Dipartimento di Scienze Chimiche
Department of Chemical Sciences

DiSC 2018

An overview of research activities at the Department of Chemical Sciences of the University of Padova

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DI PADOVA

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Introduction

The first chair of chemistry at the University of Padova dates back to 1749, when the Republic of Venice created the *"Schola Chimica Theorica et Experimentalis".* Over the years, chemistry has always been a well-established subject of study in Padova, giving rise to three departments active in the fields of physical, organic, inorganic, analytical and industrial chemistry, which merged together in 2004 to form the Department of Chemical Sciences (DiSC, www.chimica.unipd.it). Nowadays DiSC hosts 91 tenure and tenure-track professors and researchers of the University of Padova, 12 researchers of CNR-National Council of Research and one researcher of INSTM-National Interuniversity Consortium of Materials Science and Technology.

DiSC is the reference structure of four Bachelor Degree Courses (Chemistry, Industrial Chemistry, Materials Science, Science and Technology for the Environment), three Master Degree Courses (Chemistry, Industrial Chemistry, Materials Science) and a Specialization School in Evaluation and Management of Chemical Risk. Furthermore, DiSC hosts two PhD Courses: Molecular Sciences (www.chimica.unipd.it/sdsm, in collaboration with the Department of Pharmaceutical Sciences) and Science and Engineering of Materials and Nanostructures (www.chimica.unipd.it/simn, with the Department of Physics and Astronomy and the Department of Industrial Engineering). In the last three years, both courses offered, on average, 30 PhD scholarships per year. In that period, the Italian Ministry of Education funded about 50% of the scholarships; while the remaining have been financed by research Institutes and industries.

A total of about 1100 bachelor and master students, 81 PhD students and 50 post-docs are currently hosted by DiSC. 57 technicians and administrative staff provide services to support DiSC research and teaching activities. A quarter of DiSC postdocs and PhD students come from abroad, funded by European projects, international programs (UniPD-China Scholarship Council and Tianjin University, Kyungpook National University of South Korea and other specific agreements) and private foundations. A double-degree program is active between DiSC and the Jiustus-Liebig University Giessen for the Masters in Chemistry and Materials Science. DiSC delivers a wide educational offer, able to train professionals and researchers in the main fields of chemistry through teaching laboratories and an instrumentation park that has few analogues in Italy.

The Department has an internationally recognized leading role in the development of interdisciplinary aspects of chemical sciences with research projects supported by Italian and European funding. DiSC researchers contribute to molecular sciences for health, alternative energy sources, catalysis, sustainable chemistry, sensors and biomedical diagnostics. The Department was ranked second among the Chemistry departments of major Italian Universities in the national evaluation report analyzing the quality of research (VQR 2011-14) and holds a relevant position in various international rankings. DiSC is one of the 180 Italian Departments selected as Department of excellence by ANVUR (Italian National Agency for the Evaluation of University and Research Systems) to access nine million euros for the five-years period, from 2018-2022, with the project NExuS: *Nanochimica per l'Energia e la Salute* (Nanochemistry for Energy and Health).

Contacts

Address	Via Marzolo, 1 35131 Padova – Italy
Certified email	dipartimento.chimica@pec.unipd.it
Web	www.chimica.unipd.it
Tel.	+39 049 827 5051

Department Head	Prof. Michele Maggini *michele.maggini@unipd.it* *direttore.chimica@unipd.it* *+39 3347151928*
Vice-Head	Prof. Antonino Polimeno *antonino.polimeno@unipd.it*
Department Secretary	Marco Agnello *marco.agnello@unipd.it*

Research Areas

The research activities of DiSC are focused on six main research areas:

Life Chemistry
Synthesis and analysis of peptides and proteins; studies of photosynthetic systems via optic and magnetic spectroscopies.

Environment, Energy and Cultural Heritage
Development and application of chemical methods to technologies for the production and storage of energy; environment control; cultural heritage conservation.

Materials, Nanomaterials and Surfaces
Synthesis of functionalized organic, inorganic and hybrid materials; development of functional materials with controlled chemical, optic, electric, magnetic properties; studies of interfaces, films and supported nanoparticles.

Supramolecular Chemistry and Nanochemistry
Supramolecular systems and colloidal chemistry; self-assembly of nanostructures and nanoparticles.

Synthesis, Catalysis and Reactivity
Synthesis and characterization of homogeneous/heterogeneous
catalysts; coordination chemistry; organic synthesis, electrosynthesis.

Theoretical and Computational Chemistry
Molecular modeling; in silico characterization; molecular dynamics and reactivity; quantum and statistical methods; computational spectroscopy.

28 research groups develop the research activities at DiSC. They are briefly sketched in the following collection of profiles, each reporting the group name and website, some phone contacts, the structured members, an overview of their main research themes and a representative collection of references. The technical and administrative staff outline follows.

Index of DiSC research groups

Analytical Chemistry

www.chimica.unipd.it/analitica/english
+39 049 827 5182 (PP); 5207 (SB); 5178 (AT)

Denis Badocco (denis.badocco@unipd.it); Sara Bogialli (sara.bogialli@unipd.it); Luca Cappellin (luca.cappellin@unipd.it); Valerio Di Marco (valerio.dimarco@unipd.it); Gabriella Favaro (gabriella.favaro@unipd.it); Marco Frasconi (marco.frasconi@unipd.it); Chiara Giorio (chiara.giorio@unipd.it); Paolo Pastore (paolo.pastore@unipd.it); Andrea Tapparo (andrea.tapparo@unipd.it)

The research areas of the Analytical Chemistry group are focused on three main subjects: 1) mass spectrometry, 2) environmental chemistry and 3) sensoring. The Analytical Chemistry laboratories are equipped with various instrumentations such as high resolution LC-MS (Q-TOF by Agilent and Q-Exactive by Thermo), ICP-MS (Agilent), GC-MS/MS (Thermo) and many other instruments dedicated to the following topics: optical sensors; emerging contaminants in the environment and food; metabolomics; metallomics; atmosphere chemistry; PTR-MS for food and environment; metal-ligand complexation in aqueous solutions for chelation therapy.
The group is currently involved in various collaborations in national and international projects.

- *Ion Pair Formation between Tertiary Aliphatic Amines and Perchlorate in the Biphasic Water/Dichloromethane System,* J. Phys. Chem. B, **2017**,121, 9403-9410.
- *Liquid chromatography-high resolution mass spectrometric methods for the surveillance monitoring of cyanotoxins in freshwaters,* Talanta, **2017**, 170, 322-330.
- *Porous graphite oxide pillared with tetrapod-shaped molecules*, Carbon, **2017**, 120, 145-156.
- *Ornamental plants on sale to the public are a significant source of pesticide residues with implications for the health of pollinating insects,* Environ. Pollution, **2017**, 228, 297-304.
- *Online Quantification of Criegee Intermediates of α-Pinene Ozonolysis by Stabilisation with Spin Traps and Proton Transfer Reaction Mass Spectrometry Detection*, Journal of the American Chemical Society, **2017**, 139, 3999-4008.

Applied Organometallic Chemistry

www.researchgate.net/profile/Andrea_Biffis
+39 049 827 5216 (AB); 5655 (CT)

Andrea Biffis (andrea.biffis@unipd.it); Cristina Tubaro (cristina.tubaro@unipd.it)

The focus of the research of the group lies in the design, synthesis and characterisation of selected classes of organometallic compounds with potential application as catalysts, as bioactive compounds or as active components for advanced materials and devices (luminescent devices, sensors, liquid crystals etc.). In particular, the main target are late transition metal complexes with N-heterocyclic carbene ligands (NHCs). The structure and properties of the carbene ligands are matched to the type, oxidation state, and coordination geometry of the metal centre to yield complexes with the desired properties. Ongoing research projects involve complexes with heteroditopic ligands (dicarbenes, phosphinocarbenes) as well as complexes with NHCs derived from natural compounds.

- *Gold(III) Bis(di-N-heterocyclic carbene) Square Planar Trication with Axial Ligand Interactions with Bromides from Ag/Br Counteranion Assemblies*, Organometallics, **2017**, 36, 2285-2292.
- *Advances in Transition-Metal-Catalysed Alkyne Hydroarylations*, Chem. Rec., **2016**, 16, 1742-1760.
- *Insights into the Halogen Oxidative Addition Reaction to Dinuclear Gold(I) Di(NHC) Complexes*, Chem. Eur. J., **2016**, 22, 10211-10224.
- *Chelate Palladium(II) Complexes with Saturated N-Phosphanyl-N-Heterocyclic Carbene Ligands: Synthesis and Catalysis*, Organometallics, **2016**, 35, 762-770.

Bioinorganic Chemistry

www.chimica.unipd.it/bioinorg
+39 049 827 5159 (DF); 5845 (CN), 5727 (lab)

Dolores Fregona (dolores.fregona@unipd.it); Chiara Nardon (chiara.nardon@unipd.it).

The research of the lab is at the interface between inorganic chemistry, biology and medicine.
Our experience covers the synthesis of coordination compounds, the use of several spectroscopic techniques to characterize the newly synthesized complexes, the biological investigation of the anticancer/antinflammatory activity of the compounds both *in vitro* and *in vivo*. Our researches include also the study of the in-solution properties of the new medicinal agents under physiological-like conditions, their mechanism of action and interaction with biomolecules. To achieve our goals, we exploit a highly interdisciplinary strategy which combines and merges different backgrounds and professional expertise encompassing aspects of inorganic and organic chemistry, biology, pharmacology and medicine.

- *New comprehensive studies of a gold(III) Dithiocarbamate complex with proven anticancer properties: Aqueous dissolution with cyclodextrins, pharmacokinetics and upstream inhibition of the ubiquitin-proteasome pathway,* European J. Med. Chem.,**2017,** 138, 115-127.
- *Cell and Cell-Free Mechanistic Studies on Two Gold(III) Complexes with Proven Antitumor Properties,* European J. Inorg. Chem.*,* **2017,** 12, 1737-1744.
- *Ru(III) anticancer agents with aromatic and non-aromatic dithiocarbamates as ligands: Loading into nanocarriers and preliminary biological studies,* J. Inorg. Biochem.*,* **2017***,* 165*,* 159-169.
- *Gold Complexes for Therapeutic Purposes: an Updated Patent Review (2010-2015),* Curr. Med. Chem., **2016**, 23, 3374-3403.
- *Is matching ruthenium with dithiocarbamato ligands a potent chemotherapeutic weapon in oncology?,* Future Med. Chem.*,* **2016,** 8, 211-226.

Biomolecular Structures

www.chimica.unipd.it/stefano.mammi
+39 049 827 5293 (SM)

Stefano Mammi (stefano.mammi@unipd.it); Roberto Battistutta (roberto.battistutta@unipd.it); Massimo Bellanda (massimo.bellanda@unipd.it); Elisabetta Schievano (elisabetta.schievano@unipd.it); Andrea Calderan (andrea.calderan@unipd.it); Paolo Ruzza (paolo.ruzza@unipd.it)

The research of the Biomolecular Structure Group is addressed to the study of peptides and proteins. We investigate their chemical and structural properties with the goal to elucidate the molecular mechanisms at the basis of their biological activity in natural processes. We then apply this knowledge to try to modify the properties of selected targets (for instance for biotechnological applications) or to correct them when correlated to pathological states. The main experimental techniques we employ are multidimensional NMR and protein crystallography. Another focus of our research is the application of NMR, in combination with multivariate statistical analysis, to the metabolomic study of complex matrices such as food extracts and biological fluids. The applications range from the development of new methods to the traceability of food products to the development of new analytical tools to establish the *in vivo* effects of exogenous substances. Our main research lines are the following:

- Structural, functional and inhibition studies of oncogenic protein kinases CK2 and CDK2;
- Structural and functional characterization of SulP/SLC26 anion transporters;
- Enzyme engineering for industrial applications;
- Structure and interactions of proteins involved in the peculiar redox metabolism of pathogenic organisms;
- Fragment-based drug discovery by NMR and crystallography;
- Metabolomic analysis of food extracts and biological fluids;
- Traceability of foodstuff;
- Synthesis and characterization of peptide and peptidomimetics.

- *Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters*, Nat. Comm., **2014**, 5, 3622-35.
- *Objective Definition of Monofloral and Polyfloral Honeys Based on NMR Metabolomic Profiling*, J. Agric. Food Chem., **2016**, 64, 3645-3652.
- *Interactions of GFAP with ceftriaxone and phenytoin: SRCD and molecular docking and dynamic simulation*, Biochim. Biophys. Acta-Gen. Subj., **2016**, 1860, 2239-2248.
- *NMR Quantification of Carbohydrates in Complex Mixtures. A Challenge on Honey*, Anal. Chem., **2017**, 89, 13405-13414.
- *Polyamine-Based Thiols in Trypanosomatids: Evolution, Protein Structural Adaptations, and Biological Functions.* Antioxid. Redox Signal., **2018**, 28, 463– 486.

Bio-Organic Chemistry

www.chimica.unipd.it/bocgroup
+39 049 827 5277 (FF)

Fernando Formaggio (fernando.formaggio@unipd.it); Barbara Biondi (barbara.biondi@unipd.it); Marco Crisma (marco.crisma@unipd.it); Marta De Zotti (marta.dezotti@unipd.it); Marina Gobbo (marina.gobbo@unipd.it); Alessandro Moretto (alessandro.moretto.1@unipd.it); Cristina Peggion (cristina.peggion@unipd.it)

The research activity of the Bio-Organic Chemistry group is focused on the exploitation of peptides and conformationally constrained peptides for applications in organic, physical, biophysical and supramolecular chemistry. The group is currently engaged in the following research lines:

- synthesis, conformation, mechanism of action and bioactivities (antibacterial and antitumor) of the naturally-occurring peptaibiotics;
- textiles functionalized with antibacterial peptides for biomedical applications;
- peptide nanotechnology: peptido-rotaxanes, self-assembled peptide polymers, peptide-decorated metal nanoparticles for nanomedicine;
- synthesis and conformation of peptides with rigid and well-defined 3D-structure as structural elements for spectroscopic studies and for electron transfer and photovoltaic applications.

- *Spectroscopic Insights into Carbon Dot Systems*, J. Phys. Chem. Lett., **2017**, 8, 2236–2242.
- *Enhanced EGFR Targeting Activity of Plasmonic Nanostructures with Engineered GE11 Peptide,* Adv. Healthcare Mater., **2017**, 6, 2192-2201.
- *A terminally protected dipeptide: from crystal structure and self-assembly, through co-assembly with carbon-based materials, to a ternary catalyst for reduction chemistry in water*, Soft Matter, **2016**, 12, 238-245.
- *The peculiar N- and C-termini of trichogin GA IV are needed for membrane interaction and human cell death induction at doses lacking antibiotic activity*, BBA Biomembranes, **2015**, 1848, 134-144.
- *Cotton functionalized with peptides: characterization and synthetic methods*, J. Pept. Sci., **2014**, 20, 547-553.

Chemistry of Cultural Heritage

+39 049 827 5204 (RB); 5854 (lab); 5173 (lab)

Renzo Bertoncello (renzo.bertoncello@unipd.it);
Luca Nodari (luca.nodari@ieni.cnr.it)

The investigation in material science of Cultural Heritage Artefacts are mainly devoted to the study of inorganic materials (glass, ceramics and metals) by using non-conventional spectroscopic techniques, as X-rays photoelectron spectroscopy (XPS) and Mössbauer spectroscopy. By using these facilities, we investigate about technology processes and alteration phenomena in various cultural heritage materials since the beginning of the ’90.

Recently the group has worked in Cappella degli Scrovegni in Padua, in the San Marco church mosaics and in the artistic glasses of San Giovanni e Paolo churches in Venice. Nowadays the equipment provided to Cultural Heritage Research group are: portable LIBS (Laser Induced Breakdown Spectroscopy); portable micro-XRF (X-Ray Fluorescence); 57Fe Mössbauer spectroscopy operating in transmission (micro-invasive) and reflection (micro-invasive, non-invasive mode); XPS (X-ray Photoelectron Spectroscopy); AFM (Atomic Force Microscopy); FEG-ESEM equipped with detector for EDS analyses; optical microscopy; climatic chamber. Also accessible to the group Raman, IR, UV- Vis spectroscopies together with SIMS (Secondary Ion Mass Spectrometry) and in collaboration with Louvre museum laboratories we have access to IBA (Ion Beam Analyses) techniques. Moreover, the group has reached an optimum research experience in projecting and synthetizing silica based coating for glass, ceramic and metallic substrates.

- *Photoelectrochemical Behavior of Electrophoretically Deposited Hematite Thin Films Modified with Ti(IV)*, Molecules, **2016**, 21, 942.
- *Potash‐lime‐silica glass: protection from weathering*, Herit. Sci., **2015**, 3, 22.
- *Sol–gel silica coating for potash–lime–silica stained glass: Applicability and protective effect*, Journal of Non-Crystalline Solids, **2014**, 390, 45–50.
- *Non-invasive multitechnique methodology applied to the study of two 14th century canvases by Lorenzo Veneziano*, Journal of Cultural Heritage 14S, **2013**, e153–e160.

Electrocatalysis and Applied Electrochemistry

www.chimica.unipd.it/electrochem/
+39 049 827 5132 (AG), 5677 (AAI), 5112 (CD)

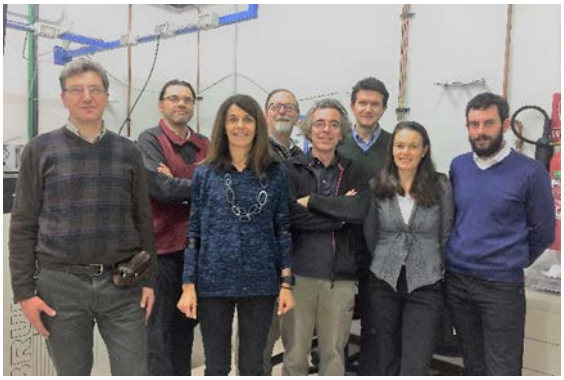
Armando Gennaro (armando.gennaro@unipd.it); Abdirisak Ahmed Isse (abdirisak.ahmedisse@unipd.it); Christian Durante (christian.durante@unipd.it)

The research group applies electrochemical methods to the study of chemical problems, conducting investigations in electro-organic chemistry,
electrochemical surface science, catalysis and environmental electrochemistry. The research activity is centered in the field of molecular electrochemistry with particular attention to electrosynthesis and electrocatalysis, especially the study of mechanisms of organic electrochemical processes, the development of eco-friendly electrosyntheses for industrial applications and the development of electrocatalytic materials and/or electrocatalytic processes. The main topics of the research activity are electrocatalytic reduction of organic halides, mechanisms of electron transfers, electrochemical approaches to controlled radical polymerizations, electrochemical activation of carbon dioxide, electrocarboxylation and electrosyntheses of fine chemicals and pharmaceutical compounds, and development of electrocatalytic materials for Oxygen Reduction Reaction (ORR).

- *Absolute Potential of the Standard Hydrogen Electrode and the Problem of Interconversion of Potentials in Different Solvents,* J. Phys. Chem. B, **2010**, 114, 7894-7899.
- *Electrochemically Mediated Atom Transfer Radical Polymerization*, Science, **2011**, 332, 81-84.
- *Electrocatalytic properties of transition metals towards reductive dechlorination of polychloroethanes*, Electrochim. Acta, **2012**, 70, 50-61.
- *Electrochemical triggering and control of Atom Transfer Radical Polymerization,* Curr. Opin. Electrochem., **2018**, 8, 1-7.
- *One Step forward to a Scalable Synthesis of Platinum-Yttrium alloyed Nanoparticles on Mesoporous Carbon for Oxygen Reduction Reaction,* J. Mater. Chem. A, **2016**, 4, 12232-12240.

EPR Spectroscopy

www.chimica.unipd.it/eprgroup/
+39 049 827 5144 (DC); 5123 (MB)



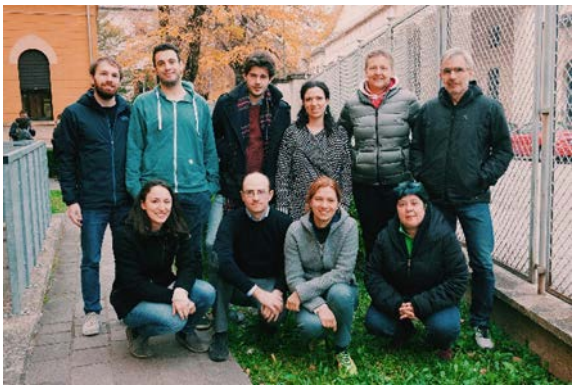
Donatella Carbonera (donatella.carbonera@unipd.it); Antonio Toffoletti (antonio.toffoletti@unipd.it); Lorenzo Franco (lorenzo.franco@unipd.it); Marilena Di Valentin (marilena.divalentin@unipd.it); Marco Ruzzi (marco.ruzzi@unipd.it); Alfonso Zoleo (alfonso.zoleo@unipd.it); Antonio Barbon (antonio.barbon@unipd.it); Marco Bortolus (marco.bortolus@unipd.it).

The research activity of the group is focused on the development and application of Electron Paramagnetic Resonance (EPR) techniques to **Material Science** (graphene, metal nanoparticles, organic photovoltaics, cultural heritage materials), and **Biology** (natural and artificial photosynthetic systems, hydrogenases and bio-inspired analogs for the bio-production of hydrogen, protein motions as detected by spin labelling techniques).
The facilities of the EPR Laboratory include: - X-band CW- and pulsed-EPR spectrometer, equipped with pulsed ENDOR and PELDOR accessories - Two CW and ENDOR X band spectrometers - Time-resolved EPR spectrometer for analysis of light-induced processes - Q-band EPR spectrometer with CW, pulsed, ENDOR, PELDOR and time-resolved accessories - Optically detected Magnetic Resonance (ODMR) spectrometer.

- *Identifying conformational changes with site-directed spin labeling reveals that the GTPase domain of HydF is a molecular switch*, Scientific Reports**, 2017**, 7, 1714.
- *Light-Induced Porphyrin-Based Spectroscopic Ruler for Nanometer Distance Measurement*, Chemistry-A European Journal, **2016**, 22, 17059-17064.
- *Time-Resolved EPR of Photoinduced Excited States in a Semiconducting Polymer/PCBM Blend*, J. Phys. Chem. C, **2013**, 117, 1554–1560.
- *Au-25(SEt)(18), a Nearly Naked Thiolate-Protected Au-25 Cluster: Structural Analysis by Single Crystal X-ray Crystallography and Electron Nuclear Double Resonance*, ACS Nano, **2014**, 8, 3904-3912.
- *Radical-Enhanced Intersystem Crossing in New Bodipy Derivatives and Application for Efficient Triplet-Triplet Annihilation Upconversion*, J. Am. Chem. Soc., **2017**, 139, 7831–7842.

Laser Spectroscopy and Nanophotonics

www.chimica.unipd.it/lsnp/
+39 049 827 5148 (CF); 5131 (EC); 5118 (RS)



Camilla Ferrante (camilla.ferrante@unipd.it); Danilo Pedron (danilo.pedron@unipd.it); Raffaella Signorini (raffaella.signorini@unipd.it); Elisabetta Collini (elisabetta.collini@unipd.it); Roberto Pilot (roberto.pilot@unipd.it).

The group has a long standing experience in the investigation of inter- and intra-molecular charge and energy transfer, fast coherent and incoherent dynamics, and nonlinear optical response in complex systems like molecular crystals, molecular aggregates, metal and semiconductor nanoparticles. Recently optical properties of properly synthetized nanostructured materials, like core-shells, spherical nanoparticles and metallic substrates have been investigated, with particular attention to the near-field spectral distribution, in view of application as optical sensors, and to the nanoparticles-proteins/cells interactions. Nonlinear optical properties of these materials have also been exploited for the realization of optical devices, like optical limiters, nanolasers and microfluidic circuits.

- *Correlated Fluctuations and Intraband Dynamics of J-Aggregates Revealed by Combination of 2DES Schemes,* J. Phys. Chem. Lett., **2016***,* 7, 4996-5001.
- *Oxidation effects on the SERS response of silver nanoprism arrays,* RSC Adv., **2017***,* 7, 369-378.
- *Mechanistic insight into internal conversion process within Q-bands of chlorophyll a,* Sci. Rep., **2017***,* 7, 11389/1-7.
- *Spectroscopic insights into carbon dot systems,* J. Phys. Chem. Lett., **2017***,* 8(7), 2236-2242.
- *Bridging Energetics and Dynamics of Exciton Trapping in Core–Shell Quantum Dots,* J. Phys. Chem. C, **2017***,* 121(1), 896-902.

Molecular Electrochemistry and Nanosystems

www.chimica.unipd.it/flavio.maran/
+39 049 827 5147 (FM); 5193 (SA); 5194 (SB); 5117-5133 (labs)



Flavio Maran (flavio.maran@unipd.it); Sabrina Antonello (sabrina.antonello@unipd.it); Sara Bonacchi (sara.bonacchi@unipd.it)

The M.E.N. Group focuses on molecular aspects of electrochemical reactions and nanosystems, from both fundamental and applied viewpoints. Specific research topics include:

- Electron transfer through molecular bridges and interfaces;
- Dissociative electron transfer;
- Monolayer-protected clusters: electrochemical, optical and magnetic properties, redox catalysis, drug-delivery systems;
- Electrochemical sensors for cancer biomarkers and volatile chemicals;
- Self-assembled monolayers of conformationally constrained peptides.

The M.E.N. group is equipped with state-of-the-art electrochemical instrumentations, including electrogenerated chemiluminescence and SECM, STM and AFM, PM-IRRAS and UV-visible spectrometers, HPLC.

- *Electrocrystallization of Monolayer Protected Gold Clusters: Opening the Door to Quality, Quantity and New Structures,* J. Am. Chem. Soc., **2017**, 139, 4168-4175.
- *Magnetic Ordering in Gold Nanoclusters,* ACS Omega, **2017**, 2, 2607-2917.
- *From Blue to Green: Fine Tuning of Photoluminescence and Electrochemiluminescence in Bifunctional Organic Dyes,* J. Am. Chem. Soc., **2017**, 139, 2060-2069.
- *Molecular Electrochemistry of Monolayer-Protected Clusters,* Curr. Opinion Electrochem., **2017**, 2, 18-25.
- *A Magnetic Look into the Protecting layer of Au25 Clusters,* Chem. Sci., **2016**, 7, 6910-6918.

Molecular Materials, Colloids & Modeling (M_2CM)

www.chimica.unipd.it/m2cm/links.html
+39 049 827 5236 (LA); 5164 (MC); 5736 (SG)

Lidia Armelao (lidia.armelao@unipd.it); Gregorio Bottaro (gregorio.bottaro@unipd.it); Silvia Carlotto (silvia.carlotto@unipd.it); Maurizio Casarin (maurizio.casarin@unipd.it); Daniel Forrer (daniel.forrer@unipd.it); Silvia Gross (silvia.gross@unipd.it); Marta Maria Natile (martamaria.natile@unipd.it); Marzio Rancan (marzio.rancan@unipd.it); Andrea Vittadini (andrea.vittadini@unipd.it); Pier Luigi Zanonato (pierlugi.zanonato@unipd.it)

Design, synthesis, characterization, and modeling of supramolecular structures and of nanocrystalline inorganic colloids with applications ranging from energy to nanomedicine by way of catalysis and optics are at the core of our scientific activity. Innovative inorganic nanostructures are obtained in the former case through strategies of molecular self-assembly by exploiting non-covalent, selective and directional interactions, in the latter one by sustainable wet chemistry and colloidal routes. Furthermore, organic-inorganic hybrid materials are prepared starting from suitably functionalized inorganic building blocks. All the systems are studied and characterized with advanced experimental and computational techniques. Advanced synchtron-assisted analytical methods (XAS, photoemission, SAXS) complement the chemico-physical and structural characterizations at Home.

- *Pursuing the Crystallization of Mono- and Polymetallic Nanosized Crystalline Inorganic Compounds by Low-Temperature Wet-Chemistry and Colloidal Routes*, Chem. Rev., **2015**, 115, 11449-11502.
- *Hampered Subcomponent Self-Assembly Leads to an Aminal Ligand: Reactivity with Silver(I) and Copper(II)*, Eur. J. Inorg. Chem., **2017**, 30-34.
- *Energetics of CO oxidation on lanthanide-free perovskite systems: the case of Co-doped SrTiO3*, Phys. Chem. Chem. Phys., **2016**, 18, 33282-33286.
- *Very high temperature tiling of tetraphenylporphyrin on rutile TiO2(110)*, Nanoscale, **2017**, 9, 11694-11704.
- *Cu(I) and Ag(I) complex formation with the hydrophilic phosphine 1,3,5-triaza-7-phosphadamantane in different ionic media. How to estimate the effect of a complexing medium*, Dalton Trans.**, 2017**, 46, 1455–1466.

Molecular Recognition and Catalysis

www.chimica.unipd.it/lab108/
+39 049 827 5289 (GL); 5244 (CZ)

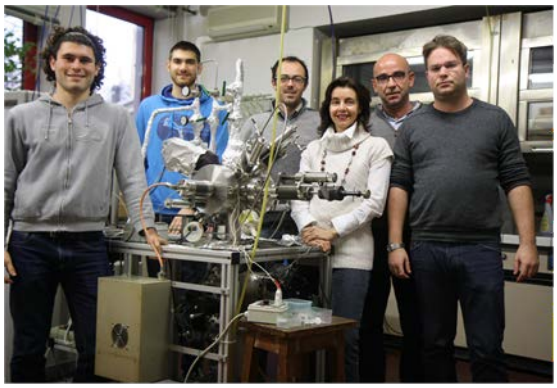
Giulia Licini (giulia.licini@unipd.it); Cristiano Zonta (cristiano.zonta@unipd.it).

The Molecular Recognition and Catalysis group is interested in all aspects of selective catalytic transformations and molecular recognition, and especially in the design, discovery, and study of systems that catalyze fundamentally useful organic reactions, in particular Lewis Acid catalysis and oxidations. In addition, we apply the tools of physical-organic chemistry to gain insight into the transition structure geometries and molecular recognition events that control reactivity and selectivity. The following topics are currently under investigation in our laboratories: - Activation of Small Molecules (CO2, O2, H2O2) - Mimics of Physiologically Important Metallo-Enzymes (haloperoxidases, ligninperoxidases); - New Approaches to Catalyst Design and Recycling in Green Chemistry; - Self-Assembled Molecular Cages and Catalysis in Confined Spaces; - Stereodynamic Chiral Probes for e.e. Determination.

- *Concentration-Independent Stereodynamic g-Probe for Chiroptical Enantiomeric Excess Determination*, J. Am. Chem. Soc., **2017**, 139, 15616–15619, DOI: 10.1021/jacs.7b09469.
- *Triggering Assembly and Disassembly of a Supramolecular Cage*, J. Am. Chem. Soc., **2017**, 139, 6456–6460 DOI: 10.1021/jacs.7b02341.
- *Vanadium(V) Catalysts with High Activity for the Coupling of Epoxides and CO2: Characterization of a Putative Catalytic Intermediate,* ACS Catalysis, **2017**, 7, 2367–2373, DOI: 10.1021/acscatal.7b00109.
- *Heterolytic (2 e) vs Homolytic (1 e) Oxidation Reactivity: N-H versus C-H Switch in the Oxidation of Lactams by Dioxirans*, Chem. Eur. J., **2017**, 23, 259-262. DOI: 10.1002/chem.201604507.
- *Effective bromo and chloro peroxidation catalysed by tungsten(VI) amino triphenolate complexes,* Dalton Trans., **2016**, 45, 14603-14608. DOI**:** 10.1039/C6DT01780K.

Multi-functional Nanomaterials

www.chimica.unipd.it/multi-functional-material-group/index.htm
+39 049 827 5234 (CM); 5192 (AG); 5170 (DB)



Chiara Maccato (chiara.maccato@unipd.it); Alberto Gasparotto (alberto.gasparotto@unipd.it); Davide Barreca (davide.barreca@unipd.it).

The Multi-functional Nanomaterials Group has an internationally recognized know-how in the fabrication of inorganic nanoarchitectures (thin films, supported nanoparticles, nanowires, nanoplatelets,…) by chemical vapor deposition (CVD), plasma enhanced-CVD, and radio frequency-sputtering. Attention is also devoted to the synthesis of novel molecular precursors for CVD and PE-CVD processes.
The developed nanosystems are deeply characterized to unravel structure-property relationships and investigated for sustainable end-uses, encompassing photo-activated applications (H2 production by photocatalysis and photoelectrochemical water splitting, air/water purification, self-cleaning and anti-fogging systems), molecular detection of flammable/toxic gases, but also anodes for Li-ion batteries and magnetic materials.

- *Surface functionalization of nanostructured Fe2O3 polymorphs: from design to light-activated applications*, ACS Appl. Mater. Interfaces, **2013**, 5, 7130-7138.
- *Enhanced hydrogen production by photoreforming of renewable oxygenates through nanostructured Fe2O3 polymorphs*, Adv. Funct. Mater., **2014**, 24, 372-378.
- *Pt-functionalized Fe2O3 Photoanodes for Solar Water Splitting: the Role of Hematite Nano-organization and Platinum Redox State*, Phys. Chem. Chem. Phys., **2015**, 17, 12899-12907.
- *Advances in photocatalytic NOX abatement through the use of Fe2O3/TiO2 nanocomposites*, RSC Adv., **2016**, 6, 74878-74885.
- *Vapor phase fabrication of nanoheterostructures based on ZnO for photoelectrochemical water splitting*, Adv. Mater. Interfaces, **2017**, 4, 1700161-1 1700161-9.

Nano & Molecular Catalysis

www.chimica.unipd.it/NanoMolCat
Tel.: +39 049 827 5670 (MB); 5256 (MC); 5252 (AS)

Marcella Bonchio (marcella.bonchio@unipd.it); Mauro Carraro (mauro.carraro@unipd.it); Andrea Sartorel (andrea.sartorel@unipd.it); Luca Dell'Amico (luca.dellamico@unipd.it); Giacomo Saielli (giacomo.saielli@unipd.it)

The group has established a highly interdisciplinary activity on the study of novel bio-inspired catalytic systems, molecular materials and functional hybrid architectures. Main topics include: (i) artificial photosynthesis: development of multi-redox routines powered by light irradiation for water splitting, CO2 fixation and stereoselective light-driven reactions for the synthesis of biologically relevant molecules with application to flow photochemistry; (ii) design of synthetic enzymes (synzymes), bio-conjugate nanomaterials and hybrid membranes for the interaction with diverse biological targets involved in ROS-related diseases, with applications in catalysis and nanomedicine; (iii) computational modeling in collaboration with ITM-CNR: DFT calculations of spectroscopic properties of organic and organometallic systems and MD simulations of ionic liquids and ionic liquid crystals.

- *Hydrogen Evolution by FeIII Molecular Electrocatalysts Interconverting between Mono and Di-Nuclear Structures in Aqueous Phase,* ChemSusChem, **2017**, 10, 4430–4435.
- *Photo-assisted water oxidation by high-nuclearity cobalt-oxo cores: tracing the catalyst fate during oxygen evolution turnover*, Green Chem.**, 2017**, 19, 2416-2426.
- *Merged Heme and Non-Heme Manganese Cofactors for a Dual Antioxidant Surveillance in Photosynthetic Organisms,* ACS Catal., **2017**, 7, 1971-1976.
- *Tuning Iridium Photocatalysts and Light Irradiation for Enhanced CO2 reduction*, ACS Catal., **2017**, 7, 154-160.
- *Dynamic Anti-Fouling of Catalytic Pores Armed with Oxygenic Polyoxometalates*, Adv. Mater. Interfaces*,* **2015**, 2, 1500034-1500034.

Nanostructures & (Bio)molecules Modeling

www.tame-plasmons.eu
+39 049 827 5295 (SC)

Stefano Corni (stefano.corni@unipd.it)

The group is developing and applying multiscale computational methods for hybrid systems, such as organic and biological molecules interacting with inorganic nanoparticles. The exploited methods range from ab initio atomistic calculations and classical molecular dynamics to classical electrodynamics. The main research topics are:

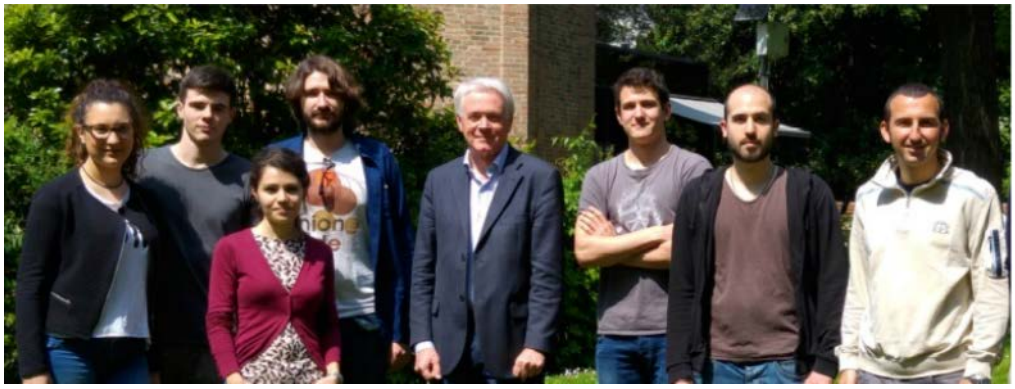
- ultrafast spectroscopy and optical properties of molecules close to plasmonic nanostructures & in solution, including surface enhanced optical phenomena. -the quantum nature of plasmonics excitations at the nanoscale.
- the interactions of inorganic surfaces and nanoparticles with proteins.

Currently the group is funded by the ERC CoG Grant TAME-Plasmons (2016-2021), dedicated to develop simulation approaches for the optical properties of molecules close to plasmonic nanostructures.

- *How to Identify Plasmons from the Optical Response of Nanostructures,* ACS Nano, **2017**, 11, 7321–7335.
- *The interaction with gold suppresses fiber-like conformations of the amyloid β (16–22) peptide,* Nanoscale, **2016**, 8, 8737-8748
- *Probing the influence of citrate-capped gold nanoparticles on an amyloidogenic protein,* ACS Nano, **2015**, 9, 2600-2613.
- *Facet selectivity in gold binding peptides: exploiting interfacial water structure,* Chem. Sci., **2015**, 6, 5204-5214.
- *Surface packing determines the redox potential shift of cytochrome c adsorbed on gold,* J. Am. Chem. Soc., **2014**, 136, 12929-12937.

Nanostructures & Optics

www.chimica.unipd.it/nanostructures.optics/
+39 049 827 5127 (MM)



Moreno Meneghetti (moreno.meneghetti@unipd.it)

Research activities at NOL are on the synthesis, characterization and applications of nanostructures for fields like nanobiotechnology and related fields, new materials for photovoltaic cells and in cultural heritage. All these activities are based on plasmonic and magnetoplasmonic nanostructures obtained by laser ablation of bulk materials under solvents. The plasmonic properties are exploited in particular for the SERS effect, whereas the magnetic ones for magnetophoresis. For the nanobiotechnological applications the nanostructures are functionalized with molecules (peptides and antibodies) for cell targeting and their activity is studied as a function of their organization on the nanostructure surface. SERS properties of the nanostructures are exploited in cultural heritage studies and new materials are obtained for perovskite solar cells.

- *Enhanced EGFR Targeting Activity of Plasmonic Nanostructures with Engineered GE11 Peptide,* Adv. Healthcare Mater., **2017**, 1700596 (DOI: 10.1002/adhm.201700596).
- *High-Quality, Ligands-Free, Mixed-Halide Perovskite Nanocrystals Inks for Optoelectronic Applications,* Adv. Energy Mater., **2017**, 7, 1601703 (DOI: 10.1002/aenm.201601703).
- *A new integrated TLC/MU-ATR/SERS advanced approach for the identification of trace amounts of dyes in mixtures,* Analytica Chimica Acta, **2017***,* 991, 104-112 (DOI: 10.1016/j.aca.2017.08.020).
- *Degradation-by-design: Surface modification with functional substrates that enhance the enzymatic degradation of carbon nanotubes,* Biomaterials*,* **2015**, 72, 20-28 (DOI: 10.1016/j.biomaterials.2015.08.046).
- *Perylene Derivatives As Useful SERRS Reporters, Including Multiplexing Analysis,* ACS Appl. Mater. Interfaces, **2015**, 7, 28042−28048 (DOI: 10.1021/acsami.5b03586).

New materials for energy conversion and storage

+39 049 827 5232 (GC)

Gianni Cavinato (gianni.cavinato@unipd.it)

Main research interests are in the field of the synthesis and reactivity of transition metals complexes and their applications in homogeneous and heterogeneous catalysis. The laboratory is equipped with a carbonylation plant, GC, HPLC and other instruments dedicated to the following research lines:

- synthesis, structural investigation and reactivity of palladium complexes;
- organic synthesis catalyzed by transition metals via carbonylation and hydrogenation;
- catalytic copolymerization (carbon monoxide-olefins) for polyketones production.

The group is currently involved in two projects for the synthesis and functionalization of materials for energy conversion and storage.

- *A polyketone-based anion exchange membrane for electrochemical applications: synthesis and characterization,* Electrochimica Acta, **2017**, 226, 148-157.
- *A hybrid polyketone–SiO2 support for palladium catalysts and their applications in cinnamaldehyde hydrogenation and in 1-phenylethanol oxidation,* Applied Catalysis A: General, **2015**, 496, 40-50.
- *Carbonylation of ethene catalysed by Pd(II)-Phosphine complexes,* Molecules, **2014**, 19, 15116-15161.
- *Interplay between morphology and electrochemical performance of "core-shell" electrocatalysts for oxygen reduction reaction based on a PtNix carbon nitride "shell" and a pyrolyzed polyketone nanoball "core"*, International Journal of Hydrogen Energy, **2014**, 39, 2828-2841.
- *Synthesis, studies and fuel cell performance of "core-shell" electrocatalysts for oxygen reduction reaction based on a PtNix carbon nitride "shell" and a pyrolyzed polyketone nanoball "core"*, International Journal of Hydrogen Energy, **2014**, 39, 2812-2827.

Organic Chemistry for the Environment and Health

www.chimica.unipd.it/cristina.paradisi/
+39 049 827 5661 (CP)

Cristina Paradisi (cristina.paradisi@unipd.it), Ester Marotta (ester.marotta@unipd.it).

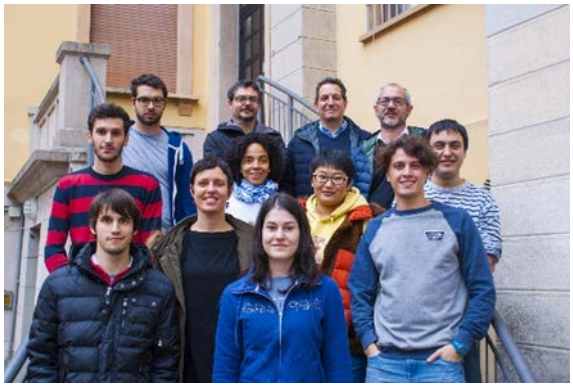
We pursue two lines of research:

1. *Non-thermal* (alias *non-equilibrium*) plasmas as a novel means to induce chemical processes of interest for the environment, energy and agrifood applications
   - advanced oxidation for air and water remediation
   - CO_2 conversion
   - conservative treatment of fresh food and stimulation of algal growth
2. Design and synthesis of mitochondria-targeted small molecules to report on or to affect mitochondrial function and dysfunction.

- *Complete mineralization of organic pollutants in water by treatment with air non-thermal plasma*, Chem. Eng. J., doi.org/10.1016/j.cej.2017.12.107
- *Oxidation of clofibric acid in aqueous solution using a non-thermal plasma discharge or gamma radiation*, Chemosphere, **2017**, 187, 395-403.
- *Investigation on plasma-driven methane dry reforming in a self-triggered spark reactor*, Plasma Process. Polym., **2015**, 12, 808-816.
- *Direct pharmacological targeting of a mitochondrial ion channel selectively kills tumor cells in vivo,* Cancer Cell, **2017**, 31, 516-531.
- *Novel lipid-mimetic prodrugs delivering active compounds to adipose tissue.* Eur. J. Med. Chem., **2017**, 135, 77-88.

Organic Materials

www.chimica.unipd.it/lab205
+39 049 827 5662 (MM)



Tommaso Carofiglio (tommaso.carofiglio@unipd.it); Michele Maggini (michele.maggini@unipd.it); Miriam Mba (miriam.mba@unipd.it); Enzo Menna (enzo.menna@unipd.it)

Organic synthesis towards functional materials is at heart of the group, whose research focuses mainly on the chemical functionalization of carbon nanostructures for solar energy conversion and biomedical applications, the use of nanocellulose as a platform for bio-inspired functional materials and the preparation of functional supramolecular gels. We often use the microfluidics toolbox to study reactions or surface absorption kinetics, the controlled functionalization of nanosystems or the batch-to-flow transposition of active pharmaceutical ingredients of industrial interest. Main characterization techniques for organic synthesis and materials, including high-field and solid-state NMR, NIR absorption, TGA and DSC thermal analysis, AFM-STM at ambient conditions, benchtop flow reactors and cleanroom facilities are commonly accessed by the group components.

- *The Renaissance of Fullerenes with Perovskite Solar Cells*, Nano Energy, **2017**, 41, 84-100.
- *A D-π-A organic dye - reduced graphene oxide covalent dyad as a new concept photosensitizer for light harvesting applications*, Carbon, **2017**, *115*, 746-753.
- *Organic Functionalized Carbon Nanostructures for Functional Polymer-Based Nanocomposites*, Eur. J. Org. Chem. **2016**, 2016, 1071-1090.
- *Boosting perovskite solar cells performance and stability through doping a poly-3(hexylthiophene) hole transporting material with organic functionalized carbon nanostructures*, Adv. Funct. Mater., **2016**, 26, 7443-7453.
- *Tuning the Electron-Acceptor Properties of [60]Fullerene by Tailored Functionalization for Application in Bulk Heterojunction Solar Cells*, Asian J. Org. Chem., **2016**, 5, 676–684.

Physical chemistry of nano and organometallic materials

www.chimica.unipd.it/PHYNOM
+39 049 827 5119 (SS); 5673 (VA)

Saverio Santi (saverio.santi@unipd.it); Vincenzo Amendola (vincenzo.amendola@unipd.it)

PHYNOM members investigate the synthesis, properties and applications of nano and organometallic materials. PHYNOM is organized in two units.
The research of the Physical Organometallic Chemistry unit is aimed at the spectroelectrochemical study of the optical and redox properties of *ad hoc* synthetized (multi)ferrocenyl systems in which the metal-to-metal charge transfer is mediated by different organic backbones, such as peptides, aromatic polycycles and photochromic molecules.
The Laser Assisted Synthesis and Plasmonics unit focuses on laser generation of colloids to produce plasmonic and other multifunctional nanoparticles for photonics, sensor science, nanomedicine, catalysis and related fields. Mechanistic aspects of laser synthesis in liquids, which include laser ablation, laser fragmentation and laser melting, are also investigated.

- *A quarter-century of nanoparticle generation by lasers in liquids: Where are we now, and what's next?,* J. Coll. Interf. Sci., **2017**, 489, 1-2.
- *Benzodithiophene and Benzotrithiophene as π-Cores for Two- and Three-Blade Propeller-Shaped Ferrocenyl-Based Conjugated Systems*, Eur. J. Org. Chem., **2017**, 5966-5974.
- *Hydrogen-Bond-Assisted, Concentration-Dependent Molecular Dimerization of Ferrocenyl Hydantoins*, Organometallics, **2017**, *36*, 2190-2197.
- *Surface plasmon resonance in gold nanoparticles: a review,* J. Phys.: Condens. Matter, **2017**, 29, 203002.
- *Enhanced Electrocatalytic Oxygen Evolution in Au–Fe Nanoalloys,* Angew. Chem. Int. Ed.*,* **2017**, 56, 6589-6593.

Polymer Science

www.chimica.unipd.it/grsp/pubblica/indexinglese.htm
+39 049 827 5233 (CM)

Carla Marega (carla.marega@unipd.it), Valerio Causin (valerio.causin@unipd.it)

In the labs of the Polymer Science group, different kinds of polymers and nanocomposites are studied, focusing particularly on their morphological and structural aspects (crystallization, lamellar morphology, polymorphism). The study, conducted on different scales, allows to obtain a global and complete picture of the considered materials. In fact, by wide angle X-ray diffraction (WAXD) the molecular structure, the type of crystalline cell and the dimensions of crystallites are studied, by small angle X-ray scattering (SAXS) and electron microscopy the lamellar morphology is investigated. From acquired diffractograms, in order to obtain the crystallinity degree, lamellar thicknesses and distributions, sophisticated computer software is used. Once characterization data have been obtained as a function of process or formulation parameters, the influence of these latter factors on polymer morphology and physical-mechanical properties is determined, with the purpose of obtaining a structure-property correlation to be used in the design of materials. The study is completed by thermal analysis (DSC and simultaneous DSC-TGA) and optical microscopy. Besides composite polymeric fibers are prepared via electrospinning, using as fillers: silver particles, clays, carbon nanotubes, carbon quantum dots, graphene and others.

- *Nanocrystalline cellulose-fullerene: Novel conjugates,* Carbohydrate Polymers*,* **2017**, 164, 92-101.
- *Neuronal commitment of human circulating multipotent cells by carbon nanotube-polymer scaffolds and biomimetic peptides,* Nanomedicine*,* **2016**,11,1929-1946*.*
- *Synthesis and photochemical applications of processable polymers enclosing photoluminescent carbon quantum dots,* ACS nano*,* **2015**, 9, 4156-4164*.*
- *Covalent functionalization enables good dispersion and anisotropic orientation of multi walled carbon nanotubes in a poly(L-lactic acid) electrospun nanofibrous matrix boosting neuronal differentiation*, Carbon, **2015**, 95, 725-730.
- *Characteristics of TEMPO-oxidized cellulose fibril-based hydrogels induced by cationic ions and their properties,* Cellulose, **2015**, 22, 1993-2010.

Polymeric Materials for Advanced Catalysis

+39 049 827 5737 (MZ)

Marco Zecca (marco.zecca@unipd.it), Paolo Centomo (paolo.centomo@unipd.it)

The PoMACat investigates on cross-linked resins of different texture and on microgels as catalytic materials. Our research includes:

- tuning of hydro- and lipophilicity of polymeric materials to solvent or substrate compatibility in catalytic reactions
- solid acid and bifunctional catalysts for the production and transformation of biorefinery platform substances;
- supported metal catalysts for the direct synthesis of hydrogen peroxide and oxidation of alcohols;
- development of “in-operando” methods of XAFS characterization of solid catalysts under (gas)-liquid-solid conditions.

- *Influence of Metal Precursors and Reduction Protocols on the Chloride-Free Preparation of Catalysts for the Direct Synthesis of Hydrogen Peroxide without Selectivity Enhancers*, ChemCatChem, **2016**, 8, 1564–1574.
- *The distinct role of the flexible polymer matrix in catalytic conversions over immobilised nanoparticles*, RSC Advances, **2015**, 5, 56181–56188.
- *In Situ X-ray Absorption Fine Structure Spectroscopy of a Palladium Catalyst for the Direct Synthesis of Hydrogen Peroxide: Leaching and Reduction of the Metal Phase in the Presence of Bromide Ions,* ChemCatChem, **2015**, 7, 3712–3718.
- *Dry- and swollen-state morphology of novel high surface area polymers,* Microporous and Mesoporous Materials, **2014**, 185, 26–29.
- *Resin-Based Catalysts for the Hydrogenolysis of Glycerol to Propylene Glycol,* Top. Catal., **2013**, 56, 822–830.

Soft Matter Theory

www.chimica.unipd.it/alberta.ferrarini/pubblica/
+39 049 827 5682 (AF)

Alberta Ferrarini (alberta.ferrarini@unipd.it)

We use theory and computations to develop microscopic level understanding of the structure and dynamics of Soft Matter. Different methods and techniques, suitable to bridge time- and length- scales, are used to address questions of interest to biophysics and materials science. Current research topics:

- Chirality propagation across length scales in self-assembling systems (helical polymers, DNA oligomers, porphyrin conjugates, colloidal suspensions of viruses);
- Liquid crystals: elastic and flexoelectric properties, conventional and unconventional phases (cholesteric, twist-bend, Blue Phases);
- Lipid membranes and self-assembled monolayers: partitioning and translocation of molecular species, elastic properties, mutual effects of lipid matrix and protein inclusions.

- *Entropy - driven chiral order in a system of achiral bent particles,* Phys. Rev. Letters**,** **2015**, 115**,** 147801.
- *Hierarchical propagation of chirality through reversible polymerization: the cholesteric phase of DNA oligomers*, ACS Macro Letters**, 2016***,*** 5, 208-212.
- *Chiral self-assembly of helical particles,* Faraday Discuss.*,* **2016**, 186, 171–186.
- *Anomalously low twist and bend elastic constants in an oxadiazole based bent-core nematic liquid crystal; spontaneous chirality and polarity,* J. Mater. Chem. C, **2017**, 6, 980-988.
- *Spontaneous lipid flip-flop in membranes: A still unsettled picture from experiments and simulations,* in “The Biophysics of Cell Membranes - The Biological Consequences”, Eds. J.-M. Ruysschaert, R. Epand (Springer Series in Biophysics, **2017**)*, 29 – 60.*

Spectroscopic Characterization of Molecular Materials

www.chimica.unipd.it/fosca.conti/
+39 049 827 5226 (FC)

Fosca Conti (fosca.conti@unipd.it)

The Spectroscopic Characterization of Molecular Materials group is oriented to international collaborations, especially with European and Asian institutions. Materials under study are related to renewable energies and green economy. Physical-chemical properties of electro and/or photoactive molecular systems are investigated to suggest innovative devices.
Researches are carried out using magnetic, optical and thermal spectroscopies, at advanced level: NMR, EPR, UV-NIR-Raman, TGA spectroscopy. Main research topics include: (1) investigations on charge and energy transfer processes; (2) characterization of structure and dynamics of chemical species, stable and/or short-lived, excited and in ground state, interacting and isolated; (3) studies of interfacial and bulk conductivity mechanisms, spin dynamics, dipolar interactions.

- *Mixing in Biogas Digesters and Development of an Artificial Substrate for Laboratory-Scale Mixing Optimization*, Chem. Eng. Technol., **2017**, 40, 238-247.
- *Model-based assessment of partially upgraded biogas and the decentralized utilization for mobility in agriculture*, ISBN:978-88-89407-17-2, **2017**, 1358-1361.
- *Electric Response and Conductivity Mechanism in H3PO4-Doped Polybenzimidazole-4N-HfO2 Nanocomposite Membranes for High Temperature Fuel Cells*, Electrochimica Acta, **2017***, 228, 562-574.*
- *Thermogravimetric investigation on the interaction of formic acid with solder joint materials*, New J. Chem., **2016**, 40, 10482-10487.
- *Phase diagram approach to study acid and water uptake of polybenzimidazole-type membranes for fuel cells*, ECS Trans., **2016**, 72, 157-167.

Supramolecular and Systems Chemistry

www.chimica.unipd.it/suprachem
+39 049 827 5276 (PS)

Paolo Scrimin (paolo.scrimin@unipd.it); Fabrizio Mancin (fabrizio.mancin@unipd.it);
Federico Rastrelli (federico.rastrelli@unipd.it); Leonard J. Prins (leonard.prins@unipd.it)

Research in the group is focused on the development of complex chemical systems capable of bio-insipired functions as signal processing, self-organization, molecular recognition, catalysis, and sensing. Monolayer protected gold and silica nanoparticles, as well as surfactant aggregates, are the key components in these systems. Research by the group has demonstrated that their multivalent and self-organized nature gives rise to unique properties. Examples include chemical fuel driven self-organization, cooperative catalysis, high binding affinities with (bio)analytes, innovative detection protocols based, multivalent and multifunctional interaction with biological entities. We are also working with biologists and medical doctors to prepare nanoparticles for targeting cancer cells and new vaccines. The group is supported by EU (MSCA-ITN), MIUR (PRIN) and University of Padova.

- *Nanoparticle-based receptors mimic protein-ligand recognition*, Chem, **2017**, 3, 92-109.
- *Photoswitchable catalysis by a nanozyme mediated by a light-sensitive cofactor,* J. Am. Chem. Soc., **2017**, 1794-1797.
- *Dissipative self-assembly of vesicular nanoreactors,* Nature Chem., **2016**, 8, 725-731.
- *Chromatographic NMR spectroscopy with hollow silica spheres,* Angew. Chem. Int. Ed.*,* **2016**, *55*, 2733-2737.
- *Transient signal generation in a self-assembled nanosystem fueled by ATP*, Nat. Commun., **2015**, 6, 7790.

Surface Supramolecular Chemistry

www.chimica.unipd.it/mauro.sambi/pubblica/ricerca_e.html
+39 049 827 5189 (MS); 5010 (FS); 5265 (lab)

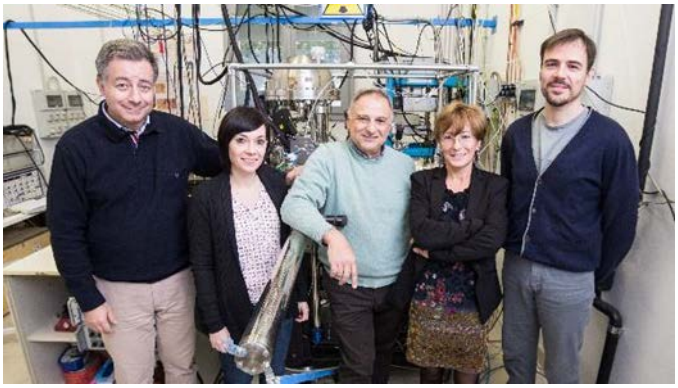

Mauro Sambi (mauro.sambi@unipd.it), Francesco Sedona (francesco.sedona@unipd.it)

The SSC Group's research activities deal with the thermo- and photoinduced on-surface synthesis of 2D materials starting from supramolecular assemblies of functionalized precursors, with a particular emphasis on the preservation of a high degree of long-range order throughout the process. The group manages an ultra-high vacuum chamber equipped with scanning tunneling microscopy (STM) and other surface science tools, interfaced with both single-wavelength and tunable laser sources for in-vacuum surface photochemistry with molecular resolution. An ambient STM/AFM instrument for solid/liquid and solid/air investigations complements the available equipment. The group has ongoing collaborations with several Italian and European groups active in the field of on-surface synthesis and molecular magnetism.

- *Metal-Free on-Surface Photochemical Homocoupling of Terminal Alkynes,* J. Am. Chem. Soc., **2016**, 138, 10151-10156.
- *Tunable Band Alignment with Unperturbed Carrier Mobility of On-Surface Synthesized Organic Semiconducting Wires,* ACS Nano*,* **2016**, 10, 2644-2651.
- *Molecules–Oligomers–Nanowires–Graphene Nanoribbons: A Bottom-Up Stepwise On-Surface Covalent Synthesis Preserving Long-Range Order,* J. Am. Chem. Soc., **2015**, 137, 1802-1808. (WOS highly cited paper)
- *Stereoselective Photopolymerization of Tetraphenylporphyrin Derivatives on Ag(110) at the Sub-Monolayer Level,* Chem. Eur. J., **2014**, 20, 14296-14304. (Hot Paper, Back Cover).
- *Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction,* Nat. Mater., **2012**, 11, 970-977.

Surfaces and Catalysts

www.chimica.unipd.it/surfacescience/
+39 049 827 5158 (GG); 5122; 5176 (AG); 5722 (GAR)



Gaetano Granozzi (gaetano.granozzi@unipd.it); Gian Andrea Rizzi (gianandrea.rizzi@unipd.it); Antonella Glisenti (antonella.glisenti.@unipd.it); Stefano Agnoli (stefano.agnoli@unipd.it); Laura Calvillo-Lamana (laura.calvillolamana@unipd.it)

The group is equipped with several experimental set-up in ultra-high-vacuum, reactors, instrumental equipments, synthesis laboratories where the following research lines are pursued:

- Structure and activity of model catalysts and (photo)electrocatalysts for advanced energy applications (fuel cells, solar fuels, electrolysers);
- Chemically modified 2D and 3D graphene as well as other 2D nanomaterials (h-BN, metal chalcogenides) for energetics and catalysis;
- Oxide-on-oxides and metal-on-oxides catalysts and devices for sustainable development: from pollutants' abatement (TWC), to green hydrogen production
- (biofuels), to energy conversion and storage (Reversible and symmetric Solid Oxide Cells, SOFC/SOEC, batteries).

The group is currently involved in two European Projects in the field of fuel cells and catalysis: H2020-NMP-2014-2015, PARTIAL-PGMs and H2020-JTI-FCH-2017-1, CRESCENDO.

- *Cobalt Spinel Nanocubes on N-Doped Graphene: A Synergistic Hybrid Electrocatalyst for the Highly Selective Reduction of Carbon Dioxide to Formic Acid,* ACS Catal., **2017**, 7, 7695–7703.
- *Single- and Multi-Doping in Graphene Quantum Dots: Unraveling the Origin of Selectivity in the Oxygen Reduction Reaction*, ACS Catal., **2015**, 5, 129−144.
- *Vanadiumoxide nanostructures on another oxide: the viewpoint from model catalysts studies* Coord. Chem. Rev., **2015,** 301–302, 106–122.
- *New Strategy for the Growth of Complex Heterostructures Based on Different 2D Materials,* Chem. Mater., **2015**, 27, 4105−4113.
- *Largely Cu-doped LaCo1-xCuxO3 perovskites for TWC: toward new PGM-free catalysts,* Appl. Catal. B Environmental, **2016**, 180, 94.

Theoretical Chemistry

www.chimica.unipd.it/theochem
Tel.: +39 049 827 5146 (AP); 5683 (GM)

Antonino Polimeno (antonino.polimeno@unipd.it); Giorgio Moro (giorgio.moro@unipd.it); Laura Orian (laura.orian@unipd.it); Barbara Fresch (barbara.fresch@unipd.it); Diego Frezzato (diego.frezzato@unipd.it); Mirco Zerbetto (mirco.zerbetto@unipd.it)

The Theoretical Chemistry group is active in several areas of theoretical and computational chemistry, including the interpretation of magnetic and optical spectroscopies, the modeling and *in silico* investigation of materials and functional molecular structures, molecular dynamics of macromolecules, microfluidics, quantum-statistical and stochastic thermodynamics. Current subjects of investigation are:

- coarse-grained description of biomolecules and supramolecular aggregates;
- multiscale methods for the self-assembly of large molecular systems;
- design of quantum nanodevices for molecular logic and sensing;
- dynamics and statistics of open quantum systems;
- dimensional reduction of complex chemical reaction networks;
- rational design of semi-natural enzymes, bio inspired drugs and catalysts.

- *Integrated computational approach to the Electron Paramagnetic Resonance characterization of rigid 310-helical peptides with TOAC nitroxide spin labels,* J. Phys. Chem. B*,* **2017***,* 121, 4379-4387.
- *The quantum molecular trajectory and its statistical properties*, J. Phys. Chem. A*,* **2017***,* 121, 5352-5360.
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Technical and administrative staff

Administration and logistics at DiSC are managed by four offices and a number of services, that include maintenance of buildings and instrumentations, laboratory safety, technical assistance to research and teaching laboratories, information systems.

The administration refers to the **Department Secretary Marco Agnello**
e-mail: marco.agnello@unipd.it

Accounting office
e-mail: contabile.chimica@unipd.it
Emanuela Andreose, Giulia Avitabile, Stefania Borin, Barbara Boscaro, Melania Brolis, Roberta Dainese, Silvia Guerzoni, Gessica Solin

Directional office
e-mail: segreteria.chimica@unipd.it
Mara Del Maschio, Vanessa D'Epiro, Santo Martino, Nicoletta Tognon

Didactics office
e-mail: didattica.chimica@unipd.it
Laura Cataldo, Carmen Mantovan, Alessandra Sperti

Research office
e-mail: scientifica.chimica@unipd.it
Daniela Longo, Anna Menna, Laura Paiola

Reception
e-mail: portineria.chimica@unipd.it
Stefania Campaner, Giulio Palermo

Machine shop and general maintenance
e-mail: manutenzione.chimica@unipd.it
Vincenzo Afelbo, Paolo Bruscagin, Massimo Dalla Benetta, Lorenzo Dainese, Roberto Inilli, Stefano Mercanzin, Paolo Roverato

Glassblowing shop
Mauro Meneghetti

Chemistry stockroom
e-mail: approvvigionamento.chimica@unipd.it
Mario Giuttari, Daniele Zanetti

Laboratory and infrastuctures safety
e-mail: sicurezza.chimica@unipd.it
Elena Campadello

Computer Service
Monica Busetto, Luigino Feltre, Michele Furlan, Gianpietro Sella

Electronics service
Claudio Comaron, Alberto Doimo

Technicians dedicated to teaching laboratories
Catia Rosaria Cucco, Andrea Nardi, Massimo Pavan, Filippo Stella, Nicola Tiso, Alberto Toniolo

Technicians dedicated to instrumental and research laboratories
Annalisa Bisello, Loris Calore, Roberta Cardena, Simone Crivellaro, Sandra Lavina, Gianni Marin, Sabrina Mattiolo, Ileana Menegazzo, Giulio Purgato, Roberta Saini, Renato Schiesari, Lidia Soldà, Emanuela Zangirolami

CNR secretariat
Lisa Bissacco, Teresa Mollo

People index

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Nanochemistry for Energy and Health.