



Chimica Verde

Energie Rinnovabili

Salute

Materiali

Modelling

Beni Culturali

CONFERENZA DI DIPARTIMENTO 2018

DS@TM

Department of Chemical Sciences and Materials Technology

24-25-26 SETTEMBRE

ASSISI

GRAND HOTEL ASSISI



Consiglio Nazionale delle Ricerche
Dipartimento Scienze Chimiche e Tecnologie dei Materiali

© Cnr Edizioni, 2019
Piazzale Aldo Moro, 7 - 00185 Roma
www.edizioni.cnr.it - bookshop@cnr.it - 06 49932287

ISBN 978 88 8080 339 3

Atti della Conferenza del Dipartimento Scienze Chimiche e Tecnologie dei Materiali
Assisi 24-25-26 settembre 2018,
a cura di **Doriano Lamba e Francesco Verginelli**

Organizzazione Giornate di Dipartimento 2018 24-25-26 Settembre, Assisi

Comitato Organizzatore (Roma)

Caterina Adinolfi
Floriana Bernabucci
Federica Criscuoli
Giuliana Quaglia
Mario Figuretti
Cinzia Frascchetti
Francesco Verginelli

Comitato Organizzatore (Perugia)

Olivia Bizzarri
Lucia Allegretti
Beatrice Bizzarri
Filippo De Angelis
Costanza Miliani
Edoardo Mosconi
Simona Fantacci
Leonardo Belpassi
Laura Cartechini
Francesca Rosi

Comitato Scientifico - Premio YIA2018

Doriano Lamba (Coordinatore)
Lucia Curri
Filippo De Angelis
Alessandro Lavacchi
Mauro Marchetti
Costanza Miliani
Alessandro Mordini
Giuseppe Palmieri
Maurizio Peruzzini
Maria Luisa Pompili
Paola Rizzarelli
Alessandra Sanson



PROGRAMMA

24 settembre 2018

13.30 - 14.30

Registrazione

14.30 - 14.40

INTRODUZIONE
Dr. Maurizio Peruzzini

Direttore Dipartimento di Scienze Chimiche e Tecnologie dei Materiali



Chimica Verde

14.40 - 14.45

Chair - Dr. Mauro Marchetti (ICB-CNR) & Dr. Alessandro Mordini (ICCOM-CNR)

14.45 - 15.05

A paper-based algal biosensor for nanoatrazine optical detection

Scognamiglio Viviana - IC

15.05 - 15.25

A coordination-driven triangle as nanoreactor

Rancan Marzio - ICMATE

15.25 - 15.45

 β -Cyclodextrin inclusion complexes of natural occurring compounds and their evaluation as insect repellents in a push-pull strategy

Delogu Giovanna - ICB

15.45 - 16.05

Green Analytical Chemistry (GAC) at ICCOM: the role of analytical methodology development

Bramanti Emilia - ICCOM

16.05 - 16.25

Permeation of Light Gases through Zeolite Membranes

Barbieri Giuseppe - ITM

16.25 - 16.45

Micro-engineered capsules: a powerful tool in green chemistry

Costa Anna - ISTECC

16.45 - 17.15

Coffee Break

17.15 - 17.45

Invited Lecture - Dr. Nicola Armaroli (ISOF-CNR)
Chemistry and the Great Energy Transition

Chimica per l'Energia Rinnovabile

17.45 - 17.50

Chair - Dr. Alessandra Sanson (ISTEC-CNR) & Dr. Alessandro Mordini (ICCOM-CNR)

17.50 - 18.10

Organic Components of Perovskite Solar Cells

Orlandi Simonetta - ISTM

18.10 - 18.30

Catalysts 2.0: a New Technology at the Forefront of Processes at the Heart of Renewable Energy Technology

Giambastiani Giuliano - ICCOM

DSCTM

18.30 - 18.50 Supported Pd and Pd-Au Membranes for Hydrogen Generation and Purification Iulianelli Adolfo - ITM

