



Anno 2013

Università degli Studi di PADOVA >> Sua-Rd di Struttura: "SCIENZE CHIMICHE - DiSC"

#### B.1.b Gruppi di Ricerca

##### 1. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Analytical Chemistry Group
Descrizione	<p>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:</p> <ul style="list-style-type: none"> <li>- optical sensors</li> <li>- emerging contaminants in the environment and food</li> <li>- atmosphere chemistry</li> <li>- metal-ligand complexation in aqueous solutions for chelation therapy</li> <li>- applied analytical chemistry</li> </ul> <p>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) TA<sub>p</sub> WAtter RAdioactivity Real Time Monitor (TAWARA_RTM).</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Signal Drift of an Oxygen Optical Sensors Part I: Rationalization of the Drift Nature and its experimental check with a light intensity detection based sensor, Sensors and Actuators B: Chem., 2013, 943-948</li> <li>- Signal Drift of an Oxygen Optical Sensors Part II: Smart Drift Correction Algorithm and its experimental check with a light intensity detection based sensor, Sensors and Actuators B: Chem., 2013, 949-954</li> <li>- Field comparison of a personal cascade impactor sampler, an optical particle counter and CEN-EU standard methods for PM10, PM2.5 and PM1 measurement in urban environment, Journal of aerosol Science, 2013, 65, 111-120</li> <li>- New Possible Chelating Agents for Iron and Aluminum: 4-hydroxy-5-methyl-3-pyridinecarboxylic Acid and 1,5-dimethyl-4-hydroxy-3-pyridinecarboxylic Acid, Eur. J. Inorg. Chem., 2013, 1310-1319</li> <li>- Application of LC-MS and LC-MS-MS to the analysis of photo-decomposed crystal violet in the investigation of cultural heritage materials aging, Journal of Mass Spectrometry, 2012, 47, 1660-1670</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/analitica/english">www.chimica.unipd.it/analitica/english</a>
Responsabile scientifico/Coordinatore	PASTORE Paolo (SCIENZE CHIMICHE - DiSC)

##### Settore ERC del gruppo:

PE4\_18 - Environment chemistry

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_5 - Analytical chemistry

PE4\_7 - Chemical instrumentation

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

PE4\_9 - Method development in chemistry

##### Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BADOCCHI	Denis	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/01
BOGIALLI	Sara	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/01
BORTOLINI	Claudio	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/01
DI MARCO	Valerio	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/01
FAVARO	Gabriella	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/01
MONDIN	Andrea	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/01
PERAZZOLO	Anna	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/12
REPICE	Carla	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/01

ROVERSO	Marco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/01
TAPPARO	Andrea	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/01

**2. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Bioinorganic Chemistry Lab
Descrizione	<p>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:</p> <ul style="list-style-type: none"> <li>- 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</li> <li>- 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</li> <li>- Development of anti-inflammatory agents for the treatment of acute and chronic inflammation</li> </ul> <p>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/antinflammatory 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.</p> <p>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.</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Beyond Platinums: Gold Complexes as Anticancer Agents, <i>Anticancer Research</i>, 2014, 34, 487-492</li> <li>- Gold(III)-Dithiocarbamato Peptidomimetics in the Forefront of the Targeted Anticancer Therapy: Preclinical Studies against Human Breast Neoplasia, <i>Plos One</i>, 2014, 9, e84248</li> <li>- Insights into the Reactivity of Gold-Dithiocarbamato Anticancer Agents toward Model Biomolecules from Multinuclear NMR Spectroscopy, <i>Chem. Eur. J.</i>, 2013, 19, 13428-13436</li> <li>- Noble metal-dithiocarbamates precious allies in the fight against cancer, <i>Mini-reviews in medicinal chemistry</i>, 2012, 12, 1216-1229</li> <li>- Targeting the ubiquitin-proteasome pathway with inorganic compounds to fight cancer: a challenge for the future, <i>Future Medicinal Chemistry</i>, 2012, 4, 525-543</li> </ul> <p>8</p>
Sito web	<a href="http://www.chimica.unipd.it/bioinorg/">http://www.chimica.unipd.it/bioinorg/</a>
Responsabile scientifico/Coordinatore	FREGONA Dolores (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

LS1\_1 - Molecular interactions

LS7\_3 - Pharmacology, pharmacogenomics, drug discovery and design, drug therapy

PE5\_11 - Biological chemistry

PE5\_18 - Molecular chemistry

PE5\_9 - Coordination chemistry

**Componenti:**

Cognome	Nome	Struttura	Qualifica	Settore
BOSCUTTI	Giulia	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
NARDON	Chiara	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03

**3. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Biomolecular Structure Group
	<p>The research of the Biomolecular Structure Group is focused on the properties and structure of peptides and proteins, with the goal to determine relationships between their biological activity and structure, to elucidate the molecular mechanisms of natural processes, and to specifically modify the latter with specific products. The main experimental techniques we employ are multidimensional NMR and protein crystallography.</p> <p>In our group, we also apply 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 trace food products to the development of new analytical tools to establish the <i>in vivo</i> effects of exogenous</p>

Descrizione	<p>substances. Our main research lines are the following:</p> <ul style="list-style-type: none"> <li>- Structural, functional and inhibition studies of oncogenic protein kinase CK2</li> <li>- Structural and functional characterization of SulP/SLC26 anion transporters</li> <li>- Enzyme engineering for industrial applications</li> <li>- Structure and interactions of proteins involved in the peculiar redox metabolism of pathogenic organisms</li> <li>- Fragment-based drug discovery by NMR and crystallography</li> <li>- Metabolomic analysis of food extracts and biological fluids</li> <li>- Traceability of foodstuff</li> <li>- Synthesis and characterization of peptide and peptidomimetics</li> </ul> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters, <i>Nat. Comm.</i> in press</li> <li>- Iron-sulfur cluster binding by mitochondrial monothiol glutaredoxin-1 of <i>Trypanosoma brucei</i>: molecular basis of iron-sulfur cluster coordination and relevance for parasite infectivity, <i>Antioxid. Redox Signal.</i>, 2013, 19, 665682,</li> <li>- Fly Cryptochrome and the Visual System, <i>Proc. Natl. Acad. Sci. U.S.A.</i>, 2013, 110, 6163-6168, Characterization of Markers of Botanical Origin and Other Compounds Extracted from Unifloral Honeys, <i>J. Agr. Food Chem.</i>, 2013, 61, 1747-1755,</li> <li>- Ceftriaxone blocks the polymerisation of <math>\alpha</math>-synuclein and exerts neuroprotective effects in vitro, <i>ACS Chem. Neurosci.</i>, 2014, 5, 30-38,</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/stefano.mammi">www.chimica.unipd.it/stefano.mammi</a>
Responsabile scientifico/Coordinatore	MAMMI Stefano (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

LS1\_10 - Structural biology (NMR)

LS1\_9 - Structural biology (crystallography and EM)

LS9\_6 - Food sciences

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BELLANDA	Massimo	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/04
BATTISTUTTA	Roberto	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/11
UDDIN	Jalal	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/04
LOLLI	Graziano	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/11
NDOUM	Emmanuel	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/04
SCHIEVANO	Elisabetta	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/04
STURLESE	Mattia	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/04

#### Altro Personale

Calderan Andrea (ICB CNR) Ruzza Paolo (ICB CNR)

#### 4. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	Bio-Organic Chemistry Group
	<p>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:</p> <ul style="list-style-type: none"> <li>- synthesis and conformation of peptides with rigid and well-defined 3D-structure (e.g., <math>\alpha</math>-, 310- and 2.05-helices or turns)</li> <li>- synthesis, conformation, mechanism of action and bioactivities (antibacterial and antitumor) of the naturally-occurring peptaibiotics</li> <li>- antimicrobial photodynamic therapy</li> <li>- textiles functionalized with antibacterial peptides for biomedical applications</li> <li>- peptide helices as rigid structural elements for spectroscopic studies and for electron transfer and photovoltaic applications</li> </ul>

<b>Descrizione</b>	<ul style="list-style-type: none"> <li>- peptide nanotechnology: peptido-rotaxanes, peptide-decorated metal nanoparticles, selfassembled peptide polymers</li> <li>Recent key publications</li> <li>- Mimicking Nature: A Novel Peptide-based Bio-inspired Approach for Solar Energy Conversion, <i>ChemPhysChem</i>, 2014, 15, 64-68</li> <li>- Reversible Chirality Control in Peptide-Functionalized Gold Nanoparticles, <i>ACS Nano</i>, 2013, 7, 9933-9939</li> <li>- Synthesis, Characterization, and Photoinduced Antibacterial Activity of Porphyrin-Type Photosensitizers Conjugated to the Antimicrobial Peptide Apidaecin 1b, <i>J. Med. Chem.</i>, 2013, 56, 10521063</li> <li>- Partial thioamide scan on the lipopeptaibiotic trichogin GA IV. Effects on folding and bioactivity, <i>Beilstein J. Org. Chem.</i>, 2012, 8, 11611171</li> <li>- A Rigid Helical Peptide Axle for a [2]Rotaxane Molecular Machine, <i>Angew. Chem. Int. Ed.</i>, 2009, 48, 8986-8989</li> </ul>
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/bocgroup">http://www.chimica.unipd.it/bocgroup</a>
<b>Responsabile scientifico/Coordinatore</b>	FORMAGGIO Fernando (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE5\_11 - Biological chemistry

PE5\_16 - Supramolecular chemistry

PE5\_17 - Organic chemistry

PE5\_7 - Biomaterials synthesis

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
GOBBO	Marina	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/06
MORETTO	Alessandro	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
MAZZIER	Daniela	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
PEGGION	Cristina	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
ORLANDIN	Andrea	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06

#### Altro Personale

Biondi Barbara (ICB CNR) Crisma Marco (ICB CNR)

#### 5. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

<b>Nome gruppo*</b>	The Biophysics Group
<b>Descrizione</b>	<p>The Biophysics Laboratory is equipped with CW- and FT-EPR, pulse-ENDOR, PELDOR (X- and Q- band), and ODMR (optically detected magnetic resonance)</p> <ul style="list-style-type: none"> <li>- Natural photosynthetic systems; The main research activity is focussed on photosynthesis and related phenomena. The spectroscopic EPR investigation, complemented with the quantum mechanical calculations, address some of the open questions on the molecular mechanisms taking place in photosynthetic systems, such as photoprotection and photoinhibition</li> <li>- Artificial bio-mimetic photosynthetic systems. Analogs of photosynthetic reaction centers and of light-harvesting systems, including the photoprotective carotenoid moiety are studied by time-resolved and pulsed EPR</li> <li>- Hydrogenase and photobioproduction of hydrogen. [FeFe]-hydrogenases are key enzymes for bio-production of H<sub>2</sub>. Research is currently underway to understand how their active site is assembled, and to improve the development of bio-inspired hydrogenase analogs in renewable energy applications</li> <li>- Motions in proteins detected by spin labelling of macromolecules</li> </ul> <p>The group is currently supported by an Italian MIUR research program on Photochemistry and by the CARIPARO foundation Excellence project Modeling and monitoring motions in proteins: cardiovascular diseases at molecular level (M3PC)</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Evidence for water-mediated triplet-triplet energy transfer in the photoprotective site of the peridinin-chlorophyll a-protein, <i>Biochem. Biophys. Acta.</i>, 2014, 1837, 85-97</li> <li>- Zeaxanthin Protects Plant Photosynthesis by Modulating Chlorophyll Triplet Yield in Specific Light-harvesting Antenna Subunits, <i>J. Biol. Chem.</i>, 2012, 287, 41820-41834</li> <li>- The [4Fe-4S]-cluster coordination of [FeFe]-hydrogenase maturation protein HydF as revealed by EPR and HYSCORE spectroscopies, <i>Biochem. Biophys. Acta.</i>, 2012, 1817, 2149-2157</li> </ul>

	<ul style="list-style-type: none"> <li>- NPQ activation reduces chlorophyll triplet state formation in the moss <i>Physcomitrella patens</i> <i>Biochem., Biophys. Acta.</i>, 2012, 1817, 1608-1615</li> <li>- Auxin-responsive genes AIR12 code for a new family of plasma membrane b-type cytochromes specific to flowering plants, <i>Plant Physiol.</i>, 2009, 150, 606-620</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/biofisica/pubblica">www.chimica.unipd.it/biofisica/pubblica</a>
Responsabile scientifico/Coordinatore	CARBONERA Donatella (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

LS1\_8 - Biophysics (e.g. transport mechanisms, bioenergetics, fluorescence)

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
DI VALENTIN	Marilena	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
ALBERTINI	Marco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02

#### 6. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Chemistry of f Elements Group
Descrizione	<p>The group engaged in the Chemistry of f Elements studies both more fundamental research in solution coordination chemistry and applications of solution chemical methodology in material sciences, environmental aquatic chemistry and problems related to nuclear waste disposal.</p> <p>The groups main interests are devoted on two topics:</p> <ul style="list-style-type: none"> <li>- The solution chemistry of f elements</li> <li>- The preparation and characterization of new materials containing f elements in a graphite matrix. resistant at very high temperatures ( 2000 °C)</li> </ul> <p>For pursuing the objectives above the Group has an authorized laboratory for processing radioactive material with all the necessary equipment for the study of the solution chemistry of f elements: two calorimeters (micro and macro), FTIR and UV-Visible spectrometers, dry boxes for working in inert atmosphere. An oven for preparations and studies on materials up to about 2000 °C completes the instrumental facilities.</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- A calorimetric study of the hydrolysis and peroxide complex formation of the uranyl(VI) ion, <i>Dalton Trans.</i>, 2014, 43(6), 2378-2383 (cover article)</li> <li>- Chemical equilibria in the UO<sub>2</sub>+H<sub>2</sub>O<sub>2</sub>F-/OH- systems and possible solution precursors for the formation of [Na<sub>6</sub>(OH<sub>2</sub>)<sub>8</sub>][UO<sub>2</sub>(O<sub>2</sub>)F]2418- and [Na<sub>6</sub>(OH<sub>2</sub>)<sub>8</sub>][UO<sub>2</sub>(O<sub>2</sub>)OH]2418- clusters, <i>Dalton Trans.</i>, 2013, 42(28), 10129-10137</li> <li>- Chemical equilibria in the uranyl(VI)peroxidecarbonate system; identification of precursors for the formation of poly-peroxometallates, <i>Dalton Trans.</i>, 2012, 41(38) 11635-11641 (cover article)</li> <li>- Chemical equilibria in the binary and ternary uranyl(VI)hydroxideperoxide systems, <i>Dalton Trans.</i>, 2012, 41(12), 3389-3386 (cover article)</li> <li>- Interaction of thorium(IV) with nitrate in aqueous solution: medium effect or weak complexation?, <i>Dalton Trans.</i>, 2011, 40 (36), 9101-9105 (cover article)</li> </ul>
Sito web	
Responsabile scientifico/Coordinatore	DI BERNARDO Plinio (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_3 - Molecular architecture and Structure

PE5\_16 - Supramolecular chemistry

PE5\_9 - Coordination chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
ZANONATO	Pier Luigi	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03

**7. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Cultural Heritage Group
	Il sistema non consente l'inserimento del componente del gruppo: dr. Luca Nodari (CNR)
Descrizione	<p>The investigation in material science of Cultural Heritage Artefacts are mainly devoted to the study of inorganic materials (glass, ceramics and metals) by using nonconventional spectroscopic techniques, as Xrays 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:</p> <ul style="list-style-type: none"> <li>- Portable LIBS (Laser Induced Breakdown Spectroscopy)</li> <li>- Portable microXRF (XRay Fluorescence)</li> <li>- <math>^{57}\text{Fe}</math> Mössbauer Spectroscopy operating in transmission (micro-invasive) and reflection (micro-invasive, noninvasive mode)</li> <li>- XPS (Xray Photoelectron Spectroscopy)</li> <li>- AFM (Atomic Force Microscopy)</li> <li>- FEGESEM equipped with detector for EDS analyses</li> <li>- Optical microscopy</li> <li>- Climatic Chamber</li> </ul> <p>Also accessible to the group Raman, IR, UVVis 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 physicchemical properties of the Fe nuclei themselves.</p>
Sito web	
Responsabile scientifico/Coordinatore	BERTONCELLO Renzo (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE4\_16 - Corrosion

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_4 - Surface science and nanostructures

PE5\_3 - Surface modification

PE5\_4 - Thin films

SH6\_1 - Archaeology, archaeometry, landscape archaeology

**Componenti:**

Cognome	Nome	Struttura	Qualifica	Settore
Altro Personale	Nodari Luca(IENI-CNR)			

**8. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The CheMaMSE Group (Chemistry of Materials for Metamorphosis and Storage of Energy)
	<p>The research lines of the CheMaMSE group are the following:</p> <ul style="list-style-type: none"> <li>- Fuel Cells: synthesis, characterization, and tests in single PEM fuel cell of new membranes and electrocatalysts</li> <li>- Redox Flow Batteries: synthesis, characterization, and tests in single fuel cell of new membranes and electrocatalysts</li> <li>- Secondary Batteries based on alkaline and alkaline-earth elements: synthesis of both electrode materials and electrolytes, characterization and tests in battery prototypes</li> </ul> <p>The laboratory is equipped with all the instrumentations needed to prepare, characterize and test in single cell devices including the above-described materials. A Broadband electrical spectroscopy laboratory is available, for the study of the electric response of materials up to 20 GHz as function of temperature (100-1000K), relative humidity and pressure (1-150 bar)</p>

<b>Descrizione</b>	<p>The group is currently involved in two important projects:</p> <ul style="list-style-type: none"> <li>- Progetto Strategico di Ateneo: MAESTRA - From Materials for Membrane-Electrode Assemblies to Electric Energy (2014 - 2016)</li> <li>- ARO with US Army: An integrated multi-scale approach for understanding ion transport in complex heterogeneous organic materials (2013-2014)</li> </ul> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Interplay between Structure and Relaxations in Perfluorosulfonic Acid Proton Conducting Membranes, Journal of the American Chemical Society, 135, 2013, 822</li> <li>- New nanocomposite hybrid inorganic-organic proton conducting membranes based on functionalized silica and PTFE, ChemSusChem, 5, 2012, 1758</li> <li>- Interplay between Mechanical, Electrical, and Thermal Relaxations in Nanocomposite Proton Conducting Membranes Based on Nafion and a [(ZrO<sub>2</sub>)-(Ta<sub>2</sub>O<sub>5</sub>)<sub>0.119</sub>] core-shell nanofiller, J. Am. Chem. Soc., 46, 2012, 19099</li> <li>- Synthesisstructuremorphology interplay of bimetalliccoreshell carbon nitride nano-electrocatalysts, ChemSusChem, 5, 2012, 2451</li> <li>- Preparation, characterization and single-cell performance of a new class of Pd-carbon nitride electrocatalysts for oxygen reduction reaction in PEMFCs, App. Catal. B, Environ, 111, 2012, 185</li> </ul>
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/lab_DiNoto">www.chimica.unipd.it/lab_DiNoto</a>
<b>Responsabile scientifico/Coordinatore</b>	DI NOTO Vito (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE3\_1 - Structure of solids and liquids

PE3\_11 - Mesoscopic physics

PE3\_13 - Structure and dynamics of disordered systems: soft matter (gels, colloids, liquid crystals...), glasses, defects

PE3\_15 - Statistical physics: phase transitions, noise and fluctuations, models of complex systems

PE3\_3 - Transport properties of condensed matter

PE3\_4 - Electronic properties of materials surfaces, interfaces, nanostructures

PE4\_1 - Physical chemistry

PE4\_10 - Heterogeneous catalysis

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_13 - Theoretical and computational chemistry

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_4 - Surface science and nanostructures

PE4\_6 - Chemical physics

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

PE5\_1 - Structural properties of materials

PE5\_10 - Colloid chemistry

PE5\_12 - Chemistry of condensed matter

PE5\_14 - Macromolecular chemistry

PE5\_15 - Polymer chemistry

PE5\_16 - Supramolecular chemistry

PE5\_2 - Solid state materials

PE5\_5 - Ionic liquids

PE5\_6 - New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles

PE5\_9 - Coordination chemistry

PE8\_6 - Energy systems (production, distribution, application)

#### Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BERTASI	Federico	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
BOARETTO	Nicola	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03

CAVINATO	Gianni	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03
ADAMI	Arianna	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
NEGRO	Enrico	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03

**Altro Personale**

Pace Giuseppe (IENI CNR) Lavina Sandra (Personale tecnico laureato Dipartimento Scienze Chimiche)

**9. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Electrocatalysis and Applied Electrochemistry (ECAE) Group
Descrizione	<p>The ECAE Laboratory is equipped with electrochemical apparatus and other analytical facilities and the group currently pursues the following research lines:</p> <ul style="list-style-type: none"> <li>- 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)</li> <li>- Electrochemical approaches to Atom Transfer Radical Polymerization and Atom Transfer Radical Cyclization</li> <li>- Electrocarboxylation of different substrates (halides, ketones, olefins) for the synthesis of fine chemicals and/or pharmaceutical compounds</li> <li>- Electrochemical reduction of organic halides in ionic liquids and characterization of inherently chiral ionic liquids</li> <li>- Electrochemical technologies for wastewater treatments</li> </ul> <p>The group is currently involved in a European Project in the field of fuel cells, started in January 2013: CH-JU-2011-1: University of Padova local coordination of CathCat (Prof. Granozzi): Novel catalyst materials for the cathode side of MEAs suitable for transportation applications (<a href="http://cathcat.eu/index.php/home">http://cathcat.eu/index.php/home</a>)</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Electrochemically Mediated Atom Transfer Radical Polymerization, <i>Science</i>, 2011, 332, 81</li> <li>- One-pot synthesis of benzoic acid by electrocatalytic reduction of bromobenzene in the presence of CO<sub>2</sub>, <i>Electrochim. Commun.</i>, 2011, 13, 810-813</li> <li>- Electrocatalytic Dechlorination of Volatile Organic Compounds at a Copper cathode. Part I: Polychloromethanes, <i>Appl. Catal. B: Environ.</i>, 2012, 126, 347-354.</li> <li>- Highly Selective Electrochemical Hydrogenation of Acetylene to Ethylene at Ag and Cu Cathodes, <i>Electrochim. Commun.</i>, 2013, 34, 90-93</li> <li>- Electrochemical behavior of N and Ar implanted highly oriented pyrolytic graphite substrates and activity toward oxygen reduction reactio</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/electrochem/">www.chimica.unipd.it/electrochem/</a>
Responsabile scientifico/Coordinatore	GENNARO Armando (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE4\_10 - Heterogeneous catalysis

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

PE5\_15 - Polymer chemistry

PE5\_5 - Ionic liquids

**Componenti:**

Cognome	Nome	Struttura	Qualifica	Settore
DURANTE	Christian	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
FANTIN	Marco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
GRADZKA	Emilia	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
AHMED ISSE	Abdirisak	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
PERINI	Lorenzo	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02

**10. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**
**Nome gruppo\***

The EPR Spectroscopy Group

<b>Descrizione</b>	The EPR spectroscopy group is focused on the development and application of Electron Paramagnetic Resonance (EPR) techniques to research in Material Science (graphene, organic electronics, organic photovoltaics), in Biomolecular Systems (peptides, membranes, protein cofactors) and Cultural Heritage conservation (degradation of ancient books, pigments and other artistic materials). The facilities of the EPR laboratory at the DiSC include: - An X-band CW- and pulsed-EPR spectrometer, equipped with pulsed ENDOR and DEER 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, DEER and time-resolved accessories All spectrometers are equipped with variable temperature systems, for measurements from 4 K to 400 K. Recent key publications - Time-resolved EPR of photoinduced excited states in a semiconducting polymer/PCBM blend, J. Phys. Chem. C, 2013, 117, 1554-1560 - Structural Characterization of a High Affinity Mononuclear Site in the Copper(II)-Synuclein Complex, J. Am. Chem. Soc., 2010, 132, 18057-18066 - Degradation Products from Naturally Aged Paper Leaves of a 16th-Century Printed Book: A Spectrochemical Study, Chem. Eur. J., 2013, 19, 9569-9577 - ENDOR Evidence of Electron-H <sub>2</sub> Interaction in a Fulleride Embedding H <sub>2</sub> , J. Am. Chem. Soc., 2010, 134, 12881-12884 - Nitroxyl Radicals for Studying Electron Transfer, Angew. Chem., 2013, 52, 8689-8692
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/eprgroup/">www.chimica.unipd.it/eprgroup/</a>
<b>Responsabile scientifico/Coordinatore</b>	MANIERO Anna Lisa (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE3\_12 - Molecular electronics

PE4\_1 - Physical chemistry

PE4\_11 - Physical chemistry of biological systems

PE4\_17 - Characterization methods of materials

PE4\_2 - Spectroscopic and spectrometric techniques

SH6\_1 - Archaeology, archaeometry, landscape archaeology

#### Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BARBON	Antonio	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
BRONZATO	Maddalena	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
BORTOLUS	Marco	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
DALZINI	Annalisa	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
FRANCO	Lorenzo	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
MARGOLA	Tommaso	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
RUZZI	Marco	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
TOFFOLETTI	Antonio	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/02
TAMPIERI	Francesco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
ZOLEO	Alfonso	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02

#### 11. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

<b>Nome gruppo*</b>	The NMRLAB Group (Experimental and computational NMR spectroscopy)
	<p>Our scientific activity is focused on experimental and computational NMR spectroscopy. Main research topics include:</p> <ul style="list-style-type: none"> <li>- Computational prediction of NMR parameters: natural substances, molecules containing heavy atoms, paramagnetic complexes and non-covalent interactions</li> <li>- Paramagnetic NMR: computational prediction of the molecular parameters that determine the NMR spectral patterns of paramagnetic substances (spin state, hyperfine couplings, g-tensor)</li> <li>- Development of experimental NMR methods for accurate determination of small coupling constants, intermolecular NOEs, weak non-covalent interactions, solvation of small molecules and nanosystems, complex matrices (e.g. food)</li> <li>- Ionic Liquid Crystals: synthesis, characterization, NMR spectroscopy and molecular dynamics (MD) simulations</li> </ul>

<b>Descrizione</b>	Departmental NMR facilities include up to 600 MHz (400 MHz for solids) instruments. The group also has agreements with European high-field NMR facilities. Computational work is carried out with Departmental facilities ( <a href="http://www.chimica.unipd.it/c3p/">www.chimica.unipd.it/c3p/</a> ) or by access to national large-scale computer centers.
Recent key publications	<ul style="list-style-type: none"> <li>- Addressing the Stereochemistry of Complex Organic Molecules by Density Functional Theory-NMR: Vannusal B in Retrospective, <i>J. Am. Chem. Soc.</i>, 2011, 133, 6072</li> <li>- Predicting the Paramagnet-Enhanced NMR Relaxation of H<sub>2</sub> Encapsulated in Endofullerene Nitroxides by DFT Calculations, <i>Phil. Trans. Royal Soc. A</i>, 2013, 20110634</li> <li>- Observation of scalar nuclear spin-spin coupling in van der Waals complexes, <i>Proc. Natl. Acad. Sci. USA</i>, 2012, 109, 12393</li> <li>- NMR chemosensing using monolayer-protected nanoparticles as receptors, <i>J. Am. Chem. Soc.</i>, 2013, 135, 11768</li> <li>- Effect of the chain length on the structure of ionic liquids: from spatial heterogeneity to ionic liquid crystals, <i>J. Phys. Chem. B</i>, 2013, 117, 1104</li> </ul>
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/nmrlab/">www.chimica.unipd.it/nmrlab/</a>
<b>Responsabile scientifico/Coordinatore</b>	BAGNO Alessandro (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE3\_13 - Structure and dynamics of disordered systems: soft matter (gels, colloids, liquid crystals...), glasses, defects

PE4\_13 - Theoretical and computational chemistry

PE4\_17 - Characterization methods of materials

PE4\_2 - Spectroscopic and spectrometric techniques

PE5\_17 - Organic chemistry

PE5\_5 - Ionic liquids

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BORGOGNO	Andrea	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06
RASTRELLI	Federico	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06

Altro Personale

Saielli Giacomo (ITM CNR)

#### 12. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

<b>Nome gruppo*</b>	The LASPEN Group (Laser Spectroscopy and Nanophotonics)
<b>Descrizione</b>	<p>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. More recently microfluidic devices for biomedical applications and synthesis of nanostructures have been also pursued. The techniques set up to investigate these phenomena are:</p> <ul style="list-style-type: none"> <li>- Micro and Macro Raman Spectroscopies: RRS, SERS</li> <li>- Two-photon induced fluorescence and Z-scan</li> <li>- Transient Absorption with fs time resolution</li> <li>- Two-Dimensional photon echo experiments</li> <li>- Time Resolved Fluorescence Microscopy: FLIM and FCS</li> </ul> <p>The group is currently involved in three European research projects and three Italian research projects, 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 (<a href="http://www.chimica.unipd.it/quenthal/">http://www.chimica.unipd.it/quenthal/</a>); FIRB2011 RBAP11X42L (R. Bozio): From single molecules to the whole animal model: an integrated approach to the study of intra- and inter-cellular signaling</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Lifetime Shortening and Fast Energy-Transfer Processes upon Dimerization of a A-pi-D-pi-A Molecule, <i>Chem. Phys. Chem.</i>, 2014, 15, 310-319</li> <li>- Investigation into the Heterostructure Interface of CdSe-Based Core-Shell Quantum Dots Using Surface-Enhanced Raman Spectroscopy, <i>ACS Nano</i>, 2013, 7, 6649-6657</li> <li>- Spectroscopic signatures of quantum-coherent energy transfers, <i>Chem. Soc. Rev.</i>, 2013, 42, 4932-4947</li> <li>- Soft-Lithographed Up-Converted Distributed Feedback Visible Lasers Based on CdSe-CdZnS-ZnS Quantum Dots, <i>Adv. Funct. Mater.</i>, 2012, 22, 337-334</li> <li>- Photophysics and Dynamics of Surface Plasmon Polaritons-Mediated Energy Transfer in the Presence of an Applied Electric Field, <i>J. Am. Chem. Soc.</i>, 2012, 134, 10061-10070</li> </ul>

Sito web	<a href="http://www.chimica.unipd.it/l.snp/">www.chimica.unipd.it/l.snp/</a>
Responsabile scientifico/Coordinatore	BOZIO Renato (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE2\_11 - Lasers, ultra-short lasers and laser physics

PE2\_9 - Optics, non-linear optics and nano-optics

PE3\_10 - Nanophysics: nanoelectronics, nanophotonics, nanomagnetism, nanoelectromechanics

PE3\_12 - Molecular electronics

PE3\_4 - Electronic properties of materials surfaces, interfaces, nanostructures

PE4\_1 - Physical chemistry

PE4\_15 - Photochemistry

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_4 - Surface science and nanostructures

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

PE5\_16 - Supramolecular chemistry

PE5\_6 - New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles

PE5\_8 - Intelligent materials - self assembled materials

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BOLZONELLO	Luca	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
COLLINI	Elisabetta	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
CIPOLLONI	Marco	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
FEDE	Caterina	SCIENZE CHIMICHE - DiSC	Assegnista	BIO/16
FERRANTE	Camilla	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/02
FRARE	Maria Chiara	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
FASSIOLI OLSEN	Francesca Daniela	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
HOSEINKHANI ASL	Sajjad	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
MINOTTO	Alessandro	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
PEDRON	Danilo	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/02
ROSSETTO	Nicola	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
SIGNORINI	Raffaella	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
TODECATO	Francesco	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
WEBER	Verena	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02

**Altro Personale**

Pilot Roberto (INSTM)

**13. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Molecular Electrochemistry and Nanosystems (MEN) Group
	<p>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:</p> <ul style="list-style-type: none"> <li>- Electron Transfer through Molecular Bridges and Interfaces</li> <li>- Dissociative Electron Transfer</li> </ul>

Descrizione	<ul style="list-style-type: none"> <li>- Molecule-like and Quantized Monolayer-Protected Gold Clusters: Properties, Redox Catalysis, Drug Delivery Systems</li> <li>- Electrochemical Sensors for Cancer Biomarkers</li> <li>- Self-Assembled Monolayers of Conformationally Constrained Peptides</li> <li>- Biomimetic Membranes</li> </ul> <p>The MEN Group is equipped with state-of-the-art electrochemical instrumentations, including electrogenerated chemiluminescence and scanning electrochemical microscopy, STM and AFM, PM-IIRRAS and UV-visible spectrometries, HPLC, mass spectrometry, etc.</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Au25(SEt)18, a Nearly Naked Thiolate-Protected Au25 Cluster: Structural Analysis by Single Crystal X-ray Crystallography and Electron Nuclear Double Resonance, ACS Nano, 2014, DOI: 10.1021/nn500805n</li> <li>- Electron Transfer through 3D Monolayers on Au25 Clusters, ACS Nano, 2014, 8, 2788-2795</li> <li>- Interplay of Charge State, Lability, and Magnetism in the Molecule-like Au25(SR)18 Cluster, J. Am. Chem. Soc., 2013, 135, 15585-15594</li> <li>- Effect of Orientation of the Peptide-Bridge Dipole Moment on the Properties of Fullerene-Peptide-Radical Systems., J. Am. Chem. Soc., 2012, 134, 10628-10637</li> <li>- Ultrasensitive Nanostructured Immunosensor for Stem and Carcinoma Cell Pluripotency Gatekeeper Protein NANOG., Nanomedicine, 2012, 7, 957-965</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/marangroup/pubblica/">www.chimica.unipd.it/marangroup/pubblica/</a>
Responsabile scientifico/Coordinatore	MARAN Flavio (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_10 - Heterogeneous catalysis

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE5\_13 - Homogeneous catalysis

PE5\_14 - Macromolecular chemistry

PE5\_15 - Polymer chemistry

PE5\_9 - Coordination chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
DAINESE	Tiziano	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
ANTONELLO	Sabrina	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
POLO	Federico	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
RENE'	Alice	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02

#### 14. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The M3 group (Molecular materials & modeling)
Descrizione	<p>Design, synthesis, characterization, and modeling of supramolecular structures 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 through strategies of molecular self-assembly by exploiting non-covalent, selective and directional interactions. 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.</p> <p>Besides spectroscopic and analytical techniques available in our department (IR and UV-Visible spectroscopy, 1H, 13C, 31P 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. The computational power available to M3 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.</p> <p>M3 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)</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Chemical tuning versus micro structure features in solid-state gas sensors: LaFe<sub>1-x</sub>GaO<sub>3</sub>, a case study, Chem. Mater., 2014, 26, 1505</li> <li>- Oxocluster-reinforced organic-inorganic hybrid materials: effect of transition metal oxoclusters on structural and functional properties, J. Mat. Chem., 2011, 48, 15853</li> <li>- A templating guest sorts out a molecular triangle from a dimer-trimer constitutional dynamic library, Chem. Commun., 2012, 48, 3115</li> </ul>

	<p>- Magnetic Properties and Vapochromic Reversible Guest-induced Transformation in a Bispyrazolato Copper(II) Polymer: an Experimental and Dispersion-Corrected Density Functional Theory Study, Inorg. Chem., 2009, 48, 4044  - Role and Effective Treatment of Dispersive Forces in Materials: Polyethylene and Graphite Crystals as Test, J. Comput. Chem., 2009, 30, 934</p>
Sito web	<a href="http://www.chimica.unipd.it/m3/">http://www.chimica.unipd.it/m3/</a>
Responsabile scientifico/Coordinatore	CASARIN Maurizio (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_13 - Theoretical and computational chemistry

PE4\_17 - Characterization methods of materials

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_3 - Molecular architecture and Structure

PE4\_4 - Surface science and nanostructures

PE4\_6 - Chemical physics

PE5\_1 - Structural properties of materials

PE5\_10 - Colloid chemistry

PE5\_12 - Chemistry of condensed matter

PE5\_13 - Homogeneous catalysis

PE5\_16 - Supramolecular chemistry

PE5\_18 - Molecular chemistry

PE5\_2 - Solid state materials

PE5\_3 - Surface modification

PE5\_4 - Thin films

PE5\_6 - New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles

PE5\_8 - Intelligent materials - self assembled materials

PE5\_9 - Coordination chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
DOLCET	Paolo	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
PANDOLFO	Luciano	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03
RANCAN	Marzio	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03

#### Altro Personale

Armelao Lidia (IENI-CNR) Bottare Gregorio (IENI-CNR) Forrer Daniel (IENI-CNR) Gross Silvia (IENI-CNR) Natile Marta Maria (IENI-CNR) Vittadini Andrea (IENI-CNR)

#### 15. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Molecular Recognition and Catalysis Group
Descrizione	<p>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 - Self-Assembled Molecular Structures; Catalytic Molecular Machines - Hybrid Receptors for Anions in Water Recent key publications</p>

	<ul style="list-style-type: none"> <li>- Revisiting the Hammett rho Parameter for the Determination of Philiicity: Nucleophilic Substitution with Inverse Charge Interaction, <i>Angew. Chem. Int. Ed.</i>, 2013, 52, 2911-2914</li> <li>- Non-Covalent Activation of a Titanium(IV) Oxygen Transfer Catalyst, <i>Chem. Eur. J.</i>, 2013, 19, 9438-9441</li> <li>- Determination of Amino Acid Enantiopurity and Absolute Configuration: Synergism between Configurationally Labile Metal-Based Receptors and Dynamic Covalent Interactions, <i>Chem. Eur. J.</i>, 2013, 19, 16809-16813</li> <li>- Recent advances in vanadium catalyzed oxygen transfer reactions, <i>Coord. Chem. Rev.</i>, 2011, 255, 2345-2357</li> <li>- Molybdenum(VI) Amino Triphenolate Complexes as Catalysts for Sulfoxidation, Epoxidation and Haloperoxidation, <i>Adv. Synth. Catal.</i>, 2010, 352, 2937-2942</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/lab108/">http://www.chimica.unipd.it/lab108/</a>
Responsabile scientifico/Coordinatore	LICINI Giulia Marina (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE5\_13 - Homogeneous catalysis

PE5\_16 - Supramolecular chemistry

PE5\_17 - Organic chemistry

PE5\_9 - Coordination chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BADETTI	Elena	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06
DI LORENZO	Rosalia	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
GJOKA	Blerina	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
ZONTA	Cristiano	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06

**16. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Multi-functional Nanomaterial Group
	<p>The Multi-functional Nanomaterial Group has an internationally recognized knowhow 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.</p> <p>The developed systems, subjected to an advanced thorough characterization, are investigated as unique multi-functional platforms for sustainable end-uses, ranging from the molecular detection of flammable/toxic gases, encompassing photo-activated applications (sustainable H<sub>2</sub> production, environmental remediation, light-triggered selfcleaning and anti-fogging systems), up to anodes for Li-ion batteries and magnetic materials.</p> <p>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:</p> <ul style="list-style-type: none"> <li>- NMP4-SL-2012-310333: Water Oxidation Nanocatalysts for Sustainable Solar Hydrogen Production through Visible-Light Activity (SOLAROGENIX) (<a href="http://www.solarogenix.eu/">http://www.solarogenix.eu/</a>)</li> <li>- FP7-PEOPLE-ITN-2008-238409 European Research Training Network of New Materials: Innovative Concepts for their Fabrication, Integration and Characterisation (ENHANCE) (<a href="http://www.enhance-itn.eu/">http://www.enhance-itn.eu/</a>)</li> </ul> <p>Despite being composed by only 3 young scientists, the group has a first-class track record, corresponding to 81 publications on ISI International Journals, 20 other publications, 3 national and international patents and 87 conference communications (of which 11 invited lectures/seminars), only in the period 2009-2013.</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Enhanced hydrogen production by photoreforming of renewable oxygenates through nanostructured Fe<sub>2</sub>O<sub>3</sub> polymorphs, <i>Advanced Functional Materials</i>, 2014, 24, 372</li> <li>- Surface functionalization of nanostructured Fe<sub>2</sub>O<sub>3</sub> polymorphs: from design to lightactivated applications, <i>ACS Applied Materials &amp; Interfaces</i>, 2013, 5, 7130</li> <li>- Columnar Fe<sub>2</sub>O<sub>3</sub> arrays via plasma-enhanced growth: interplay of fluorine substitution and photoelectrochemical properties, <i>International Journal of Hydrogen Energy</i>, 2013, 38, 14189</li> <li>- Ag/ZnO nanomaterials as high performance sensors for flammable and toxic gases, <i>Nanotechnology</i>, 2012, 23, 025502</li> </ul>
Descrizione	

	Selected for the Highlights 2012 collection of Nanotechnology - F-Doped Co <sub>3</sub> O <sub>4</sub> Photocatalysts for Sustainable H <sub>2</sub> Generation from Water/Ethanol, Journal of the American Chemical Society, 2011, 133, 19362
Sito web	
Responsabile scientifico/Coordinatore	MACCATO Chiara (SCIENZE CHIMICHE - DiSC)

Settore ERC del gruppo:
PE4_17 - Characterization methods of materials
PE4_4 - Surface science and nanostructures
PE5_4 - Thin films

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
CARRARO	Giorgio	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
GASPAROTTO	Alberto	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/03

Altro Personale	Barreca Davide (IENI CNR)
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#### 17. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Nano & Molecular Catalysis Laboratory
Descrizione	<p>The group has established a highly interdisciplinary activity on the study of bio-inspired catalysis, molecular materials and functional hybrid architectures. Topics include:</p> <ul style="list-style-type: none"> <li>- Artificial photosynthesis and sustainable photosynthetic processes, which involve the activation of multi-redox routines powered by light irradiation; Research on water splitting catalysts designed at the molecular level and evolved to complex systems for solar energy conversion schemes. Polyoxometalate chemistry as the homogeneous analogs of metal-oxide catalytic phases and surfaces</li> <li>- Bio-inspired multi-electron catalysis (synzymes) for sensing and therapy against ROS-related diseases by shaping the interfacial interaction between the synthetic synzyme and the diverse biological targets</li> <li>- Membrane science, as members of the Institute for Membrane Technology (ITM-CNR), for the development of novel synthetic and functional membranes</li> </ul> <p>The group is involved in the following European and national projects:</p> <p>FP7-NMP.2012.1.4-2 CARINHYPH Bottom-up fabrication of nano carbon-inorganic hybrid materials for photocatalytic H<sub>2</sub> production; FP7-NMP.2012.1.4-2 SACS Self-Assembly in Confined Space; FP7-NMP-2009-SMALL-3 BIONEXGEN Development of the next generation bioreactor system ; Cariparo Foundation, Excellence Project: "NANO-MODULE Design of Molecular Materials for Enhanced Catalysis and Energy"; FIRB 2011 RBAP11ETKA Nanotechnological approaches toward tumor theragnostic ; FIRB 2011 RBAP11C58Y NANOSOLAR: photocatalytic nanosystems for artificial photosynthesis and hydrogen production by solar-driven water splitting</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Supramolecular Design of Low-dimensional Carbon Nano-hybrids encoding a Polyoxometalate-bis-Pyrene Tweezer, Chem. Commun., 2014, DOI: 10.1039/C3CC49725A</li> <li>- Knitting the Catalytic Pattern of Artificial Photosynthesis to a Hybrid Graphene Nanotexture, ACS Nano, 2013, 7, 811</li> <li>- Light driven water oxidation by a single site cobalt salophen catalyst, Chem. Commun., 2013, 49, 9941</li> <li>- Water oxidation surface mechanisms replicated by a totally inorganic tetraruthenium-oxo molecular complex, Proc. Natl. Acad. Sci. U. S. A., 2013, 110, 4917</li> <li>- Photocatalytic Water Oxidation: Tuning Light-Induced Electron Transfer by Molecular Co<sub>4</sub>O<sub>4</sub> Cores, J. Am. Chem. Soc., 2012, 134, 11104</li> </ul>
Sito web	www.chimica.unipd.it/NanoMolCat
Responsabile scientifico/Coordinatore	BONCHIO Marcella (SCIENZE CHIMICHE - DiSC)

Settore ERC del gruppo:
PE5_13 - Homogeneous catalysis
PE5_17 - Organic chemistry
PE5_18 - Molecular chemistry
PE5_8 - Intelligent materials - self assembled materials

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BAZZAN	Irene	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
CARRARO	Mauro	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
SORARU'	Antonio	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
SARTOREL	Andrea	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
ZAMOLO	Valeria Anna	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06

**18. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Nanostructures & Optics Laboratory
Descrizione	<p>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.</p> <p>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.[1-2]</p> <p>These nanostructures are then functionalized with targeting units like Antibodies which show the ability of recognizing a target unit for applications in nano-biomedicine,[1] for example tumour associated antigens, or in the Cultural Heritage.[2]</p> <p>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.[3]</p> <p>Laser assisted synthetic techniques are applied to the development of plasmonic and magnetic NS.[4] also exploitable as multimodal contrast agents.[5]</p> <p>Recent key publications</p> <ul style="list-style-type: none"><li>- Plasmonic Nanostructures for SERRS Multiplexed Identification of Tumor-Associated Antigens, Small, 2012, 8, 3733-3738 (Meneghetti)</li><li>- Alternative SERRS probes for the immunochemical localization of ovalbumin in paintings: an advanced mapping detection approach, Analyst, 2013, 138, 4532-4541 (Meneghetti)</li><li>- Fluorescence dynamics and fine structure of dark excitons in semiconducting single-wall carbon nanotubes; Journal of Physics, Condensed matter, 2012, 24, 255501 (Meneghetti)</li><li>- What controls the composition and the structure of nanomaterials generated by laser ablation in liquid solution?, Phys. Chem. Chem. Phys., 2013, 15, 3027-3046 (Amendola)</li><li>- Magneto-Plasmonic Au-Fe Alloy Nanoparticles Designed for Multimodal SERS-MRI-CT Imaging, Small, 2014, doi: 10.1002/smll.201303372 (Amendola)</li></ul>
Sito web	<a href="http://www.chimica.unipd.it/nanostructures.optics">www.chimica.unipd.it/nanostructures.optics</a>
Responsabile scientifico/Coordinatore	MENEGETTI Moreno (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE3\_10 - Nanophysics: nanoelectronics, nanophotonics, nanomagnetism, nanoelectromechanics

PE4\_1 - Physical chemistry

PE4\_2 - Spectroscopic and spectrometric techniques

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
LITTI	Lucio	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
AMENDOLA	Vincenzo	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
SCARSI	Alessia	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02
SCARAMUZZA	Stefano	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02

**19. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Organic Chemistry for Environment and Health
Descrizione	<p>We have two lines of research</p> <ol style="list-style-type: none"> <li>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 <ul style="list-style-type: none"> <li>- advanced oxidation for air remediation</li> <li>- advanced oxidation for water remediation</li> <li>- syngas production via methane dry reforming conversion of the two major greenhouse gases into useful feedstock</li> </ul> </li> <li>2. Synthesis and characterization of new derivatives of polyphenols and other natural compounds to improve bioactivity <ul style="list-style-type: none"> <li>- prodrug approach: modulation of physical chemical properties of the natural compound via reversible functionalization to prevent metabolization and increase systemic levels</li> <li>- targeting approach: synthesis of mitochondriotropic derivatives for selective delivery</li> </ul> </li> </ol> <p>The group is currently involved in the European Project CMST COST Action TD1208: Electrical discharges with liquids for future applications (<a href="http://www.cost.eu/domains_actions/cmst/Actions/TD1208">http://www.cost.eu/domains_actions/cmst/Actions/TD1208</a>)</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Mitochondria-targeted resveratrol derivatives act as cytotoxic pro-oxidants, <i>Curr. Pharm. Des.</i>, 2014, 20, 172-179</li> <li>- Acetal Derivatives as Prodrugs of Resveratrol, <i>Mol. Pharmaceut.</i>, 2013, 10, 2781-2792</li> <li>- Oxidation mechanisms of CF2Br2 and CH2Br2 induced by air nonthermal plasma, <i>Environ. Sci. Technol.</i>, 2013, 47, 542-548</li> <li>- Comparison of the rates of phenol advanced oxidation in deionized and tap water within a dielectric barrier discharge reactor, <i>Water Res.</i>, 2012, 46, 6239-6246</li> <li>- A comparison of toluene removal in air at atmospheric conditions by different corona discharges, <i>Environ. Sci. Technol.</i>, 2009, 43, 9386-9392</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/cristina.paradisi/">www.chimica.unipd.it/cristina.paradisi/</a>
Responsabile scientifico/Coordinatore	PARADISI Cristina (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_18 - Environment chemistry

PE5\_17 - Organic chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
CERIANI	Elisa	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
MAROTTA	Ester	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
ROMIO	Matteo	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
RUSSO	Viviana	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06

#### 20. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Organic Materials Group
Descrizione	<p>Organic synthesis towards new functional materials is at heart of our research that focuses mainly on the chemical functionalization of carbon nanostructures for solar energy conversion; the use of nanocellulose as a platform for bio-inspired functional materials and the preparation of functional supramolecular organogels. The group is also very active in the field of microfluidics. We have developed fast prototyping techniques for the rapid fabrication of polymer microfluidic devices based on soft photolithography, and studied the surface modification of microchannels by wet chemistry methods. By using our custom prototypes, or commercial flow reactors, we study the synthesis and functionalization of organic molecular structures and nanosystems, such as metal nanoparticles, fullerenes and carbon nanotubes. We often use the microfluidics toolbox to study reaction or surface absorption kinetics. We currently work on 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 group is currently involved in four national projects on solar energy conversion:</p> <ul style="list-style-type: none"> <li>- FIRB-RBFR08DUX6 SOLIS on the engineering of bulk-heterojunctions, 2010-14</li> <li>- FIRB-RBAP11C58Y NANOSOLAR on water splitting, 2013-16</li> <li>- PRIN-20104XET32 DSSCX on dye-sensitized solar cells, 2013-15</li> <li>- PRIN-2010N3T9M4 HI-PHUTURE on carbon-neutral renewable energy, 2013-15</li> </ul> <p>Recent key publications</p>

	<ul style="list-style-type: none"> <li>- Nanocrystalline celluloseporphyrin hybrids: synthesis, supramolecular properties, and singlet-oxygen production, <i>Chem. Commun.</i>, 2013, 49, 1359-7345</li> <li>- Carbon Nanotubes and Organic Solar Cells, <i>Energy Environ. Sci.</i>, 2012, 5, 5919-5940.</li> <li>- Conjugated Polymers in Cages: Templating Poly(3-hexylthiophene) Nanocrystals by Inert Gel Matrices, <i>Adv. Mater.</i>, 2012, 114, 5636-5641</li> <li>- The continuous-flow cycloaddition of azomethine ylides to carbon nanotubes, <i>Chem. Commun.</i>, 2011, 47, 9092-9094.</li> <li>- Synthesis and self-assembly of oligo(p-phenylenevinylene)-peptide conjugates in water, <i>Chem. Eur. J.</i>, 2011, 17, 2044-2047</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/lab205">http://www.chimica.unipd.it/lab205</a>
Responsabile scientifico/Coordinatore	MAGGINI Michele (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_9 - Method development in chemistry

PE5\_17 - Organic chemistry

PE5\_8 - Intelligent materials - self assembled materials

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
CHAUHAN	Prashant	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
CAROFIGLIO	Tommaso	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/06
CRISTOFANI	Michele	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06
DE FILIPPO	Christian Corrado	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
FRISON	Enrico	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/06
MBA BLAZQUEZ	Miriam	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/06
MENNA	Enzo	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/06
ROUDGAR	Mina	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06
SILVESTRINI	Simone	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06
EVANS	Amanda Christine	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/06

#### 21. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Physical Organometallic Chemistry Group
Descrizione	<p>Il sistema non consente l'inserimento dei componenti del gruppo: dr.ssa Annalisa Bisello (tecnico universitario UNIPD), dr.ssa Roberta Cardena (tecnico universitario UNIPD).</p> <p>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. <math>^{103}\text{Rh}</math>, <math>^{57}\text{Fe}</math>, <math>^{183}\text{W}</math>, <math>^{39}\text{K}</math>). The following research lines are pursued:</p> <ul style="list-style-type: none"> <li>- Fluxionality in metal complexes</li> <li>- Electron transfer activation in multimetallic complexes of polycyclic bridging ligands</li> <li>- Electron transfer dynamic in mixed-valence bi- and trimetallic complexes (IVCT bands)</li> <li>- Reversible photochromism of ferrocenyl(bis-azobenzene) branched polymers</li> <li>- Peptides mediated electron transfer</li> </ul> <p>The group is currently involved in the Strategic Project of University of Padova From Materials for Membrane-Electrode Assemblies to Electric Energy Conversion and Storage Devices - MAESTRA, started in January 2014</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Charge transfer properties in cyclopenta[<i>b</i>]phenanthrene ferrocenyl complexes Organometallics, 2014, 33, 1135-1143</li> <li>- Charge transfer properties of multi(ferrocenyl)trindenanes, Organometallics, 2013, 32, 1029-1036</li> <li>- New bis-ferrocenyl end-capped peptides: synthesis and charge transfer properties, Biopolymers, 2013, 100, 14-24</li> <li>- Charge mapping in 310-helical peptide chains by oxidation of the terminal ferrocenyl group, Org. Lett., 2011, 13, 1282-1285</li> <li>- Synthesis of the prototypical cyclic metallocene triad: mixed-valence properties of <math>[(\text{FeCp})_3(\text{trindenyl})]</math> isomers, Angew. Chem., 2008, 47, 5331-5334</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/cinetica/">http://www.chimica.unipd.it/cinetica/</a>

Responsabile scientifico/Coordinatore

SANTI Saverio (SCIENZE CHIMICHE - DiSC)

## Settore ERC del gruppo:

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
Altro Personale	Annalisa Bisello (Personale tecnico laureato dipartimento Scienze Chimiche) Roberta Cardena (Personale tecnico laureato dipartimento Scienze Chimiche)			

## 22. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Polymer Science Group
Descrizione	<p>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.</p> <p>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.</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Self-Welding 1-Butene/Ethylene Copolymers from Metallocene Catalysts: Structure, Morphology and Mechanical Behavior, Journal of Applied Polymer Science, 2014, 131, 40119</li> <li>- The effect of different clay on the structure, morphology and degradation behavior of poly(lactic acid), Applied Clay Science, 2014, 87, 278-284</li> <li>- A Direct SAXS Approach for the Determination of Specific Surface Area of Clay in Polymer-Layered Silicate Nanocomposites, Journal of Physical Chemistry, 2012, 116, 7596-7602</li> <li>- Improvement of tensile properties and tuning of the biodegradation behavior of polycaprolactone by addition of electrospun fibers, Polymer, 2011, 52, 4054-4060</li> <li>- The effect of a synthetic double layer hydroxide on the rate of II → I phase transformation of poly(1-butene), Express Polymer Letters, 2011, 5, 1050-1061</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/grsp/pubblica/indexinglese.htm">www.chimica.unipd.it/grsp/pubblica/indexinglese.htm</a>
Responsabile scientifico/Coordinatore	MARIGO Antonio (SCIENZE CHIMICHE - DiSC)

## Settore ERC del gruppo:

PE5\_1 - Structural properties of materials

PE5\_15 - Polymer chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
CAUSIN	Valerio	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/04
MAREGA	Carla	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/04
Altro Personale	Saini Roberta (Tecnico laureato Dipartimento di Scienze Chimiche)			

**23. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The PoMACat Group (Polymeric Materials for Advanced Catalysis)
Descrizione	<p>The PoMACat group develops and exploits polymeric materials such as microgels and cross-linked resins of different texture for application to catalysis and material chemistry. The scope of recent investigation includes:</p> <ul style="list-style-type: none"> <li>- Tuning of hydro- and lipophilicity of polymeric materials to solvent or substrate compatibility in catalytic reactions</li> <li>- Solid acid and bifunctional catalysts for the production and transformation of biorefinery platform substances</li> <li>- Supported metal catalysts for the direct synthesis of hydrogen peroxide and oxidation of alcohols</li> <li>- Microgels as exotemplates and stabilizers of nanostructured, catalytically active metals in solution</li> <li>- Development of in-operando methods of XAFS characterization of solid catalysts under (gas)-liquid-solid conditions</li> </ul> <p>Our facilities include:</p> <ul style="list-style-type: none"> <li>- 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; glass reactor equipped with membrane ultrafiltration setup;</li> <li>- HPLC, GC and GC-MS and NMR (300 MHz-1H) apparatus</li> <li>- Inverse Steric Exclusion Chromatography apparatus for the morphological characterization of swollen cross-linked polymers</li> </ul> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Novel Ion-Exchange Catalysts for Reactions Involving Lipophilic Reagents: Perspectives in the Reaction of Esterifications of Fatty Acids with Methanol, <i>Top. Catal.</i>, 2013, 56, 611-617</li> <li>- Pd-Au and Pd-Pt catalysts for the direct synthesis of hydrogen peroxide in absence of selectivity enhancers, <i>Appl. Catal. A</i>, 2013, 468, 160-174</li> <li>- Characterisation of Solute Mobility in Hypercross-Linked Resins in Solvents of Different Polarity: Two Promising Supports for Catalysis, <i>Chem. Eur. J.</i>, 2012, 18, 4706-4713</li> <li>- Highly Hydrophilic Copolymers of N,N-Dimethylacrylamide, Acrylamido-2-methylpropanesulfonic acid, and Ethylenedimethacrylate: Nanoscale Morphology in the Swollen State and Use as Exotemplates for Synthesis of Nanostructured Ferric Oxide, <i>Chem. Eur. J.</i>, 2012, 18, 6632-6643</li> <li>- Metal nanoparticles inside microgel/clay nanohybrids: Synthesis, characterization and catalytic efficiency in cross-coupling reactions, <i>J. Coll. Interface Sci.</i>, 2014, 14, 41</li> </ul>
Sito web	
Responsabile scientifico/Coordinatore	ZECCA Marco (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE4\_10 - Heterogeneous catalysis

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE5\_13 - Homogeneous catalysis

PE5\_14 - Macromolecular chemistry

PE5\_15 - Polymer chemistry

PE5\_9 - Coordination chemistry

**Componenti:**

Cognome	Nome	Struttura	Qualifica	Settore
BIFFIS	Andrea	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03
CENTOMO	Paolo	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/03

**24. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Supramolecular Chemistry and System Chemistry Group
	<p>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. State-of-the-art instrumentation is available for the synthesis and characterization of nanosystems (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). The group holds two ERC Starting Grants (L.J. Prins and F. Mancin) and is also strongly involved in other European as well as national projects. Most relevant current projects are:</p> <ul style="list-style-type: none"> <li>- DYCOCA (ERC StG): Dynamic Covalent</li> </ul>

<b>Descrizione</b>	Capture: Dynamic Chemistry for Biomolecular Recognition and Catalysis - MOSAIC (ERC StG): Patterning the surface of monolayer-protected nanoparticles to obtain intelligent nanodevices - PhosChemRec (Marie Curie ITN): Recognition and Cleavage of Biological Phosphates: Molecular Recognition, Mechanism and Biomedical Applications - READ (Marie Curie ITN): Replication and Adaptation in Molecular Networks - University of Padua Strategic Project: Nanochemistry and medicine for cancer: from diagnosis to treatment. Recent key publications - Zn <sup>2+</sup> -regulated self-sorting and mixing of phosphates and carboxylates on the surface of functionalized gold nanoparticles, Angew. Chem., Int. Ed., 2014, 53, 2104-2109 - Efficient phosphodiester cleaving nanozymes resulting from multivalency and local medium polarity control, J. Am. Chem. Soc., 2014, 136, 1158-1161 - "NMR chemosensing" using monolayer-protected nanoparticles as receptors, J. Am. Chem. Soc., 2013, 135, 11768-11771 - Factors affecting T cell responses induced by fully synthetic glyco-gold-nanoparticles, Nanoscale, 2013, 5, 390-400 - Self-assembly of a catalytic multivalent peptide-nanoparticle complex, J. Am. Chem. Soc., 2012, 134, 8396-8399
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/paolo.scrimin/pubblica/">http://www.chimica.unipd.it/paolo.scrimin/pubblica/</a>
<b>Responsabile scientifico/Coordinatore</b>	SCRIMIN Paolo Maria (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_3 - Molecular architecture and Structure

PE4\_4 - Surface science and nanostructures

PE5\_16 - Supramolecular chemistry

PE5\_17 - Organic chemistry

PE5\_8 - Intelligent materials - self assembled materials

**Componenti:**

Cognome	Nome	Struttura	Qualifica	Settore
CAZZOLARO	Alessandro	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
DIEZ CASTELLNOU	Marta	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
FRANCESCHINI	Christian	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
GOBBO	Cristian	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
GALINDO MILLAN	Jealemy Josefina	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
GAMBARIN	Alessandro	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
GARCIA MARTIN	Sergio	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
LUBIAN	Elisa	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
MANCIN	Fabrizio	SCIENZE CHIMICHE - DISC	Prof. Associato	CHIM/06
NERI	Simona	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
PRINS	Leonard Jan	SCIENZE CHIMICHE - DISC	Prof. Associato	CHIM/06
PERRONE	Barbara	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
PEZZATO	Cristian	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
RAMADORI	Federico	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
SALASSA	Giovanni	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06
SPRINGHETTI	Sara	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/06
ZARAMELLA	Davide	SCIENZE CHIMICHE - DISC	Assegnista	CHIM/06

**25. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**
**Nome gruppo\***

The Surface Supramolecular Chemistry Group

<b>Descrizione</b>	<p>The Surface Supramolecular Chemistry Group pursues the following research lines in the field of energy-targeted self-assembled supramolecular systems:</p> <ul style="list-style-type: none"> <li>- Structure and dynamics of electron donor-acceptor self-assembled molecular networks in two dimensions (2D)</li> <li>- Thermo- and photo-induced covalent stabilization of surface-supported 2D supramolecular networks</li> <li>- Interplay between local and supramolecular order in determining the electronic, magnetic and catalytic properties of surface-supported molecular species</li> <li>- Surface-supported metal coordination networks at the solid-liquid /solid-air interface</li> </ul> <p>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.</p> <p>The group is part of a National Project devoted to self-assembled supramolecular systems for energy applications started in February 2013: DESCARTES (Development of Energy-targeted Self-assembled supramolecular systems: a Convergent Approach through Resonant information Transfer between Experiments and Simulations).</p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Structurally Tunable Self-Assembled 2D Cocrystals of C60 and Porphyrins on the Ag (110) Surface, <i>J. Phys. Chem. C</i>, 2014, 118, 1587-1593</li> <li>- Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction, <i>Nat. Mater.</i>, 2012, 11, 970-977</li> <li>- Chromium wheels quasi-hexagonal 2D assembling by direct UHV sublimation, <i>Chem. Commun.</i>, 2011, 47, 5744-5746</li> <li>- Fullerene/Porphyrin Multicomponent Nanostructures on Ag(110): From Supramolecular Self-Assembly to Extended Copolymers, <i>ACS Nano</i>, 2010, 4, 5147-5154</li> <li>- Coverage-Dependent Architectures of Iron Phthalocyanine on Ag(110): a Comprehensive STM/DFT Study, <i>J. Phys. Chem. C</i>, 2010, 114, 2144-2153</li> </ul>
<b>Sito web</b>	<a href="http://www.chimica.unipd.it/mauro.sambi">www.chimica.unipd.it/mauro.sambi</a>
<b>Responsabile scientifico/Coordinatore</b>	SAMBI Mauro (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_2 - Spectroscopic and spectrometric techniques

PE4\_4 - Surface science and nanostructures

PE5\_16 - Supramolecular chemistry

#### Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BASAGNI	Andrea	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
COLAZZO	Luciano	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
EL HABRA	Naida	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
SEDONA	Francesco	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/03

#### 26. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

<b>Nome gruppo*</b>	The Surface Science and Catalysis Group
<b>Descrizione</b>	<p>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:</p> <ul style="list-style-type: none"> <li>- Structure and activity of model catalysts studied by Surface Science tools</li> <li>- Atomic Scale design of electrocatalysts for advanced electrodes (fuel cells, solar fuels)</li> <li>- Growth and functional characterization of chemically modified 2D and 3D graphene and other 2D nanosheets (h-BN, MoS2) systems for energetics and catalysis</li> <li>- Nanosystems and nanocomposites for gas- and bio-sensing</li> <li>- Oxide-on-oxides and metal-on-oxides catalysts for sustainable development: from pollutant abatement (TWC) to energy production (Solid Oxide Fuel Cells, batteries)</li> </ul> <p>The group is involved in three European Projects in the field of fuel cells and catalysts:</p> <ul style="list-style-type: none"> <li>- NMP.2012.1.1: European Coordination of DECORE: Direct ElectroChemical Oxidation Reaction of Ethanol: optimization of the catalyst/support assembly for high temperature operation (<a href="http://decure.eucoord.com/">http://decure.eucoord.com/</a>)</li> <li>- FCH-JU-2011-1: University of Padova local coordination of CathCat: Novel catalyst materials for the cathode side of MEAs suitable for transportation applications (<a href="http://cathcat.eu/index.php/home">http://cathcat.eu/index.php/home</a> )</li> <li>- NMP.2011.2.2-4 Local coordination of NEXTGENCAT "Development of NEXT GENeration cost efficient automotive CATalysts" (<a href="http://www.nextgencat.eu">http://www.nextgencat.eu</a> )</li> </ul> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Atomic Structure and Special Reactivity Toward Methanol Oxidation of Vanadia Nanoclusters on TiO2(110), <i>J. Am. Chem. Soc.</i>, 2013, 135, 17331-17338</li> <li>- A microscopic view on a chemical vapour deposition route to boron-doped graphene nanostructures, <i>Chem. Mater.</i>, 2013, 25, 1490-1495</li> </ul>

	<ul style="list-style-type: none"> <li>- Improvement in the efficiency of an Organometallic Fuel Cell by tuning the molecular architecture of the anode electrocatalyst and the nature of the carbon support, <i>Energy Environ. Sci.</i>, 2012, 5, 8608-8620</li> <li>- Evolution of electrical, chemical and structural properties of transparent and conducting chemically derived graphene thin films, <i>Adv. Funct. Mater.</i>, 2009, 19, 1-7</li> <li>- Steam reforming and oxidative steam reforming of methanol and ethanol: The behaviour of LaCo0.7Cu0.3O3, <i>Applied Catalysis A</i>, 2013, 453, 102-112</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/surfacescience/">http://www.chimica.unipd.it/surfacescience/</a>
Responsabile scientifico/Coordinatore	GRANOZZI Gaetano (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_10 - Heterogeneous catalysis

PE4\_17 - Characterization methods of materials

PE4\_4 - Surface science and nanostructures

PE4\_8 - Electrochemistry, electrodialysis, microfluidics, sensors

PE5\_3 - Surface modification

PE5\_4 - Thin films

PE5\_6 - New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles

#### Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BERSANI	Marco	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
CALVILLO LAMANA	Laura	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
CARLOTTO	Silvia	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
CATTELAN	Mattia	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
DI MARINO	Marco	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
FAVARO	Marco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
GIALLONGO	Giuseppe	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
GLISENTI	Antonella	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03
AGNOLI	Stefano	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/03
NGUYEN	Thanh Hai	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
PACELLA	Michael	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
ARTIGLIA	Luca	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/03
RIZZI	Gian Andrea	SCIENZE CHIMICHE - DiSC	Prof. Associato	CHIM/03
ZHENG	Jian	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03

#### 27. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Organometallic Group
	<p>The main research interest of the Organometallic Chemistry group lies in the design, synthesis, characterisation and applications of late transition metal complexes with poly(N-heterocyclic carbene) ligands. The relationship between structure of the carbene ligand and type, oxidation state, geometry of the metal centre is carefully studied to give metal complexes with the best stereo-electronic and reactivity properties. The final aim is their efficient application in sensors, catalysis and medicine. In particular, the research is focussed on:</p> <ul style="list-style-type: none"> <li>- Synthesis of dinuclear gold(I) complexes with bridging di(N-heterocyclic carbene) ligands: photoluminescence properties, reactivity in halogen oxidative addition, anti-cancer activity</li> <li>- Synthesis of mononuclear iridium(III) complexes with chelating di(N-heterocyclic carbene) ligands, as catalysts in water oxidation (both in dark conditions and under light activated ones) and in transfer hydrogenation</li> <li>- Catalytic properties of selected (di-NHC)complexes in standard reactions (e.g. C-H bond activation and nitrene transfer with Pd and Cu complexes)</li> </ul> <p>Recent key publications</p>
Descrizione	

	<ul style="list-style-type: none"> <li>- N-Heterocyclic dicarbene iridium(III) catalysts enabling water oxidation under visible light irradiation, <i>Eur. J. Inorg. Chem.</i>, 2014, 665-675</li> <li>- Dinuclear gold(I) complexes with propylene bridged N-heterocyclic dicarbene ligands: Synthesis, structures, and trends in reactivities and properties, <i>Dalton Trans.</i>, 2013, 42, 10952-10963</li> <li>- Blue-emitting dinuclear N-heterocyclic dicarbene gold(I) complex featuring a nearly unit quantum yield, <i>Inorg. Chem.</i>, 2012, 51, 1778-1784</li> <li>- Dinuclear N-heterocyclic dicarbene gold complexes in I-III and III-III oxidation states: Synthesis and structural analysis, <i>Organometallics</i>, 2011, 30, 4607-4615</li> <li>- Alkyne hydroarylation in ionic liquids catalyzed by palladium(II) complexes, <i>ChemSusChem</i>, 2010, 3, 834-839</li> </ul>
Sito web	
Responsabile scientifico/Coordinatore	BASATO Marino (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE5\_13 - Homogeneous catalysis

PE5\_9 - Coordination chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BARON	Marco	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03
TUBARO	Cristina	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/03
VOLPE	Andrea	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/03

#### 28. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):

Nome gruppo*	The Theoretical Chemistry- 1 Group
Descrizione	<p>The group 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. Our multiscale protocols combine quantum methods, atomistic molecular dynamics and coarse-grained descriptions and seek to understand the connections between different levels of analysis, from molecules (microscopic) through local structures (mesoscopic), to phases (macroscopic). Main current subjects of investigations are:</p> <ul style="list-style-type: none"> <li>- statistics and dynamics of quantum pure states</li> <li>- modeling motions in flexible macromolecules</li> <li>- modeling of energy-transfer processes via hybrid methods</li> <li>- dimensional reduction of chemical kinetics in complex systems</li> <li>- multiscale methods for photo and thermo responsive organic/inorganic hybrid systems</li> </ul> <p>The group is currently involved in a CARIPARO Excellence Project: Modelling and Monitoring Motions in Proteins - <a href="http://www.chimica.unipd.it/m3p">www.chimica.unipd.it/m3p</a> and in the CMST Action CM1002 - CODECS: COnvergent Distributed Environment for Computational Spectroscopy - <a href="http://codecs.sns.it">codecs.sns.it</a></p> <p>Recent key publications</p> <ul style="list-style-type: none"> <li>- Role of gamma carboxylated Glu47 in connexin 26 hemichannel regulation by extracellular Ca<sup>2+</sup>: Insight from a local quantum chemistry study, <i>Biochem. Biophys. Res. Comm.</i>, 2014, 445, 1, 10-15</li> <li>- Analysis of N-15-H-1 NMR Relaxation in Proteins by a Combined Experimental and Molecular Dynamics Simulation Approach, <i>J. Phys. Chem. B</i>, 2013, 117, 174-184</li> <li>- A Computational tools for the interpretation of electron spin resonance spectra in solution, <i>Mol Phys.</i>, 2013, 111, 18, 2746-2756</li> <li>- A Charge Transfer in Model Bioinspired Carotene-Porphyrin Dyads, <i>J. Phys. Chem. A</i>, 2012, 116, 15, 3926-3933</li> <li>- Beyond quantum microcanonical statistics, <i>J. Chem. Phys.</i>, 2011, 134, 5, 054510</li> </ul>
Sito web	<a href="http://www.chimica.unipd.it/theochem">www.chimica.unipd.it/theochem</a>
Responsabile scientifico/Coordinatore	POLIMENTO Antonino (SCIENZE CHIMICHE - DiSC)

#### Settore ERC del gruppo:

PE3\_14 - Fluid dynamics (physics)

PE3\_15 - Statistical physics: phase transitions, noise and fluctuations, models of complex systems

PE3\_3 - Transport properties of condensed matter

PE4\_11 - Physical chemistry of biological systems

PE4\_12 - Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

PE4\_13 - Theoretical and computational chemistry

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
CODEN	Maurizio	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
FORTUNATI	Nicola	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
FREZZATO	Diego	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
MORO	Giorgio	SCIENZE CHIMICHE - DiSC	Prof. Ordinario	CHIM/02
ORIAN	Laura	SCIENZE CHIMICHE - DiSC	Ricercatore	CHIM/02
TORSELLO	Mauro	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
ZERBETTO	Mirco	SCIENZE CHIMICHE - DiSC	Ric. a tempo determ.	CHIM/02

**29. Scheda inserita da questa Struttura ("SCIENZE CHIMICHE - DiSC"):**

Nome gruppo*	The Theoretical Chemistry-2 group
Descrizione	<p>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 theories, Fokker-Planck equations, 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.</p> <p>Current research topics:</p> <ul style="list-style-type: none"><li>- Chirality propagation across length scales in self-assembling systems (helical polymers, DNA oligomers, porphyrin conjugates, colloidal suspensions of viruses); [MIUR-PRIN project Building with DNA: an experimental, computational and theoretical study]</li><li>- Liquid crystals: elastic and flexoelectric properties, conventional and unconventional phases (cholesteric, twist-bend, Blue Phases) [collaborative project Molecular modelling of liquid crystal materials for electrooptic applications with Merck Chemicals Ltd]</li><li>- NMR in ordered media: solutions of polymers (PBLG), proteins and thermotropic liquid crystals</li><li>- Lipid membranes and Self-Assembled Monolayers: order, partitioning and translocation of molecular solutes and nanoparticles, elastic properties</li></ul> <p>Recent key publications</p> <ul style="list-style-type: none"><li>- The flip-flop of steroids in phospholipid bilayers: effects of the chemical structure on transbilayer diffusion, J. Am. Chem. Soc., 2012, 134, 12198</li><li>- Crucial role of molecular curvature for the bend elastic and flexoelectric properties of liquid crystals: mesogenic dimers as a case study, J. Mat. Chem., 2011, 21, 12303</li><li>- Chirality transfer across length-scales in nematic liquid crystals: fundamentals and applications, Chem. Soc. Rev., 2011, 40, 258</li><li>- Monomeric fullerenes in lipid membranes: effects of molecular shape and polarity, Langmuir, 2011, 27, 12560</li><li>- Right- and left-handed liquid crystalline assemblies of oligonucleotides: phase chirality as a reporter of changes in non-chiral interactions?, Soft Matter, 2011, 7, 9291</li></ul>
Sito web	<a href="http://www.chimica.unipd.it/alberta.ferrarini/pubblica/">www.chimica.unipd.it/alberta.ferrarini/pubblica/</a>
Responsabile scientifico/Coordinatore	FERRARINI Alberta (SCIENZE CHIMICHE - DiSC)

**Settore ERC del gruppo:**

PE3\_13 - Structure and dynamics of disordered systems: soft matter (gels, colloids, liquid crystals...), glasses, defects

PE4\_1 - Physical chemistry

PE4\_13 - Theoretical and computational chemistry

PE4\_6 - Chemical physics

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
FREZZA	Elisa	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
GRECO	Cristina	SCIENZE CHIMICHE - DiSC	Dottorando	CHIM/02
PARISIO	Giulia	SCIENZE CHIMICHE - DiSC	Assegnista	CHIM/02

**30. Scheda inserita da altra Struttura ("INGEGNERIA DELL'INFORMAZIONE - DEI"), tra i componenti risultano persone afferenti a questa Struttura:**

Nome gruppo*	Center for the development of Photovoltaic materials, devices and systems.
Descrizione	L'Università di Padova si occupa da tempo di tematiche legate alle energie rinnovabili e al fotovoltaico. In quest'ottica, si è fatta promotrice di un'iniziativa progettuale per la creazione di un Polo per la R&S e il trasferimento tecnologico nel fotovoltaico. Il Polo si propone di costituire un soggetto in grado di rispondere ai bisogni delle aziende operanti nel settore, agendo da attrattore e moltiplicatore di iniziative indirizzate alla R&S di nuove tecnologie, materiali, dispositivi, metodi di produzione e installazione, nella prospettiva futura di creare un Distretto Veneto del Fotovoltaico.
Sito web	<a href="http://www.polofotovoltaicoveneto.it/index.php/en">http://www.polofotovoltaicoveneto.it/index.php/en</a>
Responsabile scientifico/Coordinatore	MENEHESO Gaudenzio (INGEGNERIA DELL'INFORMAZIONE - DEI)

**Settore ERC del gruppo:**

PE3\_5 - Semiconductors and insulators: material growth, physical properties

PE7\_2 - Electrical and electronic engineering: semiconductors, components, systems

PE7\_3 - Simulation engineering and modelling

PE8\_6 - Energy systems (production, distribution, application)

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BARBATO	Marco	INGEGNERIA DELL'INFORMAZIONE - DEI	Dottorando	ING-INF/01
CESTER	Andrea	INGEGNERIA DELL'INFORMAZIONE - DEI	Ricercatore	ING-INF/01
DUGHIERO	Fabrizio	INGEGNERIA INDUSTRIALE - DII	Prof. Ordinario	ING-IND/31
DEL COL	Davide	INGEGNERIA INDUSTRIALE - DII	Ricercatore	ING-IND/10
MAGGINI	Michele	SCIENZE CHIMICHE - DiSC	Prof. Ordinario	CHIM/06
MENEIGHINI	Matteo	INGEGNERIA DELL'INFORMAZIONE - DEI	Assegnista	ING-INF/01
SPIAZZI	Giorgio	INGEGNERIA DELL'INFORMAZIONE - DEI	Prof. Associato	ING-INF/01
VILLORESI	Paolo	INGEGNERIA DELL'INFORMAZIONE - DEI	Prof. Associato	FIS/01
WRACHIEN	Nicola	INGEGNERIA DELL'INFORMAZIONE - DEI	Assegnista	ING-INF/01
ZANONI	Enrico	INGEGNERIA DELL'INFORMAZIONE - DEI	Prof. Ordinario	ING-INF/01

**31. Scheda inserita da altra Struttura ("MEDICINA MOLECOLARE - DMM"), tra i componenti risultano persone afferenti a questa Struttura:**

Nome gruppo*	Anatomia Umana
Descrizione	<p>Si elencano di seguito i principali ambiti di ricerca del Gruppo.</p> <p>Neuroscienze.</p> <p>Centri bulbari di regolazione cardiorespiratoria: Neuroanatomia (morfometria); Neuropatologia (lesioni ipossico-ischemiche). Glomo carotideo: Identificazione neuromodulatori; meccanismi di plasticità postnatale in iper/hipossia sperimentale; istopatologia. Neurogenesi postnatale (SVZ e GD). Interazioni tra recettori accoppiati a proteine G. Forme non sinaptiche di comunicazione intercellulare.</p> <p>Anatomia clinica.</p> <p>Basi anatomiche di nuove tecniche di mobilizzazione e segmentazione del fegato. Sviluppo di approcci chirurgici innovativi. Fasce muscolari. Approcci di medicina rigenerativa.</p>

	Azione di peptidi regolatori endogeni Surrene: Modelli sperimentali in vitro e in vivo; Iperaldosteronismo. Angiogenesi: Modelli in vitro; Modelli matematici; Studi di tossicità nanoparticelle.
Sito web	
Responsabile scientifico/Coordinatore	DE CARO Raffaele (MEDICINA MOLECOLARE - DMM)

#### Settore ERC del gruppo:

LS3 - Cellular and Developmental Biology: Cell biology, cell physiology, signal transduction, organogenesis, developmental genetics, pattern formation in plants and animals, stem cell biology

LS4 - Physiology, Pathophysiology and Endocrinology: Organ physiology, pathophysiology, endocrinology, metabolism, ageing, tumorigenesis, cardiovascular disease, metabolic syndrome

LS5 - Neurosciences and Neural Disorders: Neurobiology, neuroanatomy, neurophysiology, neurochemistry, neuropharmacology, neuroimaging, systems neuroscience, neurological and psychiatric disorders

LS7 - Diagnostic Tools, Therapies and Public Health: Aetiology, diagnosis and treatment of disease, public health, epidemiology, pharmacology, clinical medicine, regenerative medicine, medical ethics

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
FEDE	Caterina	SCIENZE CHIMICHE - DiSC	Assegnista	BIO/16
GUIDOLIN	Diego	MEDICINA MOLECOLARE - DMM	Ricercatore	BIO/16
ALBERTIN	Giovanna	MEDICINA MOLECOLARE - DMM	Ricercatore	BIO/16
MACCHI	Veronica	MEDICINA MOLECOLARE - DMM	Prof. Associato	BIO/16
PORZIONATO	Andrea	MEDICINA MOLECOLARE - DMM	Prof. Associato	BIO/16
STECCO	Carla	MEDICINA MOLECOLARE - DMM	Ricercatore	M-EDF/02
STOCCHIO	Elena	SCIENZE DEL FARMACO - DSF	Dottorando	CHIM/06
TIENGO	Cesare	MEDICINA MOLECOLARE - DMM	Ricercatore	BIO/16
TORTORELLA	Cinzia	MEDICINA MOLECOLARE - DMM	Ricercatore	BIO/16

#### Altro Personale

Dott.ssa Silvia Barbon

**32. Scheda inserita da altra Struttura ("MEDICINA - DIMED"), tra i componenti risultano persone afferenti a questa Struttura:**

Nome gruppo*	DIABETOLOGIA E DIETETICA
Descrizione	LINEE DI SVILUPPO SCIENTIFICO: PATOGENESI E COMPLICANZE CRONICHE NEL DIABETE; DIABETE IN GRAVIDANZA
Sito web	<a href="http://www.medicinadimed.unipd.it/">http://www.medicinadimed.unipd.it/</a>
Responsabile scientifico/Coordinatore	LAPOLLA Annunziata (MEDICINA - DIMED)

#### Settore ERC del gruppo:

LS4\_3 - Endocrinology

Componenti:

Cognome	Nome	Struttura	Qualifica	Settore
BURLINA	Silvia	MEDICINA - DIMED	Specializzando	MED/13

CHILELLI	Nino Cristiano	MEDICINA - DIMED	Specializzando	MED/13
ROVERSO	Marco	SCIENZE CHIMICHE - DISC	Dottorando	CHIM/01
SARTORE	Giovanni	MEDICINA - DIMED	Ricercatore	MED/13

**Altro Personale**

PIARULLI F., BAX G., CARDONE C. (DIRIGENTI MEDICI); COSMA C., TRALDI P., SERAGLIA R. (BORSISTI E CNR); DALFRA' MG., MASIN M.(MD); BONSEMBIANTE B., GALLO A. (SUMAI)

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