CIVIS A European Civic University

# CIVIS call for researchers MSCIF 2020

# PANEL: Chemistry (CHE)

Co-funded by the Erasmus+ Programme of the European Union

| AIX MARSEILLE UNIVERSITE - France | | | | contact person: civis@univ-amu.fr | |
|---|---|---|---|---|---|
| SUPERVISOR | RESEARCH LAB/GROUP | AREA OF EXPERTISE | LINES OF INVESTIGATION | KEY FACILITIES | WEBSITE |
| **Sylvain Marque** | chemistry | organic synthese, electron paramagnetic resonance, radical chemistry, materials scineces, chemical biology | Development of new radical probes for imaging developement of radical initiators for smart materials developement of smart objects for applications against cancer, parasites, bacteria, and fungi | all devices for organic synthesis all current analysis for chemistry electron paramagnetic resonance machines | http://icr-amu.cnrs.fr/ |
| **Cristinel Diaconu** | Centre de Physique des Particules de Marseille | Physique des Particules, Astro-Particules, Cosmology, Medical Imaging, Computing | CPPM, the Marseille Particle Physics Centre is a Joint Research Unit (UMR 7346). The laboratory is part of the Institut national de physique nucléaire et de physique des particules (IN2P3), under the joint supervision of the French National Centre for Scientific Research (CNRS) and Aix-Marseille University. The research conducted at CPPM is at the crossroads of two infinites; ranging from the study of the elementary components of matter - the infinitely small - to the exploration of the cosmos - the infinitely large. To follow these we design and build state-of-the-art detector systems, often required to operate under extreme conditions: deep under the sea, in space or underground. Most of our research is carried out within leading international scientific collaborations and our contributions are recognized worldwide. We participate in the training of young people for research careers, directly through our research programs and also through their university education. Our laboratory is also very active in promoting technological developments resulting from its research. We seek to understand the Universe and its composition through laboratory experiments and observations of often violent celestial phenomena. Our research is aligned along three main axes: - Particle physics: of the infinitely small, to identify the most basic constituents of matter, measure their properties and understand their interactions (Experiments: ATLAS and LHCb at LHC/CERN, Belle II at KEK/Japan) - Astroparticle physics: the infinitely large seen through the infinitely small: studying the most violent phenomena in the Universe to look for the origins of very high energy cosmic rays and radiation. Experiments: KM3NeT, CTA. - Observational cosmology: direct studies of the infinitely large to determine and understand the history of the Universe, its origins, evolution and the nature of its constituents. Observational surveys : LSST, EUCLID, DESI. In addition to these three main axes of fundamental research leading to frontiers of scientific and associated technology, we are strongly committed to interdisciplinary themes and their societal applications, such as biomedical imaging, modern intensive computing and studies of the deep-sea environment. | We contribute to several very large multinational infrastructures essential to today's research. We are committed to many international collaborations: some having more than 3,000 collaborators. Examples include large experiments (ATLAS and LHCb) operating at the CERN LHC (Large Hadron Collider) in Geneva, the French "Grille" national computing infrastructure, and the CTA and LSST terrestrial telescopes. In addition CPPM is a major participant in the ANTARES and KM3NeT deep sea neutrino telescope collaborations, serving as the host laboratory for the ANTARES infrastructure and the KM3NeT western site, both located at a depth of around 2400m near Toulon. We are also involved in the construction of major elements of the Euclid space telescope satellite, which is partly supported by CNES and ESA (the French and European space agencies). From a technological point of view, these contributions require cutting edge know-how developed by CPPM experts in the fields of electronics, mechanics, computer science and instrumentation. Our highly qualified staff design and build innovative tools and are nationally and internationally recognized for their technological accomplishments. The laboratory benefits from a state-of-the-art infrastructure: including experimental areas located within clean rooms as well as a modern, well-equipped mechanical workshop and a large assembly hall with overhead crane facilities. | https://www.cppm.in2p3.fr/web/en/index.html |

| NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS – Greece | | | | | |
|---|---|---|---|---|---|
| SUPERVISOR | RESEARCH LAB/GROUP | AREA OF EXPERTISE | LINES OF INVESTIGATION | KEY FACILITIES | WEBSITE |
| **KOKOTOS Christoforos** | Laboratory of Organic Chemistry | Organic Chemistry, Catalysis, Green Chemistry, Sustainable Catalysis | Organocatalysis, Photocatalysis, Green Chemistry, Sustainable Catalysis, Study of reaction mechanisms | All facilities for Organic Chemistry | http://www.chem.uoa.gr/?page_id=2898&lang=el |
