIII ([aprecupas@icf.ro](mailto:aprecupas@icf.ro))
- 2) Dr. Mirela Enache, CSII, ([menache@icf.ro](mailto:menache@icf.ro))
- 3) Dr. Adina Magdalena Musuc, CSII, ([amusuc@icf.ro](mailto:amusuc@icf.ro))
- 4) Dr. Vlad Tudor Popa, CSI, ([vtpopa@icf.ro](mailto:vtpopa@icf.ro))

### Other research collaborators:

- Dr. Gabriela Ionita, CSI ([ige@icf.ro](mailto:ige@icf.ro))  
Dr. Irina Atkinson, CSII, ([iatkinson@icf.ro](mailto:iatkinson@icf.ro))  
Dr. Romica Sandu, CSIII ([rsandu@icf.ro](mailto:rsandu@icf.ro))  
Dr. Anca Leonties, CSIII ([aleonties@icf.ro](mailto:aleonties@icf.ro))  
Dr. Ana Maria Toader, CSIII ([amtoader@icf.ro](mailto:amtoader@icf.ro))  
Dr. Andreea Neacsu, CS ([addneacsu@icf.ro](mailto:addneacsu@icf.ro))

### Main research equipment:

<https://eeris.eu/ERIF-2000-000U-1234>



Jasco V-550 UV-VIS spectrophotometer + Jasco ETC-505T cell-temperature controller

### Research cooperation:

“Carol Davila” University of Medicine and Pharmacy  
University of Bucharest  
“Cantacuzino” National Institute  
Institute of Biology of the Romanian Academy

### Selected publications:

- 1.1) A. Precupas, R. Sandu, A.V.F. Neculae, A. Neacsu, V.T. Popa, *Calorimetric, spectroscopic and computational investigation of morin binding effect on bovine serum albumin stability*, J. Mol. Liq. 333, 115953 (2021).
- 1.2) A. Precupas, V.T. Popa, *Microcalorimetric investigation of ligand binding to BSA and its influence on the protein stability, in Bovine Serum Albumin. Properties and Applications*, Nova Science Publisher, New York 157–197 (2020).
- 1.3) A. Precupas, A. Neacsu, A. R. Leonties, R. Sandu, V.T. Popa, *Gallic acid influence on bovine serum albumin thermal stability*, New J. Chem. 43, 3891-3898 (2019).
- 2.1) M. Enache, A.M. Toader, M.I. Enache, *Mitoxantrone – surfactant interactions: a physicochemical overview*, Molecules 21 (10), 1356 (2016).
- 2.2) M. Enache, A.M. Toader, V. Neacsu, G.E. Ionita, M.I. Enache, *Spectroscopic investigation of the interaction of the anticancer drug mitoxantrone with sodium taurodeoxycholate (NaTDC) and sodium taurocholate (NaTC) bile salts*, Molecules 22 (7), 1079 (2017).
- 2.3) M. Enache, A.M. Toader, *Insights into molecular interaction of antitumor drug mitoxantrone with anionic surfactant sodium dodecyl sulfate at different temperatures*, Journal of Surfactants and Detergents 21, 31-41 (2018).
- 3.1) A.M. Musuc, V. Anuta, I. Atkinson, V.T. Popa, I. Sarbu, C. Mircioiu, G.A. Abdalrb, M.A. Mitu, E.A. Ozon, *Development and Characterization of Orally Disintegrating Tablets Containing a Captopril-Cyclodextrin Complex*, Pharmaceutics 12(8), 744 (2020).
- 3.2) A.M. Musuc, V. Anuta, I. Atkinson, I. Sarbu, V.T. Popa, C. Munteanu, C. Mircioiu, E.A. Ozon, G.M. Nitulescu, M.A. Mitu, *Formulation of chewable tablets containing carbamazepine- $\beta$ -cyclodextrin inclusion complex and F-melt disintegration excipient: the mathematical modeling of the release kinetics of carbamazepine*, Pharmaceutics 13(6), 915 (2021).
- 4.1) V.T. Popa, *Monod’s Bacterial Growth Model. Kinetic Arguments for ‘Simple, But Not Too Simple’, in Prokaryotes: Physiology, Biochemistry and Cell Behavior*, Nova Science Publisher, New York 221-246 (2014).
- 4.2) M.G. Popa, A.A. Muntean, V.T. Popa, C.C. Dragomirescu, I. Eremia, S. Nica, M.I. Popa, C. Cirstoiu, *Microcalorimetric growth evaluation of Candida albicans in different conditions*, Rom Biotechnol Lett. 25(6), 2140-2147 (2020).
- 4.3) M.I.G. Popa, A. Cursaru, B. Serban, B. Crețu, A.A. Muntean, V.T. Popa, M.C. Chifiriuc, C. Cirstoiu, *Microcalorimetry - Versatile Method of Describing Bacterial Growth*, Applied Sciences 11(20), 9740 (2021).
- 4.4) M. Popa, A. Cursaru, V. Popa, A. Munteanu, B. Șerban, B. Crețu, S. Iordache, C. G. Smarandache, C. Orban, C. Cirstoiu, *Understanding orthopedic infections through a different perspective: Microcalorimetry growth curves*, Experimental and Therapeutic Medicine 23(4), 1-6 (2022).

