Arii tematice cercetare - Doctorat in Chimie - 2026
PhD research areas- Chemistry - 2026

Topic : **Heterotrispin complexes**
Name of supervisor: **acad. prof. univ. dr. Marius Andruh**
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Background information: Coordination compounds constructed from three different spin carriers (2p-3d-4f; 3d-4d-4f, 3d-3d'-4f, etc.) represent a new class of magnetic materials of high interest in modern chemistry and materials science. Such compounds are still rare, and their synthesis is challenging for chemists. Two types of systems will be designed: coordination compounds containing: (a) three different paramagnetic metal ions and (b) two different metal ions and a nitronyl-nitroxide radical. An important problem to be solved consists of the analysis of the factors that influence the synergy between the three spin carriers in order to improve the performances of the new magnetic materials (Single Molecule Magnets and Single Chain Magnets).

Special requirements : The candidate is expected to have at least background knowledge in coordination chemistry (synthesis of new ligands and complexes; crystallogenesis; characterization of the new compounds using various spectroscopic techniques (FTIR, NMR), molecular magnetism.

References

1. J. Ribas, Coordination Chemistry, Wiley, 2008.
2. M. Andruh, *Chem. Commun*., **2018**, *54*, 3559.
3. M. Andruh, *Dalton Trans*.,**2015**, *44*, 16633.
4. S. Demir, I.-R. Jeon, J. R. Long, T. D. Harris, *Coord. Chem. Rev*., **2015**, *289-290*, 149.
5. M. Zhu, L. Li, J.-P. Sutter, *Inorg. Chem. Front*., **2016**, *3*, 994.

Topics :
1. New stationary phases for ion exchange chromatography.
2. Non-conventional stationary phases for environmental analysis.

Name of supervisor: **prof. univ. dr. Irinel Adriana Badea**
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Background information: Nowadays the quality of water is a social concern even if the term "quality" is not very familiar to many people. You are thirsty, in a big city, in front of clear water running from a marvellous drinking fountain, and suddenly you see the notice: "Non-potable water". When you read them, it is not only frustration but resignation, too. And the question "Why?" arises without any chance of a direct answer. Small species in terms of both chemistry and biology sciences are responsible for the quality of water. No matter the purpose of the water, the term "good water" hides a huge scientific activity related to the monitoring of physical, chemical and biological properties. Usually, ion-exchange resins are the first choice for this purpose due to their ion-exchange capacity, good selectivity and effortless regeneration. In quest of the high selectivity of the ion-exchange process, new materials should be developed and characterized, and this is the aim of the topics proposed.

Special requirements: The candidate is expected to have at least background knowledge of Analytical Chemistry (level Master's degree)

Reference

1. Christian, G. D., Dasgupta, P. K., Schug, K.A. Analytical Chemistry, 7th Edition, Wiley Global Education, 2013.

Topic : **Biosensors based on nanostructure materials**

Name of supervisor: **prof. univ. dr. Camelia Bala**
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Background information: Biosensors are analytical devices that use a transducer and a biorecognition element in close contact to convert a biochemical event on the transducer surface into a measurable analytical signal. With the development of nanostructured materials, new possibilities have emerged for the creation of next-generation biosensors. Combining nanomaterials with the ability to control the design of the electrode interface at the nanoscale has resulted in novel biosensing platforms with improved capabilities. In recent years, biosensors made with different materials and working with different transducers have attracted considerable interest due to their numerous applications. This project focuses on developing biosensors that are highly sensitive and selective and can operate in complex media. These applications range from clinical labs, food analysis, and environmental monitoring to protein engineering, drug discovery, and security applications.

Special requirements: The candidate is expected to have a Master's degree in Chemistry, Biochemistry, Physics, or affine sectors. Previous experience in sensing, biosensing, and biomolecular assay development will be considered a strong asset. The candidates should be highly motivated to do research, communicative, creative, eager to learn, and able to work independently as well as part of a team.

References

1. A. P. F. Turner, Chem. Soc. Rev., 2013, 42, 3184.
2. KPR Castro, RNP Colombo, RM Iost, BGR da Silva, FN Crespilho, Anal. and Bioanal. Chem., 2023, 415(18), 3879.
3. S. Azzouzi, L. Rotariu, A. M. Benito, W. K. Maser, M. Ben Ali, C. Bala, Biosens. & Bioelectron, 2015, 69, 280.
4. L. Rotariu, F. Lagarde, N. Jaffrezic-Renault, C. Bala, TRAC-Trends in Analytical Chemistry, 2016, 79, 80.

Topic : **Affinity sensors**

Name of supervisor: **prof. univ. dr. Camelia Bala**

Background information: The topic addresses the sensors based on affinity reactions by integrating a biological material (e.g. cell receptors, antibodies, nucleic acids, etc.), a biologically derived material (e.g., recombinant antibodies, engineered proteins, aptamers, etc.) or a biomimetic analogue (e.g., synthetic receptors, biomimetic catalysts, combinatorial ligands, molecularly imprinted polymers, etc.) closely associated with or integrated within a physicochemical transducer, which may be optical (e.g. Surface Plasmon Resonance-SPR), electrochemical, piezoelectric or magnetic. The project will focus on the complementary intersection between molecular recognition, nanotechnology and supramolecular chemistry to improve the analytical performance and robustness of devices. The application will be driven by the label-free detection of low molecular weight molecules with application in medical diagnosis (point-of-care devices) and on-site detection of pollutants (food and environment monitoring).

Special requirements: The candidate is expected to have a Master's degree in chemistry, biochemistry, physics, or affine sectors. Previous experience in sensing, biosensing, and biomolecular assay development will be considered a strong asset. The candidates should be highly motivated to do research, communicative, creative, eager to learn, and able to work independently as well as part of the team.

References

1. M. Puiu, A. Idili, D. Moscone, F. Ricci, C. Bala, Chem. Commun., 2014, 50(64), 8962
2. M. Puiu, O.-M. Istrate, V. Mirceski, C. Bala, Analytical Chemistry, 2023, 95(44), 16185.
4. G. M. Danila, M. Puiu, L. Gabriel Zamfir, C. Bala, Analytical Chemistry, 2019, 91(23), 14812
5. M Puiu, V Mirceski, C. Bala, Current Opinion in Electrochemistry 2021, 100726

Topic: **Electrochemical sensors for monitoring biological molecules**

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Background information: Electrochemical sensors have attracted considerable interest due to their wide range of applications in pharmaceutical analysis, clinical diagnostics, experimental medicine, and other areas of interest, such as industry, food safety, cultural heritage, and environmental protection. These sensors are characterized by their affordability, quick response times, ease of manufacturing, and ability to detect multiple analytes simultaneously. In addition, electroanalytical techniques are useful for characterizing electrochemical systems. They allow us to study the reversibility and irreversibility conditions of reactions, determine if the process is diffusion- or surface-controlled, calculate some kinetic parameters, and quantitatively determine the electroactive compounds involved in the process. Electrochemical methods are appropriate and practical when used with suitable working electrode materials. Although various materials have been successfully used to develop electrochemical sensors, challenges remain. These include electrode surface fouling, interference from substances in complex matrices (such as biological ones) that affect selectivity, maintaining stability and reproducibility in complex environments, and achieving low detection limits.

Special requirements: The candidate should have a basic understanding of analytical chemistry and electrochemistry.

References:

1. G.D. Christian, P.K. Dasgupta, K.A. Schug, Analytical chemistry, 7th Edition, Wiley Global Education, 2013.
2. A.J. Bard, L.R. Faulkner, H.S. White, Electrochemical methods. Fundamentals and applications, 3rd Edition, John Wiley & Sons, 2022.
3. J. Wang, Analytical electrochemistry, 3rd Edition, John Wiley & Sons, 2006.
4. C.M.A. Brett, A.M. Oliveira Brett, Electrochemistry. Principles, methods and applications, Oxford University Press, 1993.

