DiSC 2016/2017

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

The Department of Chemical Sciences (Dipartimento di Scienze Chimiche, DiSC) is one of the largest of the University of Padova; it hosts several academic courses in all areas of chemistry at all levels, including doctorates. The most recent national evaluation and ranking places DiSC first among chemistry departments of large Italian Universities.

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Research Areas

The research activities of DiSC are focused on six main research areas: chemistry for life sciences; chemistry for energy, environment and cultural heritage; materials, nanomaterials and surface science; supramolecular chemistry and nanochemistry; synthesis, reactivity and catalysis; theoretical and computational chemistry.

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
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The Department of Chemical Sciences – an overview

The Department of Chemical Sciences - DiSC - was founded in 2004, from a merger of three existing Departments: Inorganic, Metallorganic and Analytical Chemistry, Physical Chemistry, and Organic Chemistry. 79 Faculty members and 60 technical and administrative employees work at DiSC that hosts also 17 scientists of the National Research Council. State-of-the-art facilities are available at DiSC, such as high-field NMR, mass and EPR spectrometers, autonomous computational facility, AFM, STM, XPS, XRD, Mössbauer and time-resolved, femtosecond laser equipments are also available to researchers at DiSC, as well as all key instrumentation to run full-equipped laboratories for the synthesis and characterization of chemical compounds.

DiSC offers three B.Sc. programs (Chemistry, Industrial Chemistry, Materials Science, Science and Technology for the Environment) three M.Sc. (Chemistry, Industrial Chemistry and Materials Science) and two graduate programs: Molecular Sciences and Science and Engineering of Materials and Nanostructures. Recently signed MoU include those with the University of Giessen, the Indian Institute of Chemical Technology-Hyderabad, the Korean Kyungpook National University, the University of Tianjin, the Beijing University of Chemical Technology and the Shanghai Institute of Organic Chemistry-CAS.

Graduates programs

The Graduate Course of Molecular Sciences (Corso di Dottorato in Scienze Molecolari, SM) offers a highly competitive PhD program for a comprehensive education in the fields of Chemistry, Biochemistry, Materials Chemistry and Pharmaceutical Chemistry. Research activities are complemented by advanced courses in novel areas of molecular sciences. The program offers a wide variety of topics: synthesis, characterization and applications of molecular and supramolecular systems towards new materials, surfaces and interfaces; development of innovative methodological approaches in theoretical, physical, organic and analytical chemistry; design, synthesis and characterization of bioactive molecular systems. The SM reference Departments are Chemical Sciences and Pharmaceutical Sciences.

The Graduate Course in Science and Engineering of Materials and Nanostructures (Corso di Dottorato in Scienza e Ingegneria dei Materiali e delle Nanostrutture, SIMN) offers a program that combines complementary expertise in nanoscience and nanotechnology for the development of innovative materials. SIMN students deal effectively with the design, production, characterization and modeling of materials and innovative devices, through the understanding and use of nanostructure-function relationships for the material under investigation, in view of a specific application. The SIMN reference Departments are Chemical Sciences, Physics and Astronomy and Industrial Engineering.
Analytical Chemistry

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The Analytical Chemistry Laboratories are equipped with high resolution LC-MS (Q-TOF by Agilent and Q-Exactive by Thermo), ICP-MS (Agilent), GC-MS (Thermo) and many other instruments dedicated to the following research lines:
- optical sensors;
- emerging contaminants in the environment and food;
- atmosphere chemistry;
- metal-ligand complexation in aqueous solutions for chelation therapy;
- applied analytical chemistry.
The group is currently involved in some national and international Projects. The international one is coordinated by a research group of the Department of Physics to which the present group adheres: (FP7-SEC-2012-1 n. 312713) TAp WAter RAdioactivity Real Time Monitor (TAWARA_RTM).

Recent key publications
- Definition of the limit of quantification in the presence of instrumental and non-instrumental errors. Comparison among the various definitions applied to the calibration of zinc by ICP-MS, Spectrochim. Acta B, 2015, 114, 81-86.
- The metallome of human placenta in gestational diabetes mellitus, Metallomics, 2015, 7, 1146-1154.
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 building blocks for advanced materials and devices (luminescent devices, liquid crystals etc.). In particular, the main target are late transition metal complexes with stable 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 are the following:

- synthesis of dinuclear gold complexes with di-NHC ligands: photoluminescence properties, reactivity of gold(I) complexes in oxidative addition, anti-cancer activity;
- synthesis characterization and application of transition metal complexes with novel heteroditopic di-NHC ligands (imidazol-ylidene and triazol-ylidene);
- synthesis of iridium(III) complexes with chelating di-NHC ligands as catalysts for water oxidation and transfer hydrogenation;
- synthesis, characterization and application of mono- and dinuclear complexes of late transition metals with novel N-phosphanyl carbene ligands;
- catalytic properties of selected carbene complexes in technologically relevant reactions (e.g. C-H bond activation, cross-couplings, nitrene transfers, alkyne additions) and under non-conventional reaction conditions (e.g. in ionic liquids).

Recent key publications

Bioinorganic Chemistry

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The research of the lab is at the interface between inorganic chemistry, biology and medicine. The following main research lines are currently being carried out:

- development of groundbreaking anticancer metal [e.g., Au(I/III), Ru(II/III), Cu(II) and Zn(II)] derivatives with a remarkable antitumor activity (AA) greatly prevailing on toxicity (TOX), contrary to most chemotherapeutic drugs;
- functionalization of antibodies with metal complexes for the developing new biosensors for clinical applications and early detection of tumor markers in blood and/or urines;
- development of anti-inflammatory agents for the treatment of acute and chronic inflammation.

In particular, our experience starts from the synthesis of coordination compounds and the close use of several spectroscopic techniques to characterize the newly synthesized complexes, and arrives to the investigation of the anticancer/antiinflammatory activity both in vitro and in vivo. Our researches include also the study of the 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 organic and inorganic chemistry, biology, pharmacology and medicine.

Recent key publications

- Gold(III)-pyrrolidinedithiocarbamato Derivatives as Antineoplastic Agents, Chemistry Open, 2015, 4, 183-191.
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.

Recent key publications
The Bio-Organic Chemistry is focusing on the exploitation of 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;
- antimicrobial photodynamic therapy;
- textiles functionalized with antibacterial peptides for biomedical applications;
- peptide nanotechnology: peptido-rotaxanes, peptide-decorated metal nanoparticles, self-assembled peptide polymers;
- synthesis and conformation of peptides with rigid and well-defined 3D-structure (e.g., α-, 310- and 2.05-helices or turns);
- peptide helices as rigid structural elements for spectroscopic studies and for electron transfer and photovoltaic applications;

Research projects recently funded:

Recent key publications
- 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.
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 Padova, 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. The mentioned facilities allow deep investigations focused on surface analyses (XPS and AFM), on local electronic environment of Fe (Mössbauer spectroscopy) and qualitative and quantitative in situ elemental analysis (XRF and LIBS). Surface analyses give important informations on the first layers (nanometric scale as magnitude order) of the investigated materials, allowing the comprehension of the possible modification induced by ageing, by corrosion etc., on the sample. Mössbauer spectroscopy plays a special role on the Fe studies. This nuclear technique describes very deeply the chemical interactions between Fe nuclei and the chemical environment, allowing the description of all the phenomena that modify the physic-chemical properties of the Fe nuclei themselves.
Electrocatalysis and Applied Electrochemistry

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The ECAE Laboratory is equipped with electrochemical apparatus and other analytical facilities and the group currently pursues the following research lines:
- preparation and physico-chemical characterization of electrocatalytic materials for electrochemical processes in the fields of energetics (fuel cells), electrosynthesis and pollution remediation (mainly halogenated volatile organic compounds);
- electrochemical approaches to Atom Transfer Radical Polymerization and Atom Transfer Radical Cyclization;
- electrochemical reduction of carbon dioxide;
- electrocarboxylation of different substrates (halides, ketones, olefins) for the synthesis of fine chemicals and/or pharmaceutical compounds;
- electrochemical reduction of organic halides in molecular solvents and in ionic liquids and characterization of inherently chiral ionic liquids;
- electrochemical technologies for wastewater treatments.

Recent key publications
The EPR spectroscopy group is focused on the development and application of Electron Paramagnetic Resonance (EPR) techniques to Material Science (graphene, metal nanoparticles, organic electronics, organic photovoltaics, cultural heritage materials), and Biology (natural and artificial photosynthetic systems, Hydrogenases and bio-inspired analogs for the photo-bioproduction of hydrogen; protein motions as detected by spin labelling techniques)

The instrumental facilities of the EPR Laboratory at DiSC include:
- An X-band CW- and pulsed-EPR spectrometer, equipped with pulsed ENDOR and PELDOR accessories
- Two X band CW and ENDOR spectrometers
- A time-resolved EPR spectrometer for analysis of light-induced processes
- A Q-band EPR spectrometer with CW, pulsed, ENDOR, PELDOR and time-resolved accessories
- Optically detected Magnetic Resonance (ODMR) spectrometer.
All spectrometers are equipped with variable temperature systems, for measurements from 4 K to 400 K.

Recent key publications
Laser Spectroscopy and Nanophotonics

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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.

The techniques set up to investigate nonlinear phenomena are:
- Micro and Macro Raman Spectroscopies: RRS, SERS, WS-SERS;
- Two-photon induced fluorescence and Z-scan;
- Transient Absorption with fs time resolution;
- Two-Dimensional photon echo experiments;
- Time Resolved Fluorescence Microscopy: FLIM and FCS;
- Fabrication of Microfluidic devices for cell growth and kinetic studies.

Most prominent financial support comes from two European grants and two Italian grants from MIUR, among these two most prominent ones are: Starting Grant of the European Research Council (E. Collini): QUantum-coherent drive of ENergy TRansfer along HELical structures by polarized ligh (http://www.chimica.unipd.it/quentrhel/); FIRB 2011 RBAP11X42L_002 (R. Bozio): Dalle single molecole al modello animale: un approccio integrato allo studio dei segnali intra e inter-cellulari; PRIN2012 (R. Bozio): New aspects of resonance energy transfer in organized media: dynamical effects and optical control.

Recent key publications
- Evaluation of gold nanoparticles toxicity towards human endothelial cells under static and flow conditions, Microvascular Res., 2015, 97, 147-155.
- Wavelength dispersion of the local field intensity in silver-gold nanocages, PCCP, 2015, 17, 7355.
Molecular Materials & Modeling

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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.

Besides spectroscopic and analytical techniques available in our department (IR, Raman and UV-Visible spectroscopies, $^1$H, $^{13}$C, $^{31}$P and bidimensional - H,H, H,P and H,C - NMR solution spectroscopy, elemental analyses, magnetic susceptibility, conductance measurements), structural studies on suitable single crystals or on powder samples are also carried out. Advanced synchtron-assisted analytical methods (XAS, photoemission, SAXS) complement the chemico-physical and structural characterization at Home. The computational power available to M$^3$ includes 4 parallel machines, with a total power of 8 TFLOPS and a file storage capacity of 5.5 TB. Open-source (Quantum Espresso), commercial (ADF and Gaussian) and in-house developed software are currently used.

M$^3$ leads a National project devoted to the Multiscale Material Modeling started in February 2013: DESCARTES (Development of Energy-targeted Self-assembled supramolecular systems: a Convergent Approach through Resonant information Transfer between Experiments and Simulations).

Recent key publications
The MEN Group focuses on molecular aspects of electrochemical reactions and nanosystems from both fundamental and applied (nanomedicine, redox catalysis) viewpoints. Specific research topics include:
- Electron Transfer through Molecular Bridges and Interfaces
- Dissociative Electron Transfer
- Molecule-like and Quantized Monolayer-Protected Metal Clusters: Properties, Redox Catalysis, Drug Delivery Systems
- Electrochemical Sensors for Cancer Biomarkers
- Self-Assembled Monolayers of Conformationally Constrained Peptides
- Biomimetic Membranes

The MEN Group is equipped with state-of-the-art electrochemical instrumentations, including electrogenerated chemiluminescence and scanning electrochemical microscopy, STM and AFM, PM-IRRAS and UV-visible spectrometers, HPLC, mass spectrometry, etc.

Recent key publications
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 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 in selective catalysis are currently under investigation in our laboratories:
- synthesis of Highly Symmetric Multidentate Ligands and their Applications in Catalysis;
- mimics of Physiologically Important Metallo-Enzymes (haloperoxidases, lignin-peroxidases);
- new Approaches to Catalyst Design and Recycling in Green Chemistry;
- self-Assembled Molecular Cages;
- hybrid Receptors for Anions in Water.

Recent key publications
The Multi-functional Nanomaterial Group has an internationally recognized know-how in the fabrication and modification of nanoarchitectures with variable dimensionality by chemical vapor deposition (CVD), either thermal- or plasma-enhanced (PE-CVD), Radio Frequency (RF)-Sputtering and their original combinations. In this regard, attention is also devoted to the synthesis of molecular precursors, endowed with high volatility, stability to air/moisture and clean decomposition patterns under both CVD and PE-CVD conditions. The developed systems, subjected to an advanced thorough characterization, are investigated as unique multi-functional platforms for sustainable end-uses, encompassing photo-activated applications (H₂ production by photocatalysis and photoelectrochemical water splitting, environmental remediation, light-triggered self-cleaning and anti-fogging systems), molecular detection of flammable/toxic gases, but also anodes for Li-ion batteries and magnetic materials.

The group is, or has been, recently involved in various national and international projects in the field of inorganic nanomaterial design, characterization and functional investigation, among which the following two European Consortia:

The group has a first-class track record, corresponding to 101 publications on ISI Journals, 20 other publications, 3 national/international patents and 110 conference communications (of which 17 invited lectures/seminars), only in the period 2010-2015.

Recent key publications
- Surface functionalization of nanostructured Fe₂O₃ polymorphs: from design to light-activated applications, ACS Appl. Mater. Interfaces, 2013, 5, 7130.
- An old workhorse for new applications: Fe(dpm)₃ as a precursor for low-temperature PECVD of iron(III) oxide, Physical Chemistry Chemical Physics, 2015, 17, 11174.
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:

- **Sustainable photosynthetic processes**: activation of multi-redox routines powered by light irradiation and water splitting catalysts;
- **Design of synthetic enzymes** (synzymes) able to interact with diverse biological targets involved in ROS-related diseases;
- **Design of hybrid materials**: synthetic membranes, capsules and polymers, nano-sized metal oxides, bio-hybrids, with applications in catalysis, energy conversion and nanomedicine;
- **Computational modelling**: DFT calculations of spectroscopic properties of organic and organometallic systems and MD simulations of ionic liquids and ionic liquid crystals.

The group is involved in the following projects:


**Recent key publications**

- Knitting the Catalytic Pattern of Artificial Photosynthesis to a Hybrid Graphene Nanotexture ACS Nano, 2013, 7, 811.
Nanostructures & (Bio)molecules Modeling

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The group is developing and applying multiscale computational methods for hybrid systems, such as organic and biological molecules interacting with inorganic surfaces and nanoparticles. The exploited methods range from ab initio atomistic calculations to classical electromagnetic modeling passing through classical molecular dynamics simulations.

In particular, the group is theoretically investigating:
- the ultrafast spectroscopy of molecules close to plasmonic nanostructures, as well as surface enhanced optical phenomena.
- the quantum nature of plasmonics excitations at the nanoscale.
- the interactions of inorganic surfaces and nanoparticles with proteins, to explore their possible biochemical effects (e.g., modification of protein fibrillation, impairing of the biological protein function) and their possible technological use (e.g., enzymatic biofuel cells).
- the solvation of molecules and its effects on optical properties.
- the effects of electronic correlation in molecules and how it impacts on scanning tunneling microscopy and photoelectron spectroscopy orbital tomography.

Currently the group is funded by the ERC Consolidator Grant TAME-Plasmons "A Theoretical Chemistry Approach to Time-Resolved Molecular Plasmonics" (2016-2021) dedicated to developing real-time approaches to simulate optical properties of molecules close to plasmonic nanostructures, and by MIUR PRIN Project "Assessing protein system dynamics and thermodynamics: a novel NMR approach at single-residue resolution" (2014-2017).

Recent Key Publications
- The interaction with gold suppresses fiber-like conformations of the amyloid β (16–22) peptide Nanoscale 2016, 8, 8737-8748.
- Quantifying the plasmonic character of optical excitations in nanostructures ACS Photonics 2016, 3, 520-525.
- 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.
New materials for energy conversion and storage

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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 carboxylation 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 carboxylation 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, coordinated by prof. Vito Di Noto (Dept. of Industrial Engineering): Progetto Strategico di Ateneo: MAESTRA - From Materials for Membrane-Electrode Assemblies to Electric Energy (2014-2017); European Project: Graphene Core 1 (2016-2018);

Recent key publications
- 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.
- Influence of the operating conditions on the catalytic activity of [PdCl₂(dapp)] in the CO-ethene copolymerization in the H₂O-CH₃COOH as a solvent (dapp=1,3-bis(di(2-methoxyphenyl)phosphino propane). Journal of Molecular Catalysis. A: Chemical, 2010, 332, 158-164.
Nanostructures & Optics

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The interest of the NOL is to engineer nanostructures (NS) with new functions and with particular attention to their linear and non-linear optical properties. The laboratory is developing NS for Surface Enhanced Raman Scattering applications in particular for detection and imaging of biological analytes in vitro, ex vivo and in vivo. These nanostructures are then functionalized with targeting units like Antibodies which show the ability of recognizing a target unit for applications in nano-biomedicine, for example tumour associated antigens, or in the Cultural Heritage. The NOL is also involved in using and in understanding on the basis of models, the properties of carbon nanostructures like functionalized carbon nanotubes and graphene nanostructures. Laser assisted synthetic techniques are applied to the development of plasmonic and magnetic NS, also exploitable as multimodal contrast agents.

Recent key publications
- Plasmonic Nanostructures for SERRS Multiplexed Identification of Tumor-Associated Antigens, Small, 2012, 8, 3733-3738.
- Fluorescence dynamics and fine structure of dark excitons in semiconducting single-wall carbon nanotubes; Journal of Physics, Condensed matter, 2012, 24, 255501.
- Magneto-Plasmonic Au-Fe Alloy Nanoparticles Designed for Multimodal SERS-MRI-CT Imaging, Small, 2014, 10, 2476–2486.
Organic Chemistry for the Environment and Health

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We have two lines of research:

1. **Non-thermal (alias non-equilibrium) plasmas** as a means to induce chemical processes of high activation energy of importance for the environment and energy
   - advanced oxidation for air remediation
   - advanced oxidation for water remediation
   - syngas production via methane dry reforming – conversion of the two major greenhouse gases into useful feedstock
2. Synthesis and characterization of new derivatives of polyphenols and other natural compounds to improve bioactivity
   - prodrug approach: modulation of physical chemical properties of the natural compound via reversible functionalization to prevent metabolization and increase systemic concentration of the parent compound
   - targeting approach: synthesis of mitochondria targetted derivatives of natural compounds for cancer therapy

The group is currently involved in the European Project **CMST COST Action TD1208: Electrical discharges with liquids for future applications** (http://www.cost.eu/domains_actions/cmst/Actions/TD1208)

Recent key publications
- **Synthesis and evaluation as prodrugs of hydrophilic carbamate ester analogues of resveratrol**, Molecular Pharmaceutics 2015, 12, 3441-3454.
- **Amino acid carbamates as prodrugs of resveratrol**, Scientific Reports, 2015, 5, 15216.
Organic Materials

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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.

Recent key publications
- 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.
Physical Organometallic Chemistry

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The Physical Organometallic Chemistry Group is equipped with two electrochemistry work stations for low current measurements with ultramicroelectrodes, one FT-vis, near-IR,-mid-IR spectrometer with a fibre optic probe and an Optical Transparent Thin Layer (OTTLE) cell for low temperature spectroelectrochemistry. Several NMR spectrometers from 200 to 600 MHz are also available together with a BBI-Z-grad probehead for the detection of low frequency nuclei (e.g. $^{103}$Rh, $^{57}$Fe, $^{183}$W, $^{39}$K). The following research lines are pursued:

- electron transfer activation in multimetallic complexes of polycyclic bridging ligands;
- charge transfer properties of mixed-valence bi- and trimetallic complexes;
- reversible photochromism of ferrocenyl(bis-azobenzene) branched polymers;
- peptides mediated electron transfer;
- hybrid aminoacid ferrocenyl arylene ethynylene systems: sensors towards metal ions.

The group is currently involved in the PRAT 2014 Project of University of Padova “Benzotriothiophene ferrocenyl end-capped electronic materials”, started in January 2015.

Recent key publications
- Charge Transfer Properties of Benzo[b]thiophene Ferrocenyl Complexes Organometallics, 2015, 34, 4451-4463.
- Key multi(ferrocenyl) complexes in the interplay between electronic coupling and electrostatic interaction, Dalton Trans., 2015, 44, 5234-5257.
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.

Recent key publications
- Synthesis and photochemical applications of processable polymers enclosing photoluminescent carbon quantum dots, ACS nano, 2015, 9, 4156.
- Covalent functionalization enables good dispersion and anisotropic orientation of multiwalled carbon nanotubes in a poly(L-lactic acid) electrospun nanofibrous matrix boosting neuronal differentiation, Carbon, 2015, 95, 725.
- Characteristics of TEMPO-oxidized cellulose fibril-based hydrogels induced by cationic ions and their properties, Cellulose, 2015, 22, 1993.
Polymeric Materials for Advanced Catalysis

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The PoMACat group develops and exploits polymeric materials such as cross-linked resins of different texture and microgels for application to catalysis and material chemistry. The scope of recent investigation 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;
- microgels as exotemplates and stabilizers of nanostructured, catalytically active metals in solution;
- development of “in-operando” methods of XAFS characterization of solid catalysts under (gas)-liquid-solid conditions.

Our facilities include:
- A semi-CFSTR for atmospheric pressure operation with on-line monitoring of the off gas; glass and steel autoclaves for low-middle to high pressure operation a ThalesNano H-Cube continuous hydrogenation reactor (10-150 °C, up to 10 MPa); glass reactor equipped with membrane ultrafiltration setup;
- HPLC, GC and GC-MS and NMR (300 MHz-1H) apparatus;
- Inverse Steric Exclusion Chromatography apparatus for the morphological characterization of swollen cross-linked polymers.

Recent key publications
- **The Distinct Role of the Flexible Polymer Matrix in Catalytic Conversions over Immobilised Nanoparticles**, RSC Adv. 2015, 5, 56181.
**Soft Matter Theory**

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We use theoretical and computational methods to investigate equilibrium properties and dynamical behavior of Soft Matter, in connection with the microscopic/molecular structure. A variety of approaches, with different resolution, are combined to bridge length- and time-scales: mean field and classical density functional theory, Fokker-Planck equation, standard quantum chemistry calculations, elastic continuum theory, Molecular Dynamics and Monte Carlo simulations, with atomistic and coarse grained models. Our research includes methodological development as well as application to problems of biological and technological interest.

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);
- NMR in anisotropic media: solutions of polymers (PBLG), proteins and thermotropic liquid crystals;
- Lipid membranes and self-assembled monolayers: order, partitioning and translocation, elastic properties.

**Recent key publications**
The Spectroscopic Characterization of Molecular Materials (SCMM) group is oriented to international collaborations, especially with European and Asian institutions.
- most of the systems under study are electro and/or photoactive materials for innovative devices useful in renewable energy systems related to green economy;
- the use of magnetic, optical and thermal spectroscopies, at advanced level, is the key factor for the success of the investigations: NMR, EPR, UV-NIR-Raman, TG spectroscopy.

Main research topics include:
- investigations on charge and energy transfer processes
- characterization of structure and dynamics of chemical species, stable and/or short-lived, excited and in ground state, interacting and isolated;
- studies of interfacial and bulk conductivity mechanisms, spin dynamics, dipolar interactions.

Collaborations:
The SCMM group is currently collaborating with three German scientific institutions:
- University of Freiburg, Department of Physical Chemistry. Magnetic resonance: NMR and EPR on biological and inorganic systems, contact: Prof. Stefan Weber (www.radicals.uni-freiburg.de/);
- Juelich Research Center, Institute of Energy and Climate Research IEK-3. Conversion technologies for an efficient energy supply, contact: Prof. Detlef Stolten (www.fz-juelich.de/iek/iek-3);

Outstanding current project: The SCMM group is currently involved in a three years Strategic Project funded by the University of Padova and called From Materials for Membrane-Electrode Assemblies to Electric Energy Conversion and Storage Devices (MAESTRA) (2014 – 2016).

Recent key publications
- Analysis of solder joint reliability of high power LEDs by transient thermal testing and transient finite element simulations, Microelectronics Journal, 2015, 1230-1238.
Research in the group is focused on the development of complex nanosystems for application in biomolecular recognition, catalysis, and sensing. Monolayer protected gold and silica nanoparticles form the key components in these systems and research by the group has demonstrated that their multivalent nature gives rise to unique properties in the above fields. Examples include cooperative catalysis, high binding affinities with (bio)analytes, innovative detection protocols, multivalent and multifunctional interaction with biological entities. In the field of nanomedicine we are working with biologists and medical doctors to prepare nanoparticles for targeting cancer cells and new, synthetic vaccines. In this research line, our interest is, on one side, in hepatocellular and colon carcinomas and, on the other, in immunization for meningitis and salmonella typhi. These are important targets for the relevance of the related diseases in the population.

State-of-the-art instrumentation is available for the synthesis and characterization of nanosystems (solution and solid-state NMR, TGA, DLS, TEM), for studying binding interactions with (bio)analytes (high field NMR, SPR, high throughput fluorescence and absorbance measurements) and for measuring reactions kinetics (absorbance, fluorescence).

Current research projects:
**MULTI-APP** (Marie Curie Initial Training Network): Multivalent molecular systems for innovative applications
**NANOCARB** (Marie Curie Individual Fellowship): Self-selection of a multivalent nanosystem for carbohydrate recognition
**NANOVAC** (Cariplo): Multifunctional gold nanoparticles as a platform for new carbohydrate-based vaccines
**NAMECA** (University of Padova Strategic Project): Nanochemistry and medicine for cancer: from diagnosis to treatment

Recent key publications
Surface Supramolecular Chemistry

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The Surface Supramolecular Chemistry Group pursues the following research lines in the field of energy-targeted self-assembled supramolecular systems:
- structure and dynamics of electron donor-acceptor self-assembled molecular networks in two dimensions (2D);
- thermo- and photo-induced covalent stabilization of surface-supported 2D supramolecular networks;
- interplay between local and supramolecular order in determining the electronic, magnetic and catalytic properties of surface-supported molecular species;
- surface-supported metal coordination networks at the solid-liquid/solid-air interface.

The group manages a multi-purpose ultra-high vacuum chamber equipped with variable-temperature scanning tunneling microscopy (STM) and other surface science tools, interfaced with both continuous wave single-wavelength and pulsed nanosecond 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.

Recent key publications
- Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction, Nat. Mater., 2012, 11, 970-977.
The Surface Science Laboratory is equipped with four experimental chambers in ultra-high-vacuum, reactors, instrumental equipments, synthesis laboratories where the following research lines are pursued:

- Structure and activity of model catalysts studied by Surface Science tools
- Atomic Scale design of electrocatalysts for advanced electrodes (fuel cells, solar fuels)
- Growth and functional characterization of chemically modified 2D and 3D graphene and other 2D nanosheets (h-BN, metal chalcogenides) systems for energetics and catalysis
- Nanosystems and nanocomposites for gas- and bio-sensing
- Oxide-on-oxides and metal-on-oxides catalysts for sustainable development: from pollutant abatement (TWC) to energy production (Solid Oxide Fuel Cells, batteries)

The group is involved in four European Projects in the field of fuel cells and catalysis:

- NMP.2012.1.1: European Coordination of DECORE: Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of the catalyst/support assembly for high temperature operation (http://decore.eucoord.com/)
- FCH-JU-2011-1: University of Padova local coordination of CathCat: Novel catalyst materials for the cathode side of MEAs suitable for transportation applications (http://cathcat.eu/index.php/home)
- NMP.2011.2.2-4 – Local coordination of NEXTGENCAT “Development of NEXT GENeration cost efficient automotive CATalysts” (http://www.nextgencat.eu)
- H2020-NMP-2014-2015, Local Coordination of PARTIAL-PGMs”Development of novel, high Performance hybrid TWV/GPF Automotive after treatment systems by raTlonAL design: substitution of PGMs and Rare earth materials”

Recent key publications

- Unveiling the Mechanisms Leading to H₂ Production Promoted by Water Decomposition on Epitaxial graphene at Room Temperature, ACS Nano, 2016, 10, 4543.
The Theoretical Chemistry Group (TCG) is active in several areas of theoretical and computational physical chemistry, including computational magnetic and optic spectroscopy, in-silico investigation of functional molecular structures, molecular dynamics of macromolecules, microfluidics. Research is focused on diverse classes of model systems, to interpret and predict molecular structures, dynamical properties and spectroscopic signatures.

Therefore, main lines of exploration at TGC deal with multiscale approaches. Our theoretical methods combine in silico molecular dynamics studies with model-based approaches and seek to understand the connections between different levels of analysis, from molecules (microscopic) through local structures (mesoscopic), to organized systems (macroscopic), to describe molecular and supramolecular systems, functional materials, biosystems.

Computational outcomes and expertise at TCG are made available to the scientific community in the form of open-source codes. In particular software tools for EPR and NMR observables can already be downloaded through the Computational Chemistry Laboratory of the Department (www.chimica.unipd.it/c3p).

Main current subjects of investigations are:
- statistics and dynamics of quantum pure states
- modeling motions in flexible macromolecules
- modeling of energy-transfer processes via hybrid methods
- dimensional reduction of chemical kinetics in complex systems
- multiscale methods for organic – inorganic hybrid systems

Recent key publications
- *Flexibility at a glycosidic linkage revealed by molecular dynamics, stochastic modeling, and $^{13}$C NMR spin relaxation: conformational preferences of $\alpha$-L-Rhap-$\alpha$ -(1 $\rightarrow$ 2)-$\alpha$-L-Rhap-OMe in water and dimethyl sulfoxide solutions*, PCCP, 2016, 18, 3086-3096.
- *Loop electrostatics asymmetry modulates the preexisting conformational equilibrium in thrombin*, Biochemistry, 2016, 55, 3984-3994.
Technical and administrative staff

Administration and logistics at DiSC is managed through four secretariats and a number of services, that include maintenance of buildings and instrumentations, laboratory safety, technical assistance to research and didactic laboratories, information systems.

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