## P7. Science of surfaces and thin layers

*Study of multifunctional semiconductor oxide systems,*

coordinated by **Dr. Mariuca Gartner**

*Transition metal tungstates with multiple applications,*

coordinated by **Dr. Simona Somacescu**

*Functionalization of the solid surface by chemical and structural modification in solution,* coordinated by **Dr. Jose Maria Calderon Moreno**

*Multifunctional materials based on TiO<sub>2</sub>, ZnO, ZnSe and SiO<sub>2</sub> for the degradation of some organic compounds and bioremediation processes,* coordinated by **Dr. Mihai Anastasescu**

### Research fields

Multifunctional oxidic semiconductor for TCO applications

Functionalization of the solid surface with organic components

Sensitive materials used in sensor devices

Interfacial properties

Optical properties (UV to Far IR spectral range)

Vibrational properties (IR and Raman)

Material Characterization

Nanomaterials

Thin Films and Nanotechnology

### Team Members

**Dr. Mariuca Gartner**, CS I, 1988 – PhD in Physics, IFTM, Ph.D. supervisor Prof. Dr. Margareta Giurgea. Post Doc: Institute of Solid State Physics in Bremen, Germany: (i) DAAD research scholarship (2003); (ii) DFG research stages (2005-2008 and 2008-2012). *Doctoral supervisor (9 Ph.D.)*.

Email: [mgartner@icf.ro](mailto:mgartner@icf.ro)

**Dr. Mihai Anastasescu**, CS I, 2005 – PhD in Physics, Romanian Academy-ICF, Ph.D. supervisor Dr. Nicolae Ionescu. Post Doc: (i) DAAD research scholarship (1999-2000) at the Institute of Physical and Theoretical Chemistry in Bonn, Germany; (ii) DFG research stage (10.2009) at the Institute of Solid State Physics in Bremen, Germany.

Email: [manastasescu@icf.ro](mailto:manastasescu@icf.ro)

**Dr. Jose Maria Calderon Moreno**, CS I, 1995 – PhD in Physics, University of Seville, Ph.D. supervisor Dr. Arturo Dominguez. Post Doc: University of London, Queen Mary College. Email: [calderon@icf.ro](mailto:calderon@icf.ro)

**Dr. Simona Somacescu**, CS I, 2009 – PhD in Chemistry, Romanian Academy-ICF, Ph.D. supervisor Dr. Viorica Parvulescu. Email: [ssimona@icf.ro](mailto:ssimona@icf.ro)

**Dr. Hermine Stroescu**, CS III, 2013 - PhD in Chemistry, Romanian Academy-ICF, Ph.D. supervisor Dr. Mariuca Gartner. Email: [hstroescu@icf.ro](mailto:hstroescu@icf.ro)