| **KOUTSELOS Andreas** | Statistical Mechanics Group at the Laboratory of Physical Chemistry of the Chemistry Department, NKUA | I am working in the field of computational physical chemistry. In my group we are developing methods for the reproduction of physical properties of the matter and produce computer codes for the calculation of physical properties. We are interested in equilibrium and nonequilibrium physical systems with emphasis to mixtures, reactive systems and transport phenomena. | We study the extension of thermodynamics, dynamic and kinetic properties of molecular systems near and far from equilibrium through the development of computational methods and relevant computer codes based on statistical mechanics and kinetic theory.<br>Far from equilibrium, we have developed non-equilibrium molecular dynamics simulation methods and relevant computer codes based on the classical and quantum mechanical description of molecular motion Applications focus on the motion of molecular ions in low density and semi-dense phases under the influence of electric and magnetic fields (Weakly ionized plasma), as well as on physical and chemical kinetic phenomena.<br>Close to equilibrium, we study the application of statistical mechanics-thermodynamics through (constrained) molecular dynamics simulation methods based on established and novel statistical ensembles for the study of adsorption and chemical activity. | The laboratory and the group have at their disposal fully-equipped offices and various computer facilities in use. The group uses three 36-core workstations and utilizes ample computer time provided by the National HPC supercomputer facility ARIS of the Greek Research & Technology Network (GRNET). | http://www.chem.uoa.gr/?page_id=2917&lang=el |
| **PROESTOS Charalampos** | | Food Chemistry | Our laboratory works on food analysis, food authenticity based on bioactive co.pounds in foods such as polyphenols, essential oils, omega 3 and omega 6 fatty acids and how through food technology these bioactive compounds can be used to produce innovative new foods based also on their nuttitive values. Also our laboratory studies food contaminants such as mycotoxins, biogenic amines, heavy metals, especially the latter on migration issues concerning food packaging. Microbiological analysis of foods concerning food pathogens is also a research field in our food laboratory. | Our laboratory is equiped with 3 hplc instruments coupled to UV, DAD, and fluorescence detectors, 2 GC instruments coupled to FID and NPD detectors, 4 spectrophotometers, 1 ELISA READER, extraction systems such as ultrasound bothuv and probe, soxhlet ectraction systems (6), rotary evaporators, microscopes, autoclave, laminar flow cabinet, ozone producing device and fully equiped food chemistry and food microbiology laboratories including colony count devices, incubators etc. Currently our laboratory works on national projects funded by the Greek government and the hellenic food authority, ministry of agriculture and food. Also we cooperate with the private sector on projects relating to new food product development and food analysis in products like olive oil, honey, wines, plant extracts and essential oil from plants. | http://www.chem.uoa.gr/?page_id=53747&lang=en |
| **THOMAIDIS Nikolaos** | Laboratory of Analytical Chemistry/Trace Analysis and Mass Spectrometry Group (TrAMS) | Sewage Epidemiology, Environmental Chemistry, Emerging Contaminants, Mass Spectrometry, Food Authenticity, Food Safety and Food Fraud | High Throuput wide-scope Non Target Sceening of Emerging Contaminants (CECs) and Bioactive Substances/Natural Products, Cheminformatics and HRMS omics technologies apllied in enviornmental, food and health studies, Wide-range monitoring and ecotoxicology of CECs, Food Authenticity of Olive Oil, Wine, Honey, Dairy Products | Wide range of Mass Spectrometers (QToFMS coupled with LC-ESI, GC-APCI, MALDI, imaging probes), Ion mobility HRMS and LC-MS/MS, GC-MS/MS, ICPAES, AAS, HPLCs and GCs, and all the supporting apparatus | http://trams.chem.uoa.gr/ |

| UNIVERSITY OF BUCHAREST - Romania | | | | contact person : Filuta Ionita filuta.ionita@cdi.unibuc.ro | |
|---|---|---|---|---|---|
| SUPERVISOR | RESEARCH LAB/GROUP | AREA OF EXPERTISE | LINES OF INVESTIGATION | KEY FACILITIES | WEBSITE |
| **Marius Andruh** | Faculty of Chemistry<br>Inorganic Chemistry Department | Metallosupramolecular Chemistry<br>Molecular magnetism<br>Crystal engineering | Molecule-based materials (single molecule magnets, single chain magnets, luminescent materials, metal-organic frameworks and covalent organic frameworks) | The laboratory is fully equipped with all facilities for synthesis and characterization of new coordination compounds : rotary evaporators, Single Crystal X-Ray diffractometer, powder X-Ray diffractometer, various spectroscopic techniques (FTIR, UV-VIS-NIR, circular dichroism, luminescence), SQUID magnetometer | |
| **Simona M. Coman** | Faculty of Chemistry/ Department of Organic Chemistry, Biochemistry and Catalysis (DOCBC) | Heterogeneous catalysis | Solid catalytic materials, biomass valorization, green catalytic processes, environmental catalysis | Our laboratory is part of the Research Center for Catalysts and Catalytic Processes (http://erris.gov.ro/Catalizatori-si-Procese-Cata) which disposes of the infrastructure for solid catalysts synthesis, solid material characterization, catalytic testing and organic chemicals analysis: catalysts' preparation setup; Magnetically stirred stainless steel autoclave reactors; Surface Area and Porosimetry System; Gas Chromatography Mass Spectrometry (GC-MS); Dynamic light scattering (DLS); Thermogravimetric (TG) and Differential Thermal Analysis (DTA); Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES); CHNS-O Elemental Analyzer; Fourier transform infrared spectroscopy (FT-IR) with DRIFT accessory; UV-vis spectrometer; Total Organic Carbon Analyzer (TOC) equipped with LAS-160 autosampler; X-ray diffractometer (XRD); Raman Spectrometer; Temperature-programmed desorption (TPD) Analyzer. | https://unibuc.ro/user/Simona.Margareta.Coman |
| **Petre IONITA** | Faculty of chemistry, Department of organic chemistry, biochemistry and catalysis | Organic chemistry. Nanomaterials. Free radicals. | Organic synthesis and characterization. Supramolecular chemistry. Free radical chemistry. Nanomaterials (gold, silver, and silica nanoparticles); graphene oxide. | NMR. Rotary evaporators. Magnetic stirrers and heaters. Glassware. | |
| **Ioan-Cezar MARCU** | Faculty of Chemistry – Laboratory of Chemical Technology and Catalysis | Heterogeneous catalysis | Oxide-based catalytic materials with acid-base and/or redox properties for alkanes oxydehydrogenation, volatile organic compounds (VOC) complete oxidation, bio-oil hydrodeoxygenation, water splitting, esterification reactions etc.; understanding of catalytic behavior of oxides in correlation with their redox and electronic properties | The laboratory is fully equipped for a research work in catalysis by metal oxides both in continuous flow and batch reactors. The following equipments are available in our lab: Catalysts' preparation setup with mechanical stirrer, pH meter and temperature controller; Universal benchtop centrifuge; Water distiller; Temperature-programmable oven and furnace; Pellet press; Catalytic test setups with quartz tube reactors and tubular furnaces, digital temperature controllers, digital flow meters or capillary flow meters; Magnetically stirred stainless steel autoclave reactors; Gas chromatographs equipped with both Thermal Conductivity and Flame Ionization Detectors; Dynamic electrical conductivity measurement setup with platinum electrodes, digital multimeter, digital temperature controller and flow meters. Our lab is part of the Research Center for Catalysts and Catalytic Processes which possesses the following equipments: Ball milling apparatus; X-ray diffractometer; Surface Area and Porosimetry measurement setup; Temperature-programmed desorption (TPD) and oxidation (TPO) Analyzer. | https://unibuc.ro/user/ioan.cezar.marcu/ |

| | | | | | |
|---|---|---|---|---|---|
| **Ludmila Otilia Cinteza** | Faculty of Chemistry - BioNanomaterials | Colloids and interfaces, nanomaterials for biomedical applications, drug delivery systems | Inorganic and organic materials as drug delivery systems (liposomes, polymeric micelles, polymeric and solid lipid nanoparticles); QDs, upconverting NPs, magnetic NPs for theranostic systems<br>Green synthesis of inorganic nanoparticles in supercritical CO2 or natural extract.<br>Surface functionalization, surface characterization, surfaces with superhydrophobic, self-cleaning and/or antibacterial properties | The laboratory possesses fully infrastructure for synthesis of inorganic and organic nanoparticles, as well as facilities for special synthesis (sonochemical, microwave techniques, supercritical fluids).<br>Instruments for characterization of materials: Tensiometer, contact angle tensiometer, UV-VIS, fluorescence and Raman spectrometers, viscosimeters, HPLC, optical microscopes (normal light, UV source, polarized light). | |
| **Augustin M. MADALAN** | University of Bucharest, Faculty of Chemistry, Inorganic Chemistry Department | Metallo-supramolecular chemistry, crystal engineering | fluorescent materials based on fluorescein derivatives, metallo-supramolecular chemistry, crystal engineering, synthesis and characterization of multifunctional heterospin systems. | The laboratory is equipped for research work in organic and inorganic chemistry. Our laboratory possesses the following equipment: single crystal X-ray diffractometers: STOE IPDS II, Rigaku XtaLAB Synergy-S (with Mo microfocus source), powder X-ray diffractometer Benchtop Proto AXRD, SQUID magnetometer, FTIR, UV-vis spectrometers, fluorescence spectrometer, circular dichroism spectrometer, elemental analyzer, rotatory evaporators, vacuum pumps. | |
| **Marilena Ferbinteanu Cimpoesu** | Faculty of Chemistry/Inorg. Chem.Dept./Advanced structural analysis of coordination compounds with special properties (magnetic and optic). | Structural chemistry and magnetic anisotropy (mechanisms and control leverages for spin bistability phenomena in terms of ligand field and spin orbit coupling effects. (experimental and computation)<br>Coordination compounds synthesis; Spectroscopy: electronic, vibrational; X-ray measurements; Quantum chemical calculations (DFT, CASSCF) and advanced modeling. | Bistability manifestations : chromotropism (FeII, FeIII, NiII, CuII complexes) and spin conversion (MnIII, CoII complexes).<br>Magnetic anisotropy (lanthanide complexes).<br>Structural chemistry: experimental and theoretical.<br>Structure-property correlations. | Synthesis Laboratory for coordination compounds with special properties (optical, magnetic) standard equipped.<br>Spectroscopy Laboratory (FT-IR, ATR-FT-IR with variable temperature, UV-VIS, optic fibre).<br>Structural Analysis Laboratory –single crystal X-ray Rigaku R-Axis Rapid II Diffractometer.<br>Computer room (Workstations and access to supercomputing facilities). Software: computational chemistry (Gaussian, ADF) and original codes related to structure-property analysis in terms of spin Hamiltonians, Ligand Field methods, electron-vibrational and spin-orbit coupling. | https://unibuc.ro/user/marilena.fierbinteanucimpoesu/ |
| **Irina ZARAFU** | Faculty of chemistry, Department of organic chemistry, biochemistry and catalysis | Organic chemistry, heterocyclic compounds, drug synthesis, nanomaterials | Synthesis and characterization of organic compounds with potential biological activity such as antibacterial, antiviral, anticancer, anti-TB activity. Synthesis and structural characterization of drugs or nanomaterials. | NMR. Rotary evaporators. Magnetic stirrers and heaters. Melting point devices (Kruss and Boetius). Glassware. Ice maker | |
| **Madalina Valentina SANDULESCU-TUDORACHE** | Faculty of Chemistry/ Department of Organic Chemistry, Biochemistry and Catalysis (DOCBC) | Biocatalysis | Enzymatic processes, enzyme immobilization, biotransformations, cascade biocatalysis, biomass valorization, green solvents, flavors and fragrances production, environmental pollution | Our laboratory is part of the Research Center for Catalysts and Catalytic Processes (http://erris.gov.ro/Catalizatori-si-Procese-Cata) which disposes of the infrastructure for (i) preparation and characterization of biocatalysts; (ii) development, optimization and implementation of biocatalysis; and (iii) monitorization of the chemical compounds by analytical methods. The facilities are: Gas Chromatography-Mass Spectrometry instrument (GC-MS); HPLC chromatograph cu DAD, RID and fluorometric detectors; GPC instrument with triple detection (RID, LSD, Visc); thermostatic incubator; surface area and porosimetry system; dynamic light scattering analyzer (DLS); thermogravimetric (TG) and differential thermal analyzer (DTA); inductively coupled plasma optical | https://unibuc.ro/user/madalinavalentina.sandulescutudorache/ |

| | | | | | |
|---|---|---|---|---|---|
| | | | | emission spectrometer (ICP-OES); CHNS-O elemental analyzer; Fourier transform infrared spectrometer (FT-IR) with DRIFT accessory; UV-vis spectrometer; total organic carbon analyzer (TOC) equipped with LAS-160 autosampler; X-ray diffractometer (XRD); Raman spectrometer; temperature-programmed desorption (TPD) analyzer. | |
| **Octavian-Dumitru PAVEL** | Faculty of Chemistry, Departament of Organic Chemistry, Biochemistry and Catalysis | Layered double hydroxides materials; Ionic liquids; Carbon-based materials; Solid characterization by different techniques; Fine chemical synthesis. | Synthesis of hydrotalcites (Mg2+; Al3+) and LDH-like basic materials with different cations (Li; Y; Dy; Ga; Sm; La; Mo; Co; etc.); Synthesis of organometallic catalysts in ionic liquids as SCILL or SILP catalysts; Synthesis of grapheme oxides and modified with different cations (Ce, Mo, etc.); Characterization of catalytic materials by solid X-ray diffraction; DRIFT; UV-Vis; BET; XPS; DTA-TG; CO2/NH3-TPD; TPR; etc.; Synthesis of different fine chemicals by different reactions as addition, condensation, oxidation, coupling, etc. | The laboratory is equipped with the necessary equipment for the synthesis of catalytic materials (agitation and heating plates, ovens, calcination furnaces, pH-meters, flow meters; peristaltic pumps; laboratory glass; and so on); with the equipment necessary for the characterization of these catalytic materials as well as with the equipment necessary for the chemical reactions to obtain some extremely important compounds for different branches of the industry as well as in the pharmaceutical field. There, also, exist some detection apparatus in order to establish the influence of the catalyst on the reaction rate, of selectivity as well as catalyst stability. All these facilities allow obtaining high quality publications recognized internationally, as well as the elaboration of bachelor's, master's and doctoral thesis. | https://unibuc.ro/user/octavian.pavel/?lang=en<br><br>https://erris.gov.ro/Catalizatori-si-Procese-Cata |
| **Bogdan Cojocaru** | Faculty of Chemistry - Department of Organic Chemistry, Biochemistry and Catalysis | Catalysis, photocatalysis, materials characterization. | Water/air photocatalytic decontamination, green fuels generation | The laboratory is fully equipped for a research work in materials synthesis, characterization and testing. Our laboratories possesses the following apparatus: rotatory evaporator, vacuum pumps, ovens, centrifuge, FTIR/DRIFT/ATR, Raman, UV-vis spectrometers, thermal analysis apparatus (TGA and DSC), XRD, DLS, Surface area, chemisorption/TPD/TPR/TPO, GCs, photoreactors,.HPLCs, mass spectrometry, | |
| **Liliana Stoicescu** | University of Bucharest, Faculty of Chemistry, Inorganic Chemistry Department | coordination chemistry. supramolecular chemistry, polydentate ligands synthesis, polynuclear transition metal compounds synthesis | polydentate ligands with amido groups, polynuclear transition metal compounds, crystal structures and magnetic properties of polynuclear transition metal compounds | The laboratory is equipped for a research work in coordination and supramolecular chemistry – ligands and transition metal compounds synthesis.<br>Our department possesses the following apparatus: FTIR and UV-vis spectrometers, thermal analysis apparatus (TGA and DSC), X-ray diffractometer, SQUID magnetometer (2-400 K) | |
| **Catalin Maxim** | Faculty of Chemistry /Inorganic Chemistry Departement | Supramolecular chemistry, coordination polymer synthesis, chiral molecular materials, crystal engineering | supramolecular materials based on chiral inorganic building blocks, synthesis of molecular based magnets, fluorescent materials | The laboratory is fully equipped for a research work in inorganic chemistry, crystal engineering and chiral coordination polymer synthesis. Our department possesses the following apparatus: rotatory evaporator, vacuum pumps, FTIR spectrometer Bruker Tensor 37, UV-Visible_NIR Spectrophotomer Jasco V670, Spectrofluorometer Jasco FP-6500, Single Crystal X-Ray Diffractometer STOE IPDS II , Powder X-Ray Diffraction PROTO AXRD , thermal analysis apparatus (TGA and DSC), SQUID Magnetometer S700X , CHNS Elemental Analyzer Euro EA3000, Single Crystal X-Ray Diffractometer SynergyS and cutting-edge JASCO J-1500 circular dichroism spectrometer. | https://www.chimie.unibuc.ro/index.php/dept-anorganica |
| **Oprea Eliza** | Faculty of Chemistry - Department of Organic Chemistry, Biochemistry and | Natural compounds, biochemistry, pharmacology | Extraction and characterisation of natural compounds (terpenes, flavonoids, anthocyanins, vitamins etc.), antioxidant evaluation and biologic assessment (antimicrobial, anti-inflammatory, cytotoxic and healing activity); biochemistry of free radicals using clinical biochemistry techniques, spectrophotometric methods for the assessment of redox | The laboratories are fully equipped for a research work in natural compounds and biochemistry. Our research group possesses the following apparatus:, UV-VIS spectrometers, flash multimode reader, microcentrifuges and centrifuges, electrophoresis systems, ultrasonic baths, refrigeration systems, various heating systems, microscopes, various | https://erris.gov.ro/Research-Center-Appl-Org-Chem |

| | | | | | |
|---|---|---|---|---|---|
| | Catalysis, Biochemistry Group | | status, ELISA techniques, enzymatic kinetics, preparation of cyclodextrin inclusion complexes with terpenic compounds by various entrapment methods, determination of entrapment efficiency. | extraction installations (Neo Clevenger, Soxhlet), rotatory evaporator, vacuum pumps, CO2 incubator, water purification systems, vortex and ultraturax mixers. | |
| **Gabriela IORGA** | Faculty of Chemistry-Dept. of Physical Chemistry, Physics Group<br>&<br>Faculty of Physics, Group of Atmospheric Physics | Atmospheric Physics, Air Pollution, Aerosol characterization | Research fields: physical and optical properties of tropospheric aerosol; the impact of aerosol on visibility and air pollution; modeling the radiative effects of the aerosol containing absorbent and non-absorbent chemical species in the troposphere; aerosol-microphysical parameterization relations of clouds and precipitations; modeling the aerosol-cloud-radiation interaction with empirical and deterministic models; air pollution and quality; wet and dry removal of pollutants from the atmosphere; radiative changes induced by anthropogenic factors | Atmospheric physics laboratory and the Experimental research facility for atmospheric measurement within the Platform for Interdisciplinary Studies in Geosciences. The main equipments are integrated in the UBFF master's and doctoral studies and are regularly used for atmosphere physics studies, including providing ambient real-time and size-resolved particle and gas concentration. The major instruments include: optical and gravimetric particle counters: LVS sampler with PM1, PM2.5, PM10 and TSP inlets, low-pressure cascade impactor Berner LPI 30/0.06/2 with 8 analysable stages, for aerosol sampling in size range 0.06 - 16.00 µm; TSI Dusttrak aerosol monitors, microbalances for gravimetric measurements, TSI integrating nephelometer for scattering coefficients, 55-gaseous compounds differential optical absorption spectroscopy system GAZMET FT-IR, ozone monitor, multi-gas monitor for SO2, NOx, two professional automatic meteorological stations (stationary and portable) with acquisition sensors and dataloggers (temperature, pressure, relative humidity, wind speed and wind direction), a ceilometer (to determine the PBL height and clouds), 2 systems (stationary and portable) for solar radiation measurements with acquisition sensors and dataloggers, a sun-photometer included in the global network AERONET, an atmospheric deposition sampling (WADOS) system to collect all wet and dry deposition samples.<br>Major equipments are available at https://sites.google.com/g.unibuc.ro/fmpe/home/infrastructura-de-cercetare/fizica-atmosferei<br>Tight collaborations with various institutions https://sites.google.com/g.unibuc.ro/fmpe/institutii-colaboratoare allow access to other complementary equipment's for air pollutants, aerosol characterization and meteorology. | https://sites.google.com/g.unibuc.ro/fmpe/home/ |

| UNIVERSITÉ LIBRE DE BRUXELLES - Belgium | | | | contact person: Emily Mainetti ulb-europe@ulb.be | |
|---|---|---|---|---|---|
| SUPERVISOR | RESEARCH LAB/GROUP | AREA OF EXPERTISE | LINES OF INVESTIGATION | KEY FACILITIES | WEBSITE |