18.50 - 19.10 Keynote Lecture - **Dr. Armida Torreggiani** (ISOF-CNR)
There isn't any science without communication: collaborative dialogue between research and school

19.10 - 20.00 Sessione Poster

20.00 Apericena

21.00 Riunione Giunta - Direttori



25 settembre 2018



Materiali Avanzati

08.30 - 08.35	Chair - Dr. Maria Lucia Curri (IPCF-CNR) & Dr. Alessandra Sanson (ISTEC-CNR)	
08.35 - 08.55	New anti-fraud method: the proteomic technique applied to the identification of luxury animal fibers	Tonetti Cinzia - ISMAC
08.55 - 09.15	Thiazole and Pyrazole-based Metal-Organic Frameworks for Gas Storage and Catalysis	Rossin Andrea - ICCOM
09.15 - 09.35	Bio-hybrid Nanostructured Cellulose Membranes as Functional Tools for Bio-separation and Bio-recognition Applications	Militano Francesca - ITM
09.35 - 09.55	From Tailored Molecules to Advanced Nanomaterials and Devices: Surface Protection, Light Absorption and NIR-Emission	Bossi Alberto - ISTM
09.55 - 10.15	Development and Application of an Analytical Method to Determine Polyethylene in Compostable Carrier Bags	Rizzarelli Paola - IPCB
10.15 - 10.35	Microstructure, wettability and surface reactivity of AlSiMg system used in additive manufacturing	Bassani Paola - ICMATE
10.35 - 10.55	Smart amphiphobic surfaces for challenging industrial applications	Blosi Magda - ISTEC
10.55 - 11.35	Coffee break	



Modeling Computazionale

11.35 - 11.40	Chair - Dr. Filippo De Angelis (ISTM-CNR)	
11.40 - 12.00	Advanced Methods and Software for the Characterization Crystalline Materials by Powder Diffraction Data	Corriero Nicola - IC
12.00 - 12.20	Exploiting Quantum Phenomena to Design Electron Transport in Nanojunctions	Trioni Mario I. - ISTM
12.20 - 12.40	Computational Multi-Scale Modeling of Metal Oxide Nanoparticles and Surfaces	Barcaro Giovanni - IPCF
12.40 - 13.10	Invited Lecture - Prof. Luigi Nicolais (Materias S.r.L) <i>The Evolution of University-Industry Relationship</i>	



13.10 - 14.30 Pranzo



Chimica per i Beni Culturali

14.30 - 14.35 **Chair - Dr. Costanza Miliani (ISTM-CNR)**

14.35 - 15.05 **Invited Lecture- Prof. Antonio Sgamellotti (Univ. Perugia)**
Chemistry for Art: a non-invasive in situ approach by MOLAB

15.05 - 15.25 Low cost, disposable and self-sustainable paper-based platforms for SERS analysis applied to the study of natural dyes **Campanella Beatrice - ICCOM**

15.25 - 15.45 Non-invasive investigations on Max Ernst's masterpieces: materials, painting technique and alterations products **Nodari Luca - ICMATE**

15.45 - 16.05 Assessment of weathering steel corrosion inhibition in NaCl solution by the natural extract of *Brassica Campestris* **Casaletto Maria Pia - ISMN**

16.05 - 16.35 **Keynote Lecture Dr. Rinaldo Psaro (ISTM-CNR)**
Materials Science and Art

16.35 - 17.15 Coffee Break



Chimica per la Salute e le Scienze della Vita

17.15 - 17.20 **Chair - Dr. Giuseppe Palmieri (ICB-CNR) & Dr. Dorian Lamba (IC-CNR)**

17.20 - 17.40 Creating neurodegenerative diseased tissue model in a membrane bioreactor **De Bartolo Loredana - ITM**

17.40 - 18.00 Mass spectrometry proteomic platforms: discovering molecular signatures in clinical proteomics studies **Desiderio Claudia - ICRM**