**Dr. Madalina Nicolescu**, CS III, 2010 - PhD in Chemistry, Romanian Academy-ICF, Ph.D. supervisor Dr. Mariuca Gartner. Email: [mnicolescu@icf.ro](mailto:mnicolescu@icf.ro)

**Dr. Paul Chesler**, CS III, 2017 - PhD in Chemistry, Romanian Academy-ICF, Ph.D. supervisor Dr. Mariuca Gartner. Email: [pchesler@icf.ro](mailto:pchesler@icf.ro)

**Dr. Mariana Chelu**, ACS, 2022 - PhD in Chemistry, Romanian Academy-ICF, Ph.D. supervisor Dr. Mariuca Gartner. Email: [mchelu@icf.ro](mailto:mchelu@icf.ro)

**PhD student Daiana Mitrea**, ACS, 2019 - present, Ph.D. supervisor Prof. Dr. Viorel Cîrcu. Email: [dmitrea@icf.ro](mailto:dmitrea@icf.ro)

### Research Equipment:

<https://eeris.eu/ERIF-2000-000B-0833>

UV-VIS-NIR and IR ellipsometer;

AFM and STM in air;

Fluorescence Spectrophotometer;

SEM & EDX;

Raman Spectrometer;

Hall measurements;

Piezoelectric measurements



IR ellipsometer.

### International collaboration

Center for Energy Research, Budapesta, Ungaria, Pannonia University, Budapesta; Tyndall Institute, Cork, Irlanda; Instituto de Tecnología Química (ITQ), Valencia, Spania; Institut für Physikalische und Theoretische Chemie, Tuebingen, Germany; Purdue University, US; National Center for Nanomaterials, Pohang, Coreea de Sud; IMDEA materials Institute, Madrid; Universitat Politecnica de Catalunya, Barcelona, Spania.

### National collaboration with research institutes

Transilvania University Brasov; IMT Bucharest, Romania; IFTM Bucharest, Romania; INFLRP Bucharest, Romania; National Institute for Materials Physics, Magurele, Romania; UPB - Polytechnic University of Bucharest; Institute of Biology (IBB) of the Romanian Academy; ICECHIM; University of Bucharest - Faculty of Biology.

**National collaborations with SRL:** ROMELGEN, Romania SRL, Bucuresti; NANOM Mems, SRL, Romania, Rasnov.

### Interacademic exchanges

- Institute of Solid State Physics, Sofia, Bulgaria 2018-2020, *Director Dr. M. Gartner*

- Institute for Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences Hungary 2019-2022, *Director Dr. M. Gartner*

### Selected research projects (2017-2022):

1. **BIOSCAF PCE 234/2021-2023** - "3D printed absorbable scaffold with prolonged biomechanical stability in human body fluids" *Director Dr. J. M. Calderon Moreno*
2. **VOC 2019-2022** - "Autonomous intelligent system for the detection of volatile organic compounds" - *Responsible ICF Dr. M. Gartner*, in collaboration with Hungary
3. **TECH4GREEN 2020-2022** - "Micro-nanotechnologies for greenhouse gas monitoring" - Project *Director Dr. M. Gartner*
4. **SENSIS 2018-2020** - "Sensors and integrated electronic and photonic systems for security of people and infrastructure", *Director for theme 4, Dr. M. Gartner and responsible for theme 2*
5. **PIEZO HARV, 2017-2019** "Energy efficient generator for hard-to-reach sensor networks and low power devices for aerospace applications" – *Responsible ICF Dr. M. Gartner*
6. **BIONANOTUBENZ 2017-2018** "Novel hybrid structures based on enzymes/1D oxide nanostructures for soil fertility increasing via accelerating bio-degradation rate-" PN-III-P2-2.1-PED-2016-1395 – *Director Dr. M. Anastasescu*
7. **WaterSafe, M-ERA.NET-2016-2018** "Sustainable autonomous system for nitrites/nitrates and heavy metals monitoring of natural water sources", Project *Director Dr. M. Gartner*