| **Franck MEYER** | Faculty of Pharmacy - Microbiology, Bioorganic and Macromolecular Chemistry unit | Supramolecular chemistry, organic and polymer synthesis, halogen bonding, crystal engineering | supramolecular materials based on halogen bonds, synthesis of pharmaceuticals, multi stimuli responsive materials | The laboratory is fully equipped for a research work in organic chemistry, crystal engineering and polymer synthesis. Our faculty possesses the following apparatus: rotatory evaporator, vacuum pumps, FTIR, UV-vis spectrometer, mass spectrometry, gel permeation chromatography (GPC), high-performance liquid chromatography, gas chromatography and chromatography with automated fraction collector, thermal analysis apparatus (TGA and DSC), and polarised optical microscopy with heating system (HPOM). | https://pharmacie.ulb.be/version-francaise/la-recherche/les-unites-de-recherche/microbiologie-chimie-bioorganique-et-macromoleculaire-mc/microbiologie-chimie-bioorganique-et-macromoleculaire-mc |
| **Hennie Valkenier-van Dijk** | Ecole Polytechnique - Engineering of Molecular NanoSystems | Supramolecular Chemistry | We synthesise organic compounds that are designed to act as receptors for anions (or cations) and that can transport these ions through lipid bilayers. We study these transmembrane transport processes in model membrane (liposomes) by various spectroscopic methods (fluorescence, NMR) and seek to understand the mechanisms of transport and the parameters that affect this process. | Organic synthesis lab, liposomes preparation and characterisation, spectrometers | https://emns.ulb.be/ |
| **Bruylants Gilles** | Ecole Polytechnique - Engineering of Molecular NanoSystems | Nanomaterials functionalization | We are focusing on is the functionalization of metal nanoparticles with organic or biological ligands in order to develop (bio)sensors and biomedical applications. | see http://emns.ulb.be/nanomaterials.html | http://emns.ulb.be/nanomaterials.html |
| **Jon Ustarroz** | ChemSIN (Chemistry of Surfaces, Interfaces and Nanomaterials) | electrochemistry ; electrodeposition ; nano-electrochemistry | The ChemSIN research group of the Université Libre de Bruxelles (ULB) is composed of 4 research units. Prof. Jon Ustarroz leads the 'Electrodeposition and Nanoscale Electrochemistry' unit and also holds a part-time research professorship at the SURF research group of the Vrije Universiteit Brussel (VUB). | Specific equipment for the electrodeposition and nano-electrochemistry unit :<br>- State-of-the-art instrumentation for SECCM: ultra-sensitive electrometers (~1pA/V) for ultra-low current detection and high precision positioning (MCL Nano-MET 10 and Nano-M250)<br>- Laser-Based Micropipette Puller (Sutter Instrument P-2000)<br><br>Available equipment in the ChemSIN research group : multiple electrochemical workstations, AFM, Confocal Fluorescence Microscopy, XPS, FIM, Contact Angle, FTIR, IRRAS, Uv-VIS, GC-MS, plasma reactors, etc.<br><br>Equipment in the SURF research group (VUB) : FE-SEM, FE-Auger, XPS, AFM, ellipsometry, SVET/SIET, SECM, multiple electrochemical workstations, etc.<br><br>Equipment available through collaboration with other groups: TEM and liquid-cell electrochemical TEM | http://cvchercheurs.ulb.ac.be/Site/unite/ULB110UK.php<br>&<br>https://www.researchgate.net/profile/Jon_Ustarroz |

| UNIVERSIDAD AUTÓNOMA DE MADRID (UAM) - Spain | | | | | |
|---|---|---|---|---|---|
| SUPERVISOR | RESEARCH LAB/GROUP | AREA OF EXPERTISE | LINES OF INVESTIGATION | KEY FACILITIES | WEBSITE |
| **Fernando Martín** | Chemistry | Atomic and Molecular Physics, Quantum Chemistry, Laser-atom and laser-molecule interactions, Unbound systems, Surfaces and Solids, Metal clusters and fullerenes, Dynamical processes, Radiation damage. | We are an interdisciplinary team of researchers that aim at developing state-of-the-art time-dependent methods to address newly emerging fundamental questions about the role of sub-fs and attosecond coherent electron and nuclear dynamics in physics and chemistry. Our research mainly focuses on: (i) the theoretical and computational modelling of photoexcitation and photoionization processes in atomic, molecular and solid-state systems induced by ultrashort laser pulses with femto- and attosecond duration and x-ray pulses from modern x-ray sources (free-electron lasers and high-order harmonic generation), with the aim of monitoring and controlling ultrafast electron and nuclear dynamics occurring in these systems, and (ii) the study and theoretical prediction of properties of materials and nano-objects of complex molecular systems, aggregates and fullerenes, isolated or deposited on metallic and nonmetallic surfaces, with emphasis on problems with potential interest in chemistry and biology and the design of novel two-dimensional materials, including graphene. This, in close collaboration with worldwide leading experimental groups. | CampuS group guarantees enough computational resources to carry out the project through projects granted by the Computing Center (CCC-UAM) and the Spanish Supercomputing Network (RES). Prof. Martín is the Chair of COST Action CA18222 (www.attochem.eu) and has been recently been awarded with an ERC-AdG to carry out the project IDEAS. | https://campusys.qui.uam.es/ |
| **Manuel Alcamí** | Chemistry | Expert in the ab initio quantum mechanical treatment of complex molecules and surfaces | - Theoretical studies of the interaction of molecules of biological interest with metal cations.<br>- Reactions of interest in atmospheric chemistry.<br>- Structure and properties of fullerenes.<br>- Fragmentation of highly charged and excited clusters.<br>- Interaction of molecules with surfaces. | MolPM group guarantees enough computational resources to carry out the project through its Computing Center (CCC-UAM), the Spanish Supercomputing Network (RES). Prof. Alcamí is the Coordinator of the Erasmus Mundus Master TCCM (www.emtccm.org), and is involved in the CA18212 COST Action (MDGAS) and the IRP-LIA-DYNAMICS. | https://molpm.qui.uam.es/ |
| **Sergio Diaz-Tendero** | Chemistry | Density functional theory in gas phase and solid state.<br>Methods based on statistical mechanics applied to the fragmentation dynamics of excited molecules.<br>Wave packet propagation methods applied to study electron dynamics in surface physics. | Fragmentation dynamics of highly excited clusters and biomolecules.<br>- Electronic and vibrational excitation in molecules and nanostructures deposited on metal surfaces.<br>- Theoretical description of reactivity in organic chemistry. | MolPM group can access computational resources of the UAM Computing Center (CCC-UAM) and the Spanish Supercomputing Network (RES). In addition, Dr. Díaz-Tendero is the WG leader of CA18212 COST Action (MDGAS), and is involved in the IRP-LIA-DYNAMICS. | https://molpm.qui.uam.es/ |
| **Antonio Picón** | Chemistry | Attosecond and ultrafast optics | We are involved in the development of new theoretical approaches to describe ultrafast experiments at advanced research laboratories that are able to produce attosecond X-ray pulses. Our main fundamental interest is the understanding of electron dynamics in complex systems and its role in the optical response and energy transfer. | Access to high-performance computing resources, collaboration with international leading laboratories in attosecond science, including front free-electron lasers, and access to a European network formed by the main experts in our field | https://campusys.qui.uam.es |
| **Florentino Borondo** | Química and Instituto de Ciencias Matemáticas (ICMAT) | Deep Learning, Reservoir Computing, Quantum Chaos, Molecular Vibrations | Deep Learning andResevoir Compting applied to the solution of Schrödinger Eq.; Quantum Manifestation of Classical Chaos in Vibrations | Excellent access to computing facilities and libraries at the group and ICMAT | https://portalcientifico.uam.es/ipublic/agent-personal/profile/iMarinaID/04-260097 |

| SAPIENZA UNIVERSITY OF ROME - Italy | | | | contact person: rosa.distefano@uniroma1.it | |
|---|---|---|---|---|---|
| **SUPERVISOR** | **RESEARCH LAB/GROUP** | **AREA OF EXPERTISE** | **LINES OF INVESTIGATION** | **KEY FACILITIES** | **WEBSITE** |
| **Sergio Brutti** | Materials for Energy | Materials Science; electrochemistry; solid state themordynamics | Synthesis, characterization and modelling of advanced materials for application in electrochemical energy storage devices (Li/Na batteries, Li-O2 batteries, supercapacitors) | Inorganic synthesis laboratory facilities (furnaces, oven, chem bench); electrochemical testing stations; Ar-glvoe box, N2 adsorption apparatus; microRaman apparatus. | https://www.chem.uniroma1.it/en/department/people/sergio-brutti |
| **Marco D'Abramo** | Modelling of chemical and biophysical systems | Computational chemistry; biophysics; modelling; statistical mechanics | Use of theoretical and computational tools to model chemical and biological processes. In particular:<br>- Molecular dynamics simulations to understand and describe the motion of biomolecules, how they affect their function<br>- QM/MM approaches to model the electronic structure of (part of) molecules in complex environments | 5 nodes cluster; PRACE and CINECA facilities | https://sites.google.com/a/uniroma1.it/marcodabramo-eng/ |

| STOCKHOLM UNIVERSITY - Sweden | | | | contact person: henrik.aspeborg@su.se | |
|---|---|---|---|---|---|
| **SUPERVISOR** | **RESEARCH LAB/GROUP** | **AREA OF EXPERTISE** | **LINES OF INVESTIGATION** | **KEY FACILITIES** | **WEBSITE** |
| **Aji Mathew** | Materials and Environmental Chemistry (MMK) | Biobased materials for water purification | The group is active in the following research areas<br>**Materials for environment**<br>• Fully biobased membranes/ filters for water purification<br>• Surface chemistry and interactions, mechanical properties, viscoelastic properties, in situ SAXS<br>• Atomic force microscopy (understanding properties at nano scale, colloidal probe)<br>**Materials for health**<br>• Biobased materials for medical applications<br>• Tissue engineering, wound dressing, antifouling and antibacterial materials<br>**Synthesis and processing of sustainable materials**<br>• Nanocellulose and nanochitin isolation and characterization<br>• Designing of recycling and circularity of materials<br>• Processing and characterisation of bionanocomposites, hybrids and crosslinked polymers | **Department of Materials and Environmental Chemistry (MMK)** has highly sophisticated scientific infrastructure which offers support for material synthesis and physical characterization, such as: two powder XRD, TGA, DSC, UV-Vis Spectroscopy, three Scanning Electron Microscopes (SEM) and three Transmission Electron Microscopes (TEM) including an aberration-corrected TEM for EELS and EDX experiments, solid-state and liquid NMR spectrometers and a fully equipped soft matter characterisation lab that will be used for structural, spatial and chemical characterisation of biobased materials. Mathew's lab has facilities for cell-wall fractionation, processing of biobased nanomaterials and synthesis of hybrid materials. We are also a frequent user of large facilities, including Max IV and DESY, to perform in-situ experiments, e.g. in-situ SAXS studies. Special equipment for in-situ studies at MMK includes combination of confocal laser scanning microscopy with atomic force microscopy | https://www.su.se/english/profiles/maji-1.227005 |
| **Alexander Lyubartsev** | Materials and Environmental Chemistry (MMK) | Molecular computer simulations | We use molecular simulations, such as molecular dynamics and Monte Carlo , to model various (bio)molecular and nanomaterial systems. Examples of studies are biomembranes, properties of drug molecules, interaction of inorganic surfaces with biomolecules, modeling of molecular mechanisms of nanotoxicity | We have a local computational cluster, as well as access to Swedish national high-perhormance computing systems. | https://www.su.se/profiles/lyuba-1.187330 |
| **Bengt Mannervik** | Biochemistry and Biophysics | Protein engineering of detoxication enzymes | Directed evolution of enzymes: fundamental studies as well as applications in molecular medicine and biotechnology | Facilities for production and functional characterization of recombinant enzymes, cell culture | https://www.su.se/english/profiles/bmann-1.188234 |
| **Berit Olofsson** | Arrhenius laboratory, Department of Organic chemistrybi | Synthetic organic chemistry | We develop sustainable, transition metal-free methodology for organic synthesis, mainly using hypervalent iodine reagents.<br>The efficiency of the methodology is demonstrated through total synthesis of small natural products or biologically interesting targets. | Our department hosts several leading research groups in synthetic organic chemistry. We have high-quality labs and access to all necessary equipment. | http://www.organ.su.se/bo/ |
| **Jiayin Yuan** | Department of Materials and Environmental Chemistry (MMK) | Functional polymer and carbon materials for energy and environmental application | We currently work very intensively with 3 topic: 1) new poly(ionic liquid) polymers and their composites with particularly 2D materials (graphene, GO and Mxene) for advanced materials (membranes, actuators, sensors, etc.); 2) heteroatom-doped porous carbons and their electrochemical energy applications (including ORR, NRR, CO2RR and single-atom catalyst); 3) biopolymer-based functional materials for energy and environmental applications, particularly in solar energy harvesting and water treatment. | We have common polymer synthesis, characterization and processing technique, including FTIR, UV, AFM, tensile testing, 3D printer, etc. We also have 3 carbonization ovens to produce porous carbons from their precursors. The gas sorption, XRD, electron microscopy up to atomic level, and 2 electrochemical work stations are available. | www.yuan-group.com |
| **Mika Sipponen** | Sustainable Materials Chemistry, Department of Materials and Environmental Chemistry (MMK) | Renewable polymers from natural sources, lignin nanomaterials, colloidal and surface chemistry, enzyme technology, polymer chemistry | The group develops new green processes and materials to replace fossil plastics and other harmful/polluting compounds by more sustainable alternatives in energy, environment, and health applications. Lignin is one of the main natural polymers that the group explores as a renewable raw material. Current projects are dealing with carbon dioxide capture and conversion, development of environmentally friendly coatings, and functional materials and systems based on lignin. | The department has a modern research infrastructure under centrally managed facilities such as MACAL, Mass spectrometry, and EMC with equipment available for material processing, sample preparation, and characterization in solid, liquid, and dispersion states. Besides basic equipment, there are solid- and liquid-state NMR spectrometers, two powder XRD, TGA, DSC, solid state UV-Vis Spectroscopy, three Scanning Electron Microscopes | https://www.su.se/english/profiles/misi6261-1.438807<br>www.sipponenlab.com |

| | | | | | |
|---|---|---|---|---|---|
| | | | | (SEM) and three Transmission Electron Microscopes (TEM) including an aberration-corrected TEM with various sample stages (Themis Z). An atomic force microscope (AFM) is available for basic imaging and morphology studies, and a Zetasizer instrument for dynamic light scattering (DLS) and zeta-potential measurements. Sipponen's sustainbale materials chemistry laboratory is equipped with adequate instrumentation (rotary evaporator, incubators, ovens, fume hoods for organic synthesis, etc.) for material synthesis and sample preparation. Many other instruments are available in the Soft Matter characterization facility. | |
| **Niklas Hedin** | Department of Materials and Environmental Chemistry (MMK) | Adsorption, Carbons, Zeolites, NMR, Gas separation, IR, Biomineralization, CCS, CCU | The main focus is currently on adsorbents for separation or reduction of carbon dioxide, and on carbon materials derived by hydrothermal carbonization. A multipronged approach is applied that includes among other tools molecular spectroscopy. | Numerous, solid-state NMR, in-situ IR, electron microscopy, X-ray diffraction, gas adsorption devices, etc. | https://www.su.se/english/profiles/nhedi-1.187310 |