Topic: **Structure-Property Relationships in New Lanthanide Coordination Compounds and Materials.**

Name of supervisor: **Assoc. Prof. Dr. Marilena Ferbinteanu Cimpoesu**
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Background information: Lanthanide systems, or in other words, rare-earth compounds are nowadays in the hot spot of the vogue targeting materials with special properties, used various high-tech domains.[1] In this quest, there is a legitimate counterpart of academic interest, in synthesizing new chemical systems, from discrete complexes[2] to MOF-type systems[3] and finding the causal roots of their various physical features, in order to achieve property-design, with potential practical applications. Applying original synthetic routes, based on the control of ligand specific affinities and tuning lattice effects, we further focus on the structural chemistry of the resulting systems. In first instance, with crystallographic and spectroscopic facilities of the owned laboratory, we pay detailed attention to the stereochemical details of the coordination units and the non-covalent assembling in lattice.[4] The geometry factors are determinant to magnetic and optic properties,[4] by leverages accounted in the general frame of ligand-field phenomenology.[5] The magnetic properties and special opto-electronic manifestations, such as luminescence[5] of the interesting newly synthesized systems can be further studied, at instrumental advanced level by national and international cooperation with other chemistry and physics laboratories. We are interested also in the modelling of properties, the primary level of simple methods being tractable in the infrastructure and know-how of the laboratory, the advanced levels benefiting also from specialized cooperation. In this way, we study in depth each system, practicing a rich interdisciplinary approach that enhances the value of our synthetic strategies and endeavours.

Special requirements from the students: The candidate should hold a MSc degree in chemistry. Applicants with strong skills in inorganic synthesis, materials chemistry and crystallography are encouraged to apply.

The candidate should be highly motivated and strive towards scientific excellence, be ambitious and able to work independently. The applicant should be confident in both written and spoken English.

References

1. A.G. Jr. Bispo*, Coord. Chem Rev.* **2025**, *537*, 216685.
2. M. Ferbinteanu, T. Kajiwara, K.Y. Choi, H. Nojiri, A. Nakamoto, N. Kojima, F. Cimpoesu, Y. Fujimura, S. Takaishi, M. Yamashita, *J. Am. Chem. Soc*., **2006**, *128*, 9008.
3. M. Ferbinteanu, F. Cimpoesu, S. Tanase, *Structure and Bonding* **2015**, *163*, 185.
4. F. Cimpoesu, F. Dahan, S. Ladera, M. Ferbinteanu, J.-P. Costes, *Inorg. Chem.* **2012**, *51*, 11279.
5. M.V. Putz, F. Cimpoesu, M. Ferbinteanu, *Structural Chemistry Principles, Methods, and Case Studies*. Springer; **2018**.

Topic: **Molecular Bistability in Coordination Compounds**

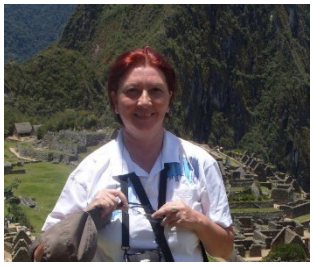
Name of supervisor: **Assoc. Prof. Dr. Marilena Ferbinteanu Cimpoesu**

Background information: This project explores molecular bistability in coordination compounds as a source of switchable functional properties. The ability of a system to function in distinct states, controlled by an accessible external parameter (temperature, pressure, light, fields) is a key functionality in the technology of processing and storing information. New generations of technologies aiming to go beyond actual silicon-based era of computers represent an explicit goal in the actual challenges, to which the coordination chemistry offers valuable material candidates and case-studies illuminating the underlying mechanisms. The research will address spin crossover,[1,2] magnetic switching,[3] phase transitions, chromotropism, and isomerization phenomena. The main objective is to establish structure–property correlations enabling control and tuning of bistable behavior.[4] The candidate will design and synthesize responsive coordination systems and study their structural, magnetic, and spectroscopic responses to external stimuli. Crystal engineering approaches will be employed to stabilize targeted switching properties.[5] The outcomes are expected to support the development of multifunctional materials for sensing, memory, and smart devices. The project sits at the interface of coordination chemistry, solid-state chemistry, and molecular materials science. With the focus on structural details, at molecular and supramolecular level, we consider non-routine crystallographic procedures, going beyond standard routine, by enriched data collection and advanced handling of the experimental electron-density maps.

Special requirements from the students: The candidate should hold a MSc degree in chemistry. Candidates with strong training in inorganic and physical chemistry are encouraged to apply. The candidate is expected to have knowledge in coordination chemistry, physical chemistry, organic synthesis, to be familiarized with various spectroscopic techniques (UV-Vis, FTIR, NMR). Experience with crystallography is considered advantageous. The candidate should be highly motivated and strive towards scientific excellence, be ambitious and able to work independently. The applicant should be confident in both written and spoken English.

References

1. S. Wang, M. Ferbinteanu, C. Marinescu, A. Dobrinescu, Q-D. Ling, W. Huang, *Inorg. Chem.* **2010**, *49*(21), 9839.
2. H. Zhu, X-T. He, C.-X. Xu, H.-Z. Zhang, C-Y. Qin, Y-H. Li, M. Ferbinteanu, C. Tang, S. Wang, *Inorg. Chem. Comm.*, **2026**, 116361.
3. M. Ferbinteanu, H. Miyasaka, W. Wernsdorfer, K. Nakata, K. Sugiura, M. Yamashita, C. Coulon, R. Clerac, *J. Am. Chem. Soc.* **2005**, *127*, 3090.
4. M.V. Putz, F. Cimpoesu, M. Ferbinteanu, *Structural Chemistry Principles, Methods, and Case Studies*. Springer; **2018**.
5. E. Fernandez-Bartolome, A. Martinez-Martinez, E. Resines-Urien, L. Piñeiro-Lopez, J.S. Costa, *Coord. Chem. Rev.* **2022**, *452*, 214281.



Topic : **Macro-and microemulsions as drug delivery systems for hydrophobic active substances**

Name of supervisor:**Assoc. prof. dr. habil. Ludmila Otilia Cinteză**
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Background information: Macroscopic emulsions and microemulsions are two of the colloidal systems widely recognized for their advantages in drug delivery applications. Microemulsions in particular, due to their thermodynamic or kinetic stability, high solubilization capacity, and nanometric droplet size, represent a modern solution for the delivery of poorly water-soluble bioactives. Their small droplet size leads to a large interfacial surface area, which enhances drug encapsulation efficiency, stabilizes labile compounds, and facilitates controlled release. These features make them especially valuable for pharmaceutical and cosmeceutical applications.

This PhD research will focus on the formulation, optimization, and detailed physicochemical characterization of microemulsions using natural (vegetable) oils and surfactants that are biocompatible, biodegradable, and safe for human use. The goal is to design next-generation delivery systems that are not only effective but also sustainable and environmentally friendly. A systematic approach will be used to study the role of oil phase composition, surfactant-to-co-surfactant ratios, and aqueous phase parameters on emulsion or microemulsion type (oil-in-water vs. water-in-oil), droplet size distribution, stability, and rheological behavior.

The potential of these systems extends beyond traditional pharmaceuticals. Their application in “green” or clean-label cosmeceuticals aligns with current consumer trends favoring natural and sustainable products. Overall, the research aims to contribute to the development of safe, high-performance colloidal systems with significant translational value in the health and personal care sectors.