8. **PiezoMEMS**, M-ERA.NET 2015-2018, “Piezoelectric MEMS for efficient energy harvesting”, **Responsible ICF Dr. M. Gartner**
9. **eNose** 2014-2017 “Instrument de tip nas electronic pentru detectia concentratiilor scazute de gaze explozive si poluante” **Director Dr. M. Gartner**

#### Selected papers:

1. S. Simeonov, A. Szekeres, D. Spassov, M. Anastasescu, I. Stanculescu, M. Nicolescu, E. Aperathitis, M. Modreanu, M. Gartner, *Investigation of the Effects of Rapid Thermal Annealing on the Electron Transport Mechanism in Nitrogen-Doped ZnO Thin Films Grown by RF Magnetron Sputtering*. *Nanomaterials* 12, 19 (2021) (IF = 5.076/2020)
2. M. Gartner, M. Stoica, M. Nicolescu, H. Stroescu, **Invited review: The ellipsometry versatility in the study of sol-gel films**. *J. Sol-Gel Sci. Technol.* 98, 1–23 (2021).
3. Ş. Neaţu, F. Neaţu, I.M. Chirica, I. Borbáth, E. Tálas, A. Tompos, S. Somacescu, P. Osiceanu, M.A. Folgado, A.M. Chaparro, et al. *Recent progress in electrocatalysts and electrodes for portable fuel cells*. *J. Mater. Chem. A* 9, 17065–17128 (2021) (IF = 12.732)
4. Ş. Neaţu, F. Neaţu, V.C. Diculescu, M.M. Trandafir, N. Petrea, S. Somacescu, F. Krumeich, J.T.C. Wennmacher, A.J. Knorpp, J.A. van Bokhoven, et al. *Undoped SnO<sub>2</sub> as a Support for Ni Species to Boost Oxygen Generation through Alkaline Water Electrolysis*. *ACS Appl. Mater. Interfaces* 12, 18407–18420 (2020) (IF = 9.229)
5. A. Stanoiu, C. Ghica, S. Somacescu, A.C. Kuncser, A.M. Vlaicu, I.F. Mercioniu, O.G. Florea, C.E. Simion, *Low temperature CO sensing under infield conditions with in doped Pd/SnO<sub>2</sub>*. *Sensors Actuators B Chem.* 308, 127717 (2020) (IF = 7.46)
6. A. Slav, I. Dascalescu, A.M. Lepadatu, C. Palade, N.C. Zoita, H. Stroescu, S. Iftimie, S. M. Lazanu, M. Gartner, D. Buca, et al. *GeSn/SiO<sub>2</sub> Multilayers by Magnetron Sputtering Deposition for Short-Wave Infrared Photonics*. *ACS Appl. Mater. Interfaces* 12, 56161–56171 (2020) (IF = 9.229)
7. G. Patrinoiu, J.M. Calderon-Moreno, S. Somacescu, A.M. Musuc, T. Spataru, P. Ionita, O. Carp, *Rational Functionalization Towards Redox-Active TEMPO Stable Free-Radical-Hydrochar Composites*. *ChemSusChem* 14, 2042–2049 (2021) (IF = 8.928)
8. C. Lete, M. Chelu, M. Marin, S. Mihaiu, S. Preda, M. Anastasescu, J.M. Calderón-Moreno, S. Dinulescu, C. Moldovan, M. Gartner, *Nitrite electrochemical sensing platform based on tin oxide films*. *Sensors Actuators, B Chem.* (2020), (IF = 7.460)
- 9 Staerz, A.; Somacescu, S.; Epifani, M.; Kida, T.; Weimar, U.; Barsan, N. *WO<sub>3</sub>-Based Gas Sensors: Identifying Inherent Qualities and Understanding the Sensing Mechanism*. *ACS Sensors* 2020, 5, 1624–1633 (IF = 7.711)
10. M. Chelu, H. Stroescu, M. Anastasescu, J.M. Calderon-Moreno, S. Preda, M. Stoica, Z. Fogarassy, P. Petrik, M. Gheorghie, C. Parvulescu, et al. *High-quality PMMA/ZnO NWs piezoelectric coating on rigid and flexible metallic substrates*. *Appl. Surf. Sci.* 529, 147135 (2020) (IF = 6.707)
11. N. Spătaru, J.M. Calderon-Moreno, P. Osiceanu, T. Kondo, C. Terashima, M. Popa, M.M. Radu, D. Culiţă, L. Preda, M.A. Mihai, et al. *Conductive diamond powder inclusion in drop-casted graphene for enhanced effectiveness as electrocatalyst substrate*. *Chem. Eng. J.* 402, 126258 (2020) (IF = 13.07/2020)
12. S. Somacescu, N. Cioatera, P. Osiceanu, J.M. Calderon-Moreno, C. Ghica, F. Neaţu, M. Florea, *Bimodal mesoporous*

*NiO/CeO<sub>2</sub>-δ-YSZ with enhanced carbon tolerance in catalytic partial oxidation of methane—Potential IT-SOFCs anode*. *Appl. Catal. B Environ.* 241, 393–406 (2019) (IF = 16.79/2019)

#### Highlights

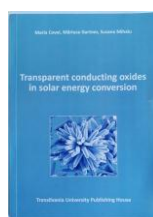
**Papers cited more than 200 times**

- **Deposition of gold nanoparticles on silica spheres: a sonochemical approach**, VG Pol, A Gedanken, J Calderon-Moreno, published in *Chemistry of Materials* 15 (5), 1111-1118 (2003) **has been cited 365 times**.
- **TiO<sub>2</sub>(Fe<sup>3+</sup>) nanostructured thin films with antibacterial properties**, Trapalis, CC; Keivanidis, P; Kordas, G; M. Zaharescu, M. Crisan, A. Szatvanyi, M. Gartner, published in *Thin Solid Films*, Volume: 433 Issue: 1-2 Pages: 186-190 (2003) **has been cited 266 times**.
- **Hydrothermal Processing of High-Quality Multiwall Nanotubes from Amorphous Carbon**, JM Calderon Moreno, M Yoshimura, published in *Journal of the American Chemical Society* 123, 741-742 (2001) **has been cited 206 times**.

#### Figure from the paper on the journal cover



Cover of the Materials Research Bulletin journal:  
XTEM and SAED on TiO<sub>2</sub>:Nb film from our paper published in: *Materials Research Bulletin*, 74 (2016) 15–20



M. Covei, M. Gartner, S. Mihaiu, *“Transparent conducting oxides in solar energy conversion”*  
Editura Universitatii Transilvania, 2015  
ISBN 978-606-19-0626-0

#### Books

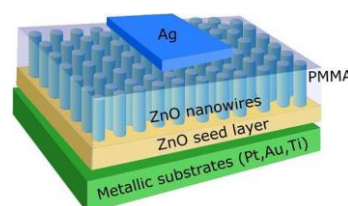


P. Chesler, C. Vladut, *“Senzori chimici rezistivi”*  
Editura Berg, August 2020,  
ISBN 978-606-9036-60-0

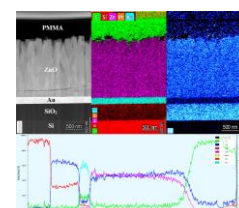
**Unique device nationwide: IR ellipsometer**- which offers information on Chemical Composition via Molecular Bond Vibrational Absorptions

For thin-films, IR ellipsometry offers increased sensitivity over FTIR and yields quantitative values for optical constants, n and k. This technique has great sensitivity to epitaxial layer thickness and substrate doping concentration, which are not seen using UV-VIS wavelengths.

**Sensitive materials** used in sensor devices to detect harmful components from air (Co, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>3</sub>H<sub>8</sub>, humidity) and from water (nitrites, nitrates, and heavy metals) were developed. The practical realization of the sensors and of the portable mini-devices was made in collaboration with IMT / ROMELGEN / NANOM / MFK-Hungary.



ICF – Romania



MFK – Hungary

## Technological Transfer Center (CTT-ICF)

CTT-ICF aims to use the results obtained from IPC's research activities to be implemented by economical operators. This will be realized by collaboration with educational and RDI units or other entities providing scientific and technological consultancy and assistance in IPC's areas of expertise. It is intended to use the IPC patents and to offer innovative concrete solutions accordingly to the requirements and needs of the market.

**Members:** Dr. Venera Giurcan, Dr. Viorica Parvulescu, Dr. Cornelia Marinescu, Dr. Razvan State.

### *The role of the CTT-ICF:*

- Promoting the offer of own services;
- Guidance and support for IPC researchers to participate at RDI projects funded from national or international sources;
- Managing the protection of intellectual property rights generated by IPC researchers;
- Promoting the activity of innovation and technological transfer;
- Negotiating research contracts, service contracts or partnership agreements with economical operators;
- Negotiating contracts for the transfer of intellectual property rights to the entities.

### *Objectives of the CTT-ICF:*

- Increasing the visibility of IPC's RDI activities;
- Development of new collaborations between CTT-ICF and economical operators to stimulate technology transfer;
- Increasing the degree of scientific and technological documentation;
- Increasing the technological absorption potential of economical operators;
- Attracting funds to increase the degree of innovation and to develop technology transfer;
- Increasing the number of patentable results at IPC level by ensuring efficient management of intellectual property rights;
- Promoting quality in research;
- Facilitate cooperation between R&D units, universities and economic agents (especially SMEs).

### *Activities of the CTT-ICF:*

- Information, technology watch, technology audit.
- Elaboration of studies and reports for SMEs or other entities.
- Providing consultancy on the exploitation of intellectual property rights.
- Providing consultancy and/or participation in partnership with other entities to national and international RDI programs and projects.
- Providing guidance on specific methodologies and technological level that can be applied/developed in industry and SMEs through concrete technological solutions or by using of IPC's patents.
- Identification of potential beneficiaries (SMEs, universities, research centers and institutes, industrial sectors, etc.) to achieve technological transfer.
- Actions to promote and increase the visibility of IPC RDI results.
- Determining the needs of potential customers to develop new innovative products.
- Organizing congresses, symposia, round tables, colloquia, workshops or exhibitions to attract new collaborations and potential beneficiaries.

### *CTT-ICF services:*

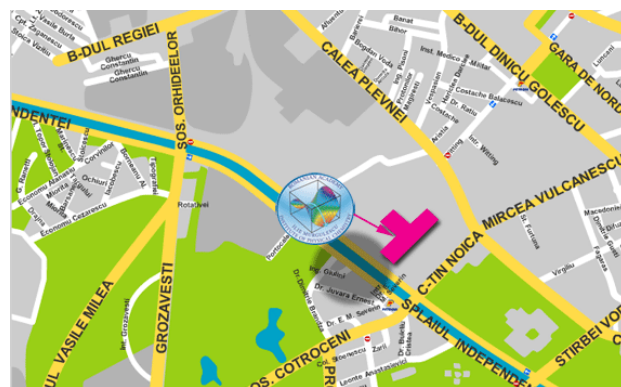
- Assistance and consultancy services for the exploitation of intellectual property rights.
- Assistance and consultancy for the implementation of innovative technology (technology audit, technological forecast, consultancy, documentation).
- Technology transfer services in the fields of IPC research activity.
- Assistance for obtaining funds from national and international programs.
- Assistance to organize colloquia, seminars, courses, conferences, scientific events and specialized exhibitions.
- Assistance and consultancy in setting up RDI partnerships and/or technology transfer between IPC and other entities.
- Assistance and consultancy for elaboration of technical (feasibility) studies.
- Assistance and consulting for development of experimental models and prototypes.

## PhD programs - School of Advanced Studies of the Romanian Academy

The institute organizes PhD programs in various fields of chemistry and physical chemistry: quantum chemistry, chemical thermodynamics and kinetics, electrochemistry and corrosion, colloid and surface science, material science and catalysis.

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