18.00 - 18.20 New Molecules for Drug Discovery by Screening Platform of Marine Natural Products **Nuzzo Genoveffa - ICB**

18.20 - 18.40 Effects of Prion Protein on β -Amyloid Peptides Oligomerization and Toxicity **Pagano Katuscia - ISMAC**

18.40 - 19.00 Toward Personalized Medicine: RGD-Peptide as Scaffold for the Comprehension of Structural Determinants for Integrin Specific Recognition **Saviano Michele - IC**

19.00 - 19.20 Nanophotosensitisers based on cyclodextrin for bio-imaging and PDT **Mazzaglia Antonio - ISMN**

19.20 - 20.00 Sessione Poster

20.30 Cena Sociale



26 settembre 2018

08.45 - 09.00	Premiazioni & Presentazioni YIA 2018
09.00 - 09.30	Chimica Verde: Guerriero Antonella - ICCOM
09.30 - 10.00	Chimica per l'Energia Rinnovabile: Gondolini Angela - ISTECH
10.00 - 10.30	Chimica per la Salute e le Scienze della Vita: Posati Tamara - ISOF
10.30 - 11.00	Coffee Break
11.00 - 11.30	Materiali Avanzati: Silvestroni Laura - ISTECH
11.30 - 12.00	Modeling Computazionale: Mosconi Edoardo - ISTM
12.00 - 12.30	Chimica per i Beni Culturali: Giuliani Chiara - ISMN
12.30 - 12.45	Menzioni d'Onore YIA2018 & Premiazioni Posters Chimica Verde: Balzarelli Fabio - ITM; Chimica per l'Energia Rinnovabile: Bossola Filippo - ISTM; Chimica per la Salute e le Scienze della Vita: Panseri Silvia - ISTECH; Materiali Avanzati: Biffi Carlo Alberto - ICMATE; Modeling Computazionale: Rinaldi Silvia - ICRM; Chimica per i Beni Culturali: Campanella Beatrice - ICCOM
12.45 - 13.00	Contributed Presentation - Dr. Mario Malinconico (IPCB-CNR) <i>2019: 100 years of IUPAC and 150 years of the Periodic Table of Chemical Elements</i>
13.00 - 13.30	DISCUSSIONE PLENARIA & CONCLUSIONI Dr. Maurizio Peruzzini Direttore Dipartimento di Scienze Chimiche e Tecnologie dei Materiali
13.30 - 14.30	Pranzo
15.00 - 17.30	Visita Basilica di Assisi



ABSTRACT

SOMMARIO

ORAL COMMUNICATION

INVITED LECTURE - KEYNOTE LECTURE - CONTRIBUTED PRESENTATION

Chemistry and the Great Energy Transition.....	12
There isn't any Science without Communication: Collaborative Dialogue between Research and School.....	13
The Evolution Of University-Industry Relationship.....	15
Chemistry for Art: a Non-Invasive <i>In Situ</i> Approach by MOLAB.....	16
Materials Science and Art.....	17
2019: 100 years of IUPAC and 150 years of the Periodic Table of Chemical Elements.....	18

GREEN CHEMISTRY.....19

A Paper-Based Algal Biosensor for Nanoatrazine Optical Detection.....	20
A Coordination-Driven Triangle as Nanoreactor.....	21
β -Cyclodextrin Inclusion Complexes of Natural Occurring Compounds and Their Evaluation as Insect Repellents in a Push-Pull Strategy.....	22
Green Analytical Chemistry (GAC) at ICCOM: the Role of Analytical Methodology Development.....	24
Permeation of Light Gases through Zeolite Membranes.....	25
Micro-Engineered Capsules: a Powerful Tool in Green Chemistry.....	27

CHEMISTRY AND ENERGY.....29

Organic Components of Perovskite Solar Cells.....	30
Catalysts 2.0: a New Technology at the Forefront of Processes at the Heart of Renewable Energy Technology.....	31
Supported Pd and Pd-Au Membranes for Hydrogen Generation and Purification.....	32