Special requirements : The candidate is expected to have a Master's degree in chemistry, pharmacy, biochemistry, chemical engineering, or affine sectors. A background knowledge in colloidal chemistry is a plus.

Strong communication skills, willingness to learn and ability to work within a team are highly appreciated.

References

1. M. Gradzielski, M. Duvail, P. M. De Molina, M. Simon, Y. Talmon, T. Zemb, Chem. Rev. 2021, 121, 5671.
2. E. S. T. Egito, L. Amaral-Machado, E. N. Alencar, A. G. Oliveira, Drug Deliv. Transl. Res. 2021, 11, 2108.
3. C. Scomoroscenco, M. Teodorescu, A. Raducan, M. Stan, S. N. Voicu, B. Trica, C. M. Ninciuleanu, C. L. Nistor, C. I. Mihaescu, C. Petcu, L. O. Cinteza, Pharmaceutics 2021, 13, 505.
4. C. Scomoroscenco, M. Teodorescu, C. L. Nistor, I. C. Gifu, C. Petcu, D. D. Banciu, A. Banciu, L. O. Cinteza, Pharmaceutics 2023, 15, 1420.

Topic : **Synergistic effect in surfactant mixtures – biomedical and cosmeceutical applications**

Name of supervisor: **Assoc. prof. dr. habil. Ludmila Otilia Cinteză**

Background information: Mixed surfactant systems are employed to enhance surfactant performance across a wide range of applications, including detergency, oil recovery, wetting, emulsification. Synergistic effects, particularly in binary systems such as cationic–anionic, ionic–nonionic, and zwitterionic–nonionic surfactant mixtures, have been extensively studied, while ternary systems, despite their frequent industrial use, remain comparatively underreported in the literature. Molecular interactions within micellar aggregates or interfacial monolayers, quantified by the β interaction parameter, tend to be less intense in systems composed exclusively of nonionic surfactants than in those involving also ionic components. The use of nonionic surfactants, with lower toxicity and improved safety profiles, are increasingly favored, due to the extensive demand for products that are better tolerated by both the skin and the environment, without sacrificing functional efficacy.

This project aims to evaluate the synergistic effects in aggregation behavior and interfacial adsorption of binary and ternary mixed systems involving pharmaceutical-grade nonionic surfactants. Mixed micelles formed with polymeric surfactants will be characterized using DLS, FTIR, TEM, and fluorescence spectroscopy. The research targets potential applications in cosmetic and pharmaceutical formulations, with a focus on developing safer and more effective surfactant systems.

Special requirements: The candidate is expected to have a Master's degree in chemistry, pharmacy, biochemistry, chemical engineering, or affine sectors. A background knowledge in colloidal chemistry is required, together with basic physico-chemical methods for characterization of materials.
Strong communication skills, willingness to learn and ability to work within a team are highly appreciated.

References

1. U. Saha, R. De, B. Das, J. Mol. Liq. 2023, 382, 121906.
2. P. Phaodee, D. A. Sabatini, J. Surfactants Deterg. 2021, 24, 551.
3. M. A. Tănase, A. Raducan, P. Oancea, L. M. Diţu, M. Stan, C. Petcu, C. Scomoroşcenco, C. M. Ninciuleanu, C. L. Nistor, L. O. Cinteza, Pharmaceutics 2021, 13, 435.

Topic : **Metal nanoparticles with tunable antimicrobial activity**

Name of supervisor: **Assoc. prof. dr. habil. Ludmila Otilia Cinteză**

Background information: Metal nanoparticles, particularly silver (Ag) and gold (Au), exhibit exceptional physicochemical properties and unique optical characteristics, that have driven their integration into a wide range of technological applications, such as optoelectronic devices, catalytic systems, biosensors, environmental remediation technologies, and components within the automotive industry. In recent decades, their antimicrobial activity has attracted growing attention for the development of medical products (wound dressings, disinfectants, antimicrobial coatings, and functional textiles), based on their broad-spectrum antimicrobial efficiency and adaptability to various formulations.
The doctoral research will focus on the facile green synthesis, physicochemical characterization and “in vitro” evaluation of silver (Ag) and copper (Cu) nanoparticles. The choice of copper, in addition to silver, reflects growing interest in cost-effective alternatives with comparable antimicrobial properties. Special emphasis will be on tailoring particle size, shape, and surface properties, in order to balance antimicrobial activity and cytotoxic effects on human cells.
The study will also investigate the integration of these nanoparticles into functional coating materials. These advanced coatings will be designed for dual-use applications: (1) in the biomedical field, such as antimicrobial surfaces for medical devices, implants, and hospital environments, and (2) in the conservation of cultural heritage objects, where microbial degradation poses a serious threat to valuable artworks and artifacts.

Special requirements: The candidate is expected to have a Master's degree in Chemistry, Chemical engineering, Physics, or affine sectors. Previous experience in synthesis and characterization of particles is considered a plus. Strong communication skills, willingness to learn and ability to work within a team are highly appreciated.

References

1. A. I. Ribeiro, A. M. Dias, A. Zille, ACS Appl. Nano Mater. 2022, 5, 3030.
2. N. T. T. Nguyen, L. M. Nguyen, T. T. T. Nguyen, T. T. Nguyen, D. T. C. Nguyen, T. V. Tran, Environ. Chem. Lett. 2022, 20, 2531.
3. T. Huang, X. Li, M. Maier, N. M. O’Brien-Simpson, D. E. Heath, A. J. O’Connor, Acta Biomater. 2023, 158, 56.
4. C. L. Nistor, C. I. Mihaescu, D. Bala, I. C. Gifu, C. M. Ninciuleanu, S. G. Burlacu, C. Petcu, M.-G. Vladu, A. Ghebaur, L. Stroea, L. O. Cinteza, Coatings 2022, 12, 253.
5. L. O. Cinteza, C. Scomoroscenco, S. N. Voicu, C. L. Nistor, S. G. Nitu, B. Trica, M.-L. Jecu, C. Petcu, Nanomaterials 2018, 8, 826.

Topic : **Superhydrophobic multifunctional coatings based on ORMOSIL materials**

Name of supervisor: **Assoc. prof. dr. habil. Ludmila Otilia Cinteză**

Background information: Smart coatings with the ability to produce superhydrophobic surfaces still represent a hot topic in the field of material science, due to the increasing demand of the functionalization of various surfaces. Among the various chemical reagents to be selected for this goal, organic modified silica materials (ORMOSILs) seem to be the most environmentally friendly, inexpensive, easy to process and scalable.
This PhD research will focus on obtaining and characterizing various nanoparticle-based coating materials with filmogenic properties, able to form effective coatings on various surfaces, from stone to metals. The

influence of the size and shape of the embedded nanoparticles on the wettability, optical properties and durability of the films will be investigated using various physicochemical methods. Such coatings, containing also nanoparticles and compounds with antimicrobial or anticorrosive properties can be valuable solutions in protection of cultural heritage monuments or artistic objects.

Special requirements: The candidate is expected to have a Master's degree in Chemistry, Chemical engineering, Material chemistry, Physics, or affine sectors. Previous experience in synthesis and characterization of nanoparticulate materials is considered a plus. Strong communication skills, willingness to learn and ability to work within a team are highly appreciated.

References

1. I. S. Bayer, Adv. Mater. Interfaces 2020, 7, 2000095.
2. H. Zhang, Z. Guo, Nano Today 2023, 51, 101933.
3. Y. Liu, X. Tan, X. Li, T. Xiao, L. Jiang, S. Nie, J. Song, X. Chen, Langmuir 2022, 38, 12881.
4. C. Petcu, E. Alexandrescu, A. Bălan, M. A. Tănase, L. O. Cinteză, Coatings 2020, 10, 1010.
5. M. Ioan, D. F. Anghel, M. Anastasescu, I. C. Gifu, E. Alexandrescu, R. I. Matei, C. Petcu, I. Stanculescu, G. A. Sanda, D. Bala, L. O. Cinteza, Coatings 2023, 13, 1193.

***Topic*: Liquid crystals with luminescent properties**

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***Background information*:** Liquid crystals, anisotropic fluids with a partial degree of ordering, a unique combination of typical properties of both the liquid state and the solid state, are commonly used in various applications, ranging from the manufacturing of LCDs to different molecular sensors and detectors, optical switches, spatial light modulator, etc. Metallomesogens (liquid crystals based on metal complexes) are a special class of liquid crystals which bring together the properties of anisotropic fluids (anisotropy of physical properties and fast orientational response to external fields) specific to liquid crystals (LC) with the particular properties of metals (geometry of coordination, electronic, magnetic or the purely structural role, depending on the metal ion). As the luminescent liquid crystals can find useful applications in emissive display devices, the required photophysical properties of such materials can be achieved by a judicious combination of metals and ligands. The project will focus on the design and preparation of new candidates as luminescent liquid crystals based on d- or f-metals with high thermal stability, lower transition temperatures and LC properties according to envisaged application (nematic and columnar phases).

***Special requirements*:** The candidate is expected to have at least background knowledge in synthetic organic chemistry, coordination chemistry and basic spectroscopic techniques (NMR, IR, UV-VIS).

References:

1. Handbook of Liquid Crystals, Second Edition, Eds. J.W. Goodby, P.J. Collings, T. Kato, C. Tschierske, H.F. Gleeson, P. Raynes, Wiley-VCH Verlag, (2014).
2. X. Wu, M. Zhu, D. W. Bruce, W. Zhu and Y. Wang, *J. Mater. Chem. C*, 2018,**6**, 9848-9860.
3. L. F Chiriac, I. Pasuk, M. Secu, M. Micutz, V. Cîrcu, *Chem. Eur. J.*, 2018, **24**, 13512-13522.

***Topic*: Metal–organic framework-derived porous materials for catalysis**

***Name of supervisor*: prof. univ. dr. Simona Margareta Coman**
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Background information: Effective transformation of biopolymers from biomass (e.g. cellulose, hemicellulose and lignin) into added-value compounds relies heavily on the development of cascade chemical reactions, where the use of multifunctional solid catalysts is indispensable. In this context, advances in material science and catalysis have provided some innovative strategies for the development of new catalytic materials with well-defined structures and efficient physicochemical characteristics. Metal-organic frameworks (MOFs), for instance, have emerged as promising materials in the areas of gas storage, magnetism, luminescence and catalysis owing to their

superior properties of highly crystalline structures. However, MOFs' stability to thermal or humidity is greatly less than carbons because they are constructed from assembly of ligands with metal ions or clusters by coordination bonds. Transforming MOFs into carbons is bringing a novel potential for MOFs to reach industrialization, and carbons with controlled pore size and surface doping are one of the most important porous materials. As compared with other carbons such as activated carbons, carbon nanotubes and graphene, MOF-derived carbons showed at least two merits: (a) MOF precursors can easily control the pores and shape; (b) heteroatoms can be easily doped with controllable configuration by the selected linkers for MOFs and carbonization condition [1, 2]. Applying MOF-derived carbons in biomass valorization, which is one of the main aims of this research, is of great potential considering their large surface areas with abundant active sites and defects in the structure.

Special requirements : The candidate is expected to have at least background knowledge in coordination chemistry, catalysis, and chemistry of materials.

References

1. T.Wang, H.-K. Kim, Y. Liu, W. Li, J. T. Griffiths, Y. Wu, S. Laha, K. D. Fong, F. Podjaski, C. Yun, R. V. Kumar, B. V. Lotsch, A. K. Cheetham, S. K. Smoukov, *J. Am. Chem. Soc*., 2018, 140, 6130.
2. J. Wang, Y. Wang, H. Hu, Q. Yang, J. Cai, *Nanoscale*, 2020,12, 4238.

Topic: **Zeolite catalysts for the biomass valorization to biofuels and biochemicals**

Name of supervisor: **prof. univ. dr. Simona Margareta Coman**

Background information: Energy shortage and environmental degradation have become worldwide problems due to the rapid exploitation and depletion of non-renewable fossil resources. The only renewable source of carbon, namely biomass, has been shown to have great potential for upgrading into valuable biochemicals and biofuels, which provides a way to address energy and environmental issues [1]. In this context, the catalytic upgrading of biomass into high-value biochemicals and biofuels has received increasing attention in the last few years and is being considered a promising strategy for the efficient utilization of biomass energy. For instance, a wide variety of value-added biochemicals and biofuels can be obtained from two well-known biobased platform molecules, namely levulinic acid (LA) and 5-hydroxymethylfurfural (HMF), able to replace the corresponding petroleum products. Zeolites with high stability and excellent tunability (mainly acid properties and porous structure) have shown remarkable catalytic performance in biomass valorization and can be used as promising heterogeneous catalysts for targeted conversion of biomass. However, zeolite design and corresponding catalytic mechanism research is necessary to facilitate the valorization of biomass. Therefore, the synthesis of efficient zeolites for biomass valorization mainly focuses on the structural modifications and the design of the active sites, which further influence the catalytic activity and reaction mechanisms [2].

Special requirements: The candidate is expected to have at least background knowledge of organic chemistry, catalysis, and chemistry of materials.

References

1. F. Rosillo-Calle, *J. Chem. Technol. Biotechnol.*, 2016, 91, 1933.
2. P. Yan, H. Wang, Y. Liao, C. Wang, *Renew. Sustain. Energy Rev*., 2023, 178, 113219

Topic: **Catalytic amino acids production from biomass-derived intermediates**

Name of supervisor: **prof. univ. dr. habil. Simona Margareta Coman**

Background information: As the basic building blocks of proteins, amino acids play an essential role in life and are widely used in food and feed supplements as precursors to biodegradable plastics, pharmaceutical products, and elsewhere. Although the current production of amino acids mainly relies on microbial cultivation processes, the issues associated with the scale limitations of microbial processes, the strict need for sterile operating conditions, and the complexity of their separation have stimulated efforts to develop efficient chemical approaches to produce amino acids and their derivatives [1-3]. As an alternative, chemocatalytic approaches to produce amino acids from renewable feedstocks, such as bio-based sugars, could offer a rapid and potentially more efficient means of amino acid synthesis. However, to date, the efforts have been limited by the development of facile chemistry and associated catalyst materials, and therefore, sustainable approaches for their direct synthesis from abundant and renewable feedstocks are still quite

rare. The main aim of this work is to develop sustainable catalytic approaches for the direct synthesis of amino acids from both biomass-derived α-hydroxyl acids and glucose.

Special requirements: The candidate is expected to have at least background knowledge of organic chemistry, catalysis, and chemistry of materials.

References

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Topic: **Electroanalysis at disposable chemically modified sensors.**

Name of supervisor: **Assoc. prof. dr. habil. Gabriela Iulia David**

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Background information: Modern electroanalytical techniques are important tools for the study of analytes belonging to different classes of compounds, in order to establish or confirm their structure, to clarify equilibria and reaction mechanisms in which they may be involved or to estimate certain physical constants (e.g. dissociation constant, charge transfer coefficient, etc.) and, finally, to quantify chemical species in varied matrices [1]. Thus, there is currently a growing trend to develop sensors with improved performance characteristics (sensitivity, selectivity, response time, stability), by using (nano)materials either as such or in combination, which leads to a huge range of such electroanalytical devices applicable in *on-site* and *in-situ* analyses in environmental, food safety or health control.

Special requirements: The candidate is expected to have at least background knowledge of analytical chemistry and physical chemistry (level Master's degree) with focus on instrumental analysis, in general, and electrochemistry, in special and statistics. The candidates should be highly motivated to do research, communicative, creative, eager to learn, and able to work independently as well as part of a team

Reference

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2. Dhanjai, A. Sinha, X. Lu, L. Wu, D. Tan, Y. Li, J. Chen, R. Jain, Voltammetric Sensing of Biomolecules at Carbon Based Electrode Interfaces: A Review. *TrAC Trends in Analytical Chemistry, 98,* 174–189*,* **2018**.
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Topic: **Non-imprinted and molecularly imprinted polymers (MIPs) as sensing materials.**

Name of supervisor: **Assoc. prof. dr. habil. Gabriela Iulia David**

Background information: Polymeric films contain functional groups that can interact with the analyte molecule, thus allowing the accumulation of the species of interest on the electrode surface and, implicitly, a more sensitive detection, but also a modification of a parameter (e.g. peak potentials, radiation intensity), following the interactions, which can lead to enhanced selectivity of the determinations. At the same time, polymer films constitute the support for the embedding or grafting of other (nano)materials through whose synergistic effect the performance characteristics of the sensor are further improved. A molecularly imprinted polymer (MIP) contains molecular recognition sites in its matrix, generated by its synthesis in the presence of a target molecule, which is subsequently removed. The behavior of MIPs is described by the "lock-and-key" concept, with the 3D cavities in the polymer matrix being the "lock" and the template molecule being the "key". MIPs can theoretically be obtained

for any analyte of interest and applied in analytes preconcentration and separation, drug delivery processes or in selective (electro)chemical sensing.

Special requirements: The candidate is expected to have at least background knowledge of analytical chemistry and physical chemistry (level Master's degree) with focus on instrumental analysis, in general, and electrochemistry, in special and statistics. The candidates should be highly motivated to do research, communicative, creative, eager to learn, and able to work independently as well as part of a team

Reference

1. O.S. Ahmad, T.S. Bedwell, C. Esen, A. Garcia-Cruz, S.A. Piletsky, Molecularly Imprinted Polymers in Electrochemical and Optical Sensors. *Trends in Biotechnology, 37*, 294–309, **2019**.
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Topic: **Investigation on the retention mechanism in hydrophilic interactions based liquid chromatography: experimental parameters and data modeling.**

Name of supervisor: **prof. univ. dr. Victor David**

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Background information: Hydrophilic interaction liquid chromatography (HILIC) is a rather new separation mechanism in liquid chromatography (LC), which is desiganted to separate various polar compounds on polar stationary phases. This mechanism represents an alternative possibility to the most used chromatographic mechanism, namely reversed-phase LC. The separation process under HILIC mechanism is influenced by nature of the stationary phase, and the composition of the mobile phase. Although some theoretical descriptions of analyte retention under this mechanism have been already published in the literature, the complete understanding of the retention behavior in HILIC mechanism is still debatable and this could have advantages in practice for its application to various types of samples investigated by LC.

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2. S.C. Moldoveanu, V. David, *Essentials in Modern HPLC Separations*, Editura Elsevier, Amsterdam, The Netherlands; ISBN: 978-0-12-385013-3; 2013.
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4. R. Kaliszan, M.A. van Straten, M. Markuszewski, C.A. Cramers, H.A. Claessens, Molecular mechanism of retention in reversed-phase high-performance liquid chromatography and classification of modern stationary phases by using quantitative structure-retention relationships; *Journal of Chromatography A*, 855; 455-86 (1999).
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6. A. Vailaya, C. Horváth, Enthalpy-entropy compensation in hydrophobic interaction chromatography; *Journal of Physical Chemistry*, 100; 2447-2455 (1996).

Topic: **Enthalpy – entropy compensation in liquid chromatography: experimental design and theoretical approaches.**

Name of supervisor: **prof. univ. dr. Victor David**

Background information: Generally, two extra-thermodynamic correlations are frequently used to discuss the mechanistic similarities of chemical equilibria and reaction kinetics: enthalpy-entropy compensation (EEC) and linear free energy relationships (LFER). A few empirical studies have been applied to liquid-chromatography deriving from thermodynamic studies on various classes of compounds based on van't Hoff plots, but they are limited to the normal-phase and reversed-phase liquid chromatography. This topic is designated to extend the research in liquid chromatography for other important retention mechanisms, such as HILIC and ZIC-HILIC mechanism for various stationary phases and mobile phase compositions, and to compare the thermodynamic results with normal-phase and reversed-phase liquid chromatography.

Special requirements: The candidate is expected to have at least background knowledge of separation science, chromatography, statistics.

References

1. S.C. Moldoveanu, V. David, *Selection of the HPLC Method in Chemical Analysis*, Elsevier, Amsterdam, The Netherlands; ISBN: 978-0-12-803684-6; 2017.
2. S.C. Moldoveanu, V. David, *Essentials in Modern HPLC Separations*, Editura Elsevier, Amsterdam, The Netherlands; ISBN: 978-0-12-385013-3; 2013.
3. Y.V. Kazakevich, High-performance liquid chromatography retention mechanisms and their mathematical descriptions; *Journal of Chromatography A*, 1126; 232-243 (2006).
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5. B. Buszewski, S. Noga, Hydrophilic interaction liquid chromatography (HILIC) - a powerful separation technique; *Analytical and Bioanalytical Chemistry*, 402; 231-247 (2012).
6. A. Vailaya, C. Horváth, Enthalpy-entropy compensation in hydrophobic interaction chromatography; *Journal of Physical Chemistry*, 100; 2447-2455 (1996).

Topic: **Organic functionalized nanometric assemblies for multivalent applications**

Name of supervisor: **prof. univ. dr. Petre Ioniță**
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Background information: This research topic is a blend between organic and materials chemistry, with the aim to obtain by synthesis nanometric assemblies that contain functional organic molecules [1-3]. These assemblies may be formed from pure organic compounds brought together by non-covalent interactions or may be hybrid structures of inorganic-organic type (such are nanoparticles), functionalized with organic compounds. The organic part will have specific properties, like paramagnetic, fluorescent, acid-base or redox. Depending on that, multivalent applications can be envisaged.

Special requirements : The candidate is expected to have at least background knowledge in organic reactions and synthesis, column chromatography, organic physical chemistry (spectroscopy). Supramolecular, materials or nanoparticles chemistry will be an asset.

References

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2. S. E. Lohse, C. J. Murphy. *Applications of colloidal inorganic nanoparticles: from medicine to energy***.** J. Am. Chem. Soc. 2012, 134, 15607. DOI: 10.1021/ja307589n
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Topic: **Stable free radicals and radicaloids derived from DPPH**
Name of supervisor: **prof. univ. dr. habil. Petre Ioniță**
Background information: The chemistry of stable free radicals is well known now-a-days [1]. A free radical is a chemical entity that contains an unpaired electron (free electron) and usually has a high reactivity due to its open-shell structure. The DPPH stable free radical (2,2-diphenyl-1-picrylhydrazyl) is a violet-colored organic compound that can be involved into redox or acid-base processes (as example, reduction yields the yellow hydrazine, and the addition of a base led to the corresponding red anion); these reversible processes are easily followed by such color-changes [2]. The aim of this research is the synthesis, characterization and the study of novel DPPH-derivatives, mainly containing a betainic structural moiety (zwitterion) that may behave as a hetero-diradical [3].
Special requirements : The candidate is expected to have at least background knowledge in organic reactions and synthesis, column chromatography, organic physical chemistry (spectroscopy). Free radicals chemistry will be an asset.
References
1. R. G. Hicks. *Stable radicals: fundamentals and applied aspects of odd-electron compounds*. John Wiley & Sons, Ltd. Chichester, UK, 2010.
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Topic: **Xanthene derivatives and complexes with xanthene derivatives**
Name of supervisor: **assoc. prof. dr. Augustin M. Mădălan**
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Background information: Xanthene derivatives such as fluorescein and rhodamine are fluorophores with excellent photophysical properties (high extinction coefficients, excellent quantum yields, great photostability, and relatively long emission wavelengths). Spirocyclic derivatives of these two xanthenes are useful molecule-based sensors because the ring opening process leads in solution to a turn-on fluorescence change.[1,2] For example, fluorescein derivatives functionalized by Mannich reactions were used as fluorescence sensors for quantifying biological Zn(II) ions.[3] The project focuses on design and synthesis of xanthene derivatives possessing coordination sites (i.e. polyamino, polyamino polycarboxylic, imines/hydrazones) able to bind selectively 3d or 4f metal ions.
Special requirements from the students: The candidate is expected to have knowledge in organic synthesis and coordination chemistry, to be familiarized with purification techniques in organic chemistry lab and characterization of the compounds using various spectroscopic techniques (UV-Vis, FTIR, NMR).
References
1. X. Chen, T. Pradhan, F. Wang, J. S. Kim, J. Yoon, *Chem. Rev.*, **2012**, *112*, 1910.
2. M. S. T. Gonçalves, *Chem. Rev.*, **2009**, *109*, 190.
3. X. Zhang, D. Hayes, S. J. Smith, S. Friedle, S. J. Lippard, *J. Am. Chem. Soc.*, **2008**, *130*, 15788.

Topic: **Complexes with compartmental ligands containing extended π systems**
Name of supervisor: **assoc. prof. dr. Augustin M. Mădălan**
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Background information: Polydentate imino/amino based ligands are important tools in designing homo- and heteropolynuclear complexes with 3d and 4f metal ions.[1] This project is devoted to the synthesis of flexible and rigid compartmental ligands containing extended π systems capable to coordinate to 3d and/or 4f metal ions. The presence of the extended π systems in the two types of ligands, flexible or rigid, can

generate the luminescent properties, but also the potential use as DNA intercalating agents. The extended π systems can also play a structural role directing the supramolecular organization of the complexes within the crystals through π–π interactions.[2,3]

Special requirements from the students: The candidate is expected to have knowledge in organic synthesis and coordination chemistry, to be familiarized with purification techniques in organic chemistry lab and characterization of the compounds using various spectroscopic techniques (UV-Vis, FTIR, NMR).

References

1. M. Andruh, *Chem. Commun.*, **2011**, *47*, 3025.
2. A. D. Popa, M. Răducă, A. M. Mădălan, *Polyhedron*, **2023**, *239*, 116441.
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Topic: ***Transition-metal-containing LDH-based catalysts for bio-oil hydrodeoxygenation***

Name of supervisor: **prof. univ. dr. Ioan-Cezar Marcu**
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Background information: Layered double hydroxides (LDH), a class of anionic clays, which can be found in nature as minerals and can also be synthesized, are currently generating an increasing attention among scientists working in catalysis [1]. Indeed, due to their special lamellar structure, these synthetic inorganic materials exhibit a set of unique properties that make them suitable for the catalysis domain, either as catalyst precursors, catalyst supports or as actual catalysts [2]. Hydrodeoxygenation is an important step in the conversion of biomass-derived oxygenates to fuels and chemicals consisting in selective deoxygenation of the intermediates derived from the fast pyrolysis step to transform them into high-value finished products [3]. To achieve this, bifunctional catalysts are needed, LDH derived materials being privileged [4]. Thus, our objective is to synthesize different multifunctional transition-metal-containing LDH-derived oxide materials and to investigate their catalytic properties in hydrodeoxygenation of some model oxygenated compounds.

Special requirements : Heterogeneous Catalysis and Basic Chemical Technology.

References

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Topic: **Oxidative dehydrogenation of light alkanes over transition-metal-based mixed oxides catalysts**

Name of supervisor: **prof. univ. dr. Ioan-Cezar Marcu**

Background information: Oxidative dehydrogenation (ODH) of light alkanes may offer a promising alternative for the production of the corresponding alkenes compared to the simple dehydrogenation as the ODH has the advantage of an exothermic reaction, without thermodynamic limitations and with a low risk of catalyst deactivation through coking because the reaction is run in an oxidative environment [1, 2]. Nevertheless, the main difficulty in obtaining high alkene yields by ODH of light alkanes arises from the fact that the alkene is more reactive than the corresponding alkane, thus being prone to further oxidation to produce carbon oxides. Indeed, the ODH of light alkanes proceeds through sequential (Alkane → Alkene → COx) and parallel (Alkane → COx) oxidation steps, the secondary reactions, i.e. the deep oxidation of both alkane and alkene, being more thermodynamically favorable than the oxidative dehydrogenation.

Consequently, our objective is to design transition-metal-based oxide catalysts [3, 4] which significantly accelerate only the chosen sequence of elementary steps and suppress all other possible elementary steps, parallel or consecutive, in ethane and propane conversion.

Special requirements : The candidate is expected to have at least background knowledge of the Principles of Heterogeneous Catalysis, including variable-valence oxide catalysts, and Basic Chemical Technology.

References

1. F. Cavani, N. Ballarini, A. Cericola, Oxidative dehydrogenation of ethane and propane: How far from commercial implementation?, Catal. Today 127 (2007) 113-131.
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Topic: **Transition-metal-based mixed oxides catalysts for volatile organic compounds abatement**

Name of supervisor: **prof. univ. dr. Ioan-Cezar Marcu**

Background information: Control of volatile organic compounds (VOC), including methane [1], emissions has become a major concern of the chemical and petrochemical industries commitment towards the environment. In this context, it is necessary to develop new eco-friendly techniques to limit and control these emissions which can affect the climate change, the growth of plants and the health of human beings [1]. Catalytic total oxidation is a suitable alternative to conventional incineration due to its practical applications both for pollution abatement and power generation. Precious metals have been widely reported in the literature as very active catalysts for the complete oxidation of short-chain hydrocarbons and VOC, but they are expensive, easily sintered and volatile at moderate temperatures [2]. Many efforts have been devoted to the replacement of noble metals by transition metals to obtain highly active metal oxide catalysts for methane combustion [2, 3]. Mn-, Co- or Cu oxides and their mixtures prepared by different methods, proved to be very promising catalysts in the combustion of VOC [2] and methane [3] as cheap and environmentally friendly systems. Consequently, our objective is to design transition-metal-based mixed oxide catalysts active for the total oxidation of methane as a model molecule for VOC.

Special requirements : The candidate is expected to have at least a background knowledge of the Principles of Heterogeneous Catalysis, including oxide-based catalysts, and Basic Chemical Technology.

References

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Topic: **Mixed oxide-derived catalysts for ammonia synthesis**

Name of supervisor: **prof. univ. dr. Ioan-Cezar Marcu**

Background information: Production of ammonia is an indispensable technological process today. Together with continuously increasing global population and widespread use of ammonia-based nitrogenous fertilisers, global ammonia production is estimated to reach 290 million metric tons by 2030 [1]. Lately, ammonia has drawn a lot of attention for being an efficient hydrogen carrier and carbon-free fuel [2]. Currently almost all ammonia is produced by Haber-Bosch process developed in the 20^{th} century. The modern industrial process relies on harsh operating conditions to overcome the kinetic barriers accounting for 2% of global energy consumption [3]. Traditional industrial ammonia synthesis relies on robust and cost-effective promoted iron-based catalysts [2]. However, their performance under mild conditions is severely limited due to substantial energy input that is required to cleave the nitrogen triple bond [2]. Furthermore, prolonged operation time leads to catalyst deactivation through irreversible sintering and poisoning, this ongoing degradation ultimately drives up the financial costs and environmental burden of large-scale production [2]. In recent years hydrides, nitrides, electrides, and non-thermal plasma systems have gained increasing research focus, but constraints such as oxidation at high temperatures, structural degradation, high

sensitivity to moisture and unfavourable reverse reactions collectively restrict their practical industrial relevance [2,4]. Mixed metal oxide-derived materials are emerging as promising catalysts for ammonia synthesis due to their ability to facilitate the reaction under mild conditions, offering robustness and stability over extended operational times [4]. Furthermore, the inherent stability and basicity of the oxide supports foster strong metal–support interactions that stabilize the active metal species and also enhance electron transfer, thereby accelerating both nitrogen activation and subsequent hydrogenation steps. To achieve the catalytic efficiency required for large-scale industrial application, future ammonia catalyst designs should incorporate various key features, such as low hydrogen poisoning, good hydrogen spillover pathway, strong electron donating ability and support involvement in ammonia formation.

Special requirements from the student: The candidate is expected to have a background knowledge of the Principles of Heterogeneous Catalysis and Fundamentals of Chemical Technology.

References

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2. S.S.S. Ganti, P.K. Roy, N. Wagh, K.N.S.S. Sai, S. Kumar, Strategically designed catalysts for ammonia synthesis under mild conditions: recent advances and challenges, J. Mater. Chem. A 13 (2025) 15361.
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Topic: **Synthesis of switching azo(hetero)arenes**

Name of supervisor: **Assoc. prof. dr. habil. Mihaela Matache**
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Background information: Molecular switches are bistable chemical systems able to reversibly interconvert under the influence of external physical or chemical triggers, by constitutional, configurational or conformational changes. The systems responsive to light are called photoswitches and they belong to classes such as *N*-acylhydrazones, azobenzenes, diarylethenes or spiropyranes. This field has significantly grown during the past two decades aimed for applications in materials chemistry for construction of smart windows, protective materials against sunlight, solar thermal fuels, data storage or medicinal chemistry, particularly for controlled drug release or photopharmacology. Heteroaryl azoswitches are a new class of photoswitches which have been developed as an alternative to azobenzenes, thanks to their broader structural diversity that result in very different spectral properties, thus solving some of the azobenzenes drawbacks. Although very promising, the field of heteroaryl azoswitches is relatively new and there are numerous unanswered questions regarding their structures, properties, and mechanisms of actions relationships. The project is based on synthesis of heterocyclic compounds containing switching units such as azo or hydrazone groups and their investigation as switches under various physical or chemical stimuli.

Special requirements from the student: The candidate is expected to hold knowledge in organic synthesis, be familiarized with purification and separation techniques in organic chemistry lab and structural analysis of organic compounds (*i.e.* UV-Vis, IR, NMR spectroscopy, mass spectrometry).

References

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Topic: **Synthesis of light-emissive small-molecules**

Name of supervisor: **Assoc. prof. dr. habil. Mihaela Matache**

Background information: Highly emissive organic-small molecules are continuously screened by structural variation and design of such compounds is directed by the desired application. Small molecules are very often preferred in biology over fluorescent proteins and seek for compounds preserving the optical properties in living organism has greatly evolved during the last years. There are numerous classes of fluorophores that have been thoroughly investigated for such purposes and synthetic approaches to these have been developed to ensure feasible pathways. The project focuses on design and multi-step synthesis of novel emissive small molecules (i.e. 1,3,4-oxadiazoles) and investigation of their properties. Depending on the target application (biological-related or materials chemistry), structures will be optimized and functionalization of the compounds will be different.

Special requirements from the student: The candidate is expected to hold knowledge in organic synthesis, be familiarized with purification and separation techniques in organic chemistry lab and structural analysis of organic compounds (*i.e.* UV-Vis, IR, NMR spectroscopy, mass spectrometry).

References

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2. E. Kozma, P. Kele, *Org. Biomol. Chem.* **2019**, *17*, 215–233.
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Topic: **Multisite coordinating ligands for metal-ion complexes**

Name of supervisor: **Assoc. prof. dr. habil. Mihaela Matache**

Background information: Chemistry of materials has been extensively developed during the past two decades in order to discover new functional materials with enhanced optoelectronic properties or able to host small molecules of interest. The design and synthesis of organic compounds that potentially lead to functional materials represent a cutting-edge research area which was born because of the chemical dynamism of the 21st century. An increasing number of publications regarding compounds useful for various fluorescence imaging techniques, as fluorescent and colorimetric sensors, phosphorescent materials or receptors for environmental and biological analytes have been reported. The project focuses on design and synthesis of compounds holding multiple sites (i.e. polyamino polycarboxylic, imines/hydrazones) able to coordinate to metal ions and investigation of the hybrid resulting molecules for optical and electronic properties.

Special requirements from the student: The candidate is expected to hold knowledge in organic synthesis, be familiarized with purification and separation techniques in organic chemistry lab and structural analysis of organic compounds (*i.e.* UV-Vis, IR, NMR spectroscopy, mass spectrometry).

References:

1. J. Wang, Q. Meng, Q. Meng, Yo. Yang, S. Zhong, R. Zhang, Y. Fang, Y. Gao, X. Cui, *ACS Sens.* **2022**, *7*, 9, 2521–2536.
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Topic: **Analytical issues for assaying target compounds having similar lipophilic character with respect to the complex matrices in which it exist.**

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Background information: Isolation of target compounds (at reduced levels) in complex matrices makes the analytical approach more quite tedious, especially when the character of the analyte of interest is quite similar to the matrix constituents. Some examples can be mentioned: polyaromatic hydrocarbons in fat or vegetal oils, active ingredients with high log P in fatty creams, ointments, or hydrophobic environments. Sample preparation in such conditions should consider some subtle differences in the properties of the target compounds with respect to the components of the matrix. Automation should be strongly considered a reliable solution to avoid random errors induced through multiple sample manipulation steps. Bidimensional chromatography should be envisaged, with a first dimension oriented versus the rough isolation of the target compound and a second direction oriented via its separation with respect to the residual co-extracted matrix. As long as the target analyte exists at a low concentration level in the initial sample, fraction transfer from one direction to the other should be attentively optimised to assist the overall sensibility of the approach.

Special requirements: The candidate is expected to have at least background knowledge of separation science, chromatography, and statistics.

Topic: **Liophilic additives in liquid chromatography**

Name of supervisor: **prof. univ. dr. Andrei-Valentin Medvedovici**

Background information: Liophilic or chaotropic agents (ChA) are weakly hydrated ions (of inorganic or organic nature), with significant charge delocalization, symmetrical conformation (usually spherical), exhibiting lyophilic properties. ChA are used as additives in mobile phases for liquid chromatography (LC) for tuning retention (and consequently selectivity) and peak symmetry for ionized analytes separated under the RP or HILIC retention mechanisms. A coherent evaluation of advantages/disadvantages related to the use of ChA in liquid chromatography is necessary, including thermodynamic approaches. The behaviour of ChA-based elution on newborn stationary phases becoming recently commercially available is emphasised. The use of ChA in applications relating to various fields (i.e. pharmaceutical, forensic) will be considered.

Special requirements: The candidate is expected to have at least background knowledge of separation science, chromatography, and statistics.

Topic: **Green solvents in sample preparation techniques for bioanalytical applications**

Name of supervisor: **prof. univ. dr. Andrei-Valentin Medvedovici**

Background information: Replacement of the usual organic solvents in mobile phases designed for RPLC elution by green solvents has already been studied in the literature. However, the potential of using green organic solvents in protein precipitation processes related to bioanalytical sample preparation schemes were not yet considered. Their use in bioanalytical protein precipitation procedures should be closely related to phenomena relating to large volume injection in LC, having as declared aim to enhance on the overall method sensitivity. Approaches related to human whole blood and plasma processing have to be considered and studied in detail, ethyl lactate and propyl carbonate being the first choice among the green solvents successfully replacing methanol or acetonitrile. Evaluation should be based through residual matrix effects appearing in mild ionization techniques used for LC-MS/MS applications.

Special requirements: The candidate is expected to have at least background knowledge of separation science, chromatography, statistics.

Topic: **Peak homogeneity in LC/DAD and LC/MS approaches**

Name of supervisor: **prof. univ. dr. Andrei-Valentin Medvedovici**

Background information: Peak homogeneity represents a major concern when validating the selectivity/specificity of the stability indicating HPLC methods. Existing methods (included in softwares assisting the data acquisition) are based on the measurement of the cosine between vectors represented in the n-dimensional space defined by the UV-Vis or MS spectra acquired during peak elution. However,

concentration/amount of the analyte reaching the detection area may induce errors with respect to the peak purity evaluation. Alternatives based on linear regression may be considered and should be tested with respect to the operational parameters used during spectral acquisition, similarity degree of spectra of the possible interfering compounds, spectral manipulation techniques (i.e. spectral derivatives) etc. Another feature of a major interest relates with the absolute differences in terms of retention time between the main compound and the interferent.

Special requirements: The candidate is expected to have at least background knowledge of separation science, chromatography, tatistics.

Topic: **Complexes developed as biologically active species**

Name of supervisor: **Assoc. prof. dr. habil. Rodica Olar**

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Background information: In the post-cisplatin era, there has been a surge in the development of complexes as biologically active species. The demand for these compounds stems from the need for new drugs and/or optimised formulations that can effectively treat various diseases, including cancers, diabetes mellitus, inflammation and viral, microbial and parasitic infections. For several of these diseases, metallodrugs have proven to be more effective than organic species due to their ability to target different biomolecules and utilise different mechanisms of action. When interacting with biomolecules, metal ions form coordinative bonds and subsequently mediate their splitting through redox processes. Additionally, selective interactions with target biomolecules can be achieved by selecting the appropriate metal ions and ligands. Furthermore, improved activity can be realised by embedding the complexes in an appropriate matrix — organic or inorganic — to develop hybrid materials. The doctoral research will therefore focus on the rational synthesis and characterisation of complexes based on essential metal ions (V, Cr, Mn, Cu and Zn) and non-essential metal ions (Pt, Ru, Au and Ag), with the aim of developing a sustainable platform for future metallodrug development. To achieve proper biological activity, ligands bearing pharmacophore moieties were selected. A plethora of characterisation techniques will be employed, including IR, UV-Vis, NMR, and EPR spectroscopy as well as single crystal X-ray diffraction. Beyond the chemical aspect, such species must also display favourable biological activity. Therefore, this research will also involve *in vitro* assessments of the complexes' antimicrobial and antitumour activity.

Special requirements from the student: The candidate is expected to have a Master's degree in Chemistry, Biochemistry, Physics, or affine fields. Previous experience in synthesis and characterization of complexes (*i.e.* through UV-Vis, IR, NMR, EPR spectroscopy) or nitrogen-based heterocycle derivatives is considered in addition.

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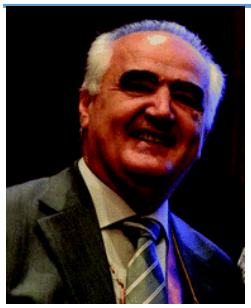

Topic : **Graphene derived catalysts for the valorisation of waste CO_2**

Name of supervisor: **prof. univ. dr. Vasile I. Parvulescu m.c.**

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Background information: The theme focuses on the investigation of the synthesis and modification of graphene structures with the aim of valorizing CO_2. CO_2 is one of the main components of greenhouse gases, and its concentration in the atmosphere presents ascendant trends. CO_2 is the main product of the burning of hydrocarbons and a residual product of many chemical processes. Its negative effects are directly related to the property of CO_2 to adsorb and release radiant energy in the thermal infrared range. These properties are completed by a very high inertness of the C=O double bond in a good concordance to the molecule's symmetry. Based on these, reducing the CO2 released concentrations is urgent and requires an efficient catalytic process. Efficiency means not only the removal of this pollutant but also its sustainable transformation into products of economic interest. The CO_2 hydrogenation to hydrocarbons is one of the very interesting alternatives for valorising this waste. In this line, the PhD thesis will follow the synthesis of graphene-based catalysts in which metal nano-particles and alloys will be deposited on surfaces of pure and doped graphene structures. The characterisation of the catalysts will be carried out through multiple techniques (texture, XRD, Raman, ATR, HRTEM, XPS, EXAFS, etc). The collected results will be correlated to catalytic results in various pressures and molar ratios. The kinetics of technological processes will be investigated as well.

Special requirements: The candidate is expected to have at least background knowledge in coordination organic chemistry, catalysis, and chemistry of materials.

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Topic : **Graphene based catalysts for chemo- and stereoselective reactions**

Name of supervisor: **prof. univ. dr. Vasile I. Parvulescu**

Background information: Graphene has been attracting a huge interest in the last period. This interest is directly related to the applications that have demonstrated their efficiency, and catalysis is among these. The catalytic properties of these materials under both pure state and as supports for metal nano-particles or grafted molecules have already been explored. The graphene properties also recommend them as catalysts for coupling reactions. These reactions are extremely important in organic synthesis and total organic synthesis in particular. Following this line, the PhD thesis will investigate chemo- and stereoselective C-C and C-N coupling reactions, including Henry synthesis. Various active 3d-4f nano-structure metal species deposited onto graphene surfaces, either in an amorphous or oriented state, will be investigated. Also, oxygen and nitrogen-functionalized graphene will be investigated. The characterisation of the catalysts will be carried out through multiple techniques (texture, XRD, Raman, ATR, HRTEM, XPS, EXAFS, etc). the kinetics of the reactions will also be investigated, taking into consideration the solvent nature.

Special requirements: The candidate is expected to have at least background knowledge in coordination organic chemistry, catalysis, and chemistry of materials.

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Topic: **2D Carbon-based magnetic materials for alcohol production**

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Background information: Recently, graphene, graphene oxides (GO), and magnetic graphene have received special attention from researchers due to the huge potential presented by various reactions. These materials can be obtained using a simple route by mixing of graphene/GO with magnetic nanoparticles [1] or in more advanced ways by in situ synthesis of magnetic materials on graphene / GO [2] as well as covalent functionalization [3] through which a strong bond is formed between graphene/GO and magnetic nanoparticles, so in the resulting nanocomposite the graphene/GO sheets cannot easily detach from the conjugated magnetic nanoparticles. Magnetic composites present some interesting properties, i.e. large surface area, improved adsorption properties, biocompatibility, etc. Usually, these materials have found different applications in medicine (drug delivery), environmental (removal of heavy metal ions, radioactive metal ions, pesticides/herbicides, pigments/dyes), and magnetic resonance imaging [4].

This project focuses on developing 2D Carbon-based magnetic materials, which will be used to obtain bioethanol from biomass.

Special requirements: The candidate is expected to have basic knowledge of the synthesis of solid carbon-based materials, catalysis, and organic chemistry.

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