ADVANCED MATERIALS.....33

New Anti-Fraud Method: the Proteomic Technique Applied to the Identification of Luxury Animal Fibers.....	34
Thiazole and Pyrazole-based Metal-Organic Frameworks for Gas Storage and Catalysis.....	35
Bio-hybrid Nanostructured Cellulose Membranes as Functional Tools for Bio-separation and Bio-recognition Applications.....	36
From Tailored Molecules to Advanced Nanomaterials and Devices: Surface Protection, Light Absorption and NIR-Emission...38	
Development and Application of an Analytical Method to Determine Polyethylene in Compostable Carrier Bags.....	40
Microstructure, Wettability and Surface reactivity of AlSiMg System Used in Additive Manufacturing.....	42
Smart Amphiphobic Surfaces for Challenging Industrial Applications.....	43

COMPUTATIONAL MODELING.....45

Advanced Methods and Software for the Characterization Crystalline Materials by Powder Diffraction Data.....	46
Exploiting Quantum Phenomena to Design Electron Transport in Nanojunctions.....	47
Computational Multi-Scale Modeling of Metal Oxide Nano-Particles and Surfaces.....	48

CHEMISTRY FOR CULTURAL HERITAGE	49
Low Cost, Disposable and Self-Sustainable Paper-Based Platforms for Sens Analysis Applied to the Study of Natural Dyes.....	50
Non-Invasive Investigations on Max Ernst's Masterpieces: Materials, Painting Technique and Alterations Products	51
Assessment of weathering steel corrosion inhibition in NaCl solution by the natural extract of <i>Brassica Campestris</i>	52
CHEMISTRY FOR LIFE SCIENCES	54
Creating Neurodegenerative Diseased Tissue Model in a Membrane Bioreactor	55
Mass Spectrometry Proteomic Platforms: Discovering Molecular Signatures in Clinical Proteomics Studies	57
New Molecules for Drug Discovery by Screening Platform of Marine Natural Products	59
Effects of Prion Protein on β -Amyloid Peptides Oligomerization and Toxicity	60
Toward Personalized Medicine: RGD-Peptide as Scaffold for the Comprehension of Structural Determinants for Integrin Specific Recognition	61
Nanophotosensitisers based on cyclodextrin for bio-imaging and PDT.....	62
POSTER COMUNICATION	63
GREEN CHEMISTRY	
Water Purification with Active Cotton Membrane: Photo- and Photoelectrochemical Treatments in Semi-Pilot Plant	64
Direct Air Capture (DAC) Of CO ₂ Accomplished By Different Alkanolamines.....	65
Environmentally Friendly Treatment of Olive Mill Wastewaters and their Valorization by using Membrane Technology	66
BiO ⁺ -Based Nanocomposite for Environmental Remediation: Modulation of the Functional Properties by Composition Tailoring	67
1D-Zigzag Lanthanides Coordination Chains endowed with temperature dependent luminescence.....	68
Advanced Membrane Operations in CO ₂ Separation	69
Axe7A: A Novel CE7 Acetylxylo Esterase for Biomass Degradation.....	71
Membrane-assisted Crystallization of Monoclonal Antibodies by Novel Customized Membranes: the AMECRYSS – Project.....	72
A Sustainable Bioprocess Based on the Marine Microorganism <i>Thermotoga Neapolitana</i> for the Production of Energy and Functional Products: Perspectives and Potential Industrial Applications.....	73
Safe-by-Design Approach for Winning the Nanorisk Challenge.....	74
New Ru-arene Complexes of the Water-soluble Ligand CAP: Synthesis, Characterization and Applications in Catalysis and Medicinal Chemistry.....	75
Pd@Sulfonated Monoliths Catalysts: Synthesis, Characterization and Application to Selective Hydrogenation Reactions under Continuous Flow.....	76
Amine Boranes Dehydrogenation Mediated by a Pyrazole-Based Unsymmetrical PCN Pincer Iridium(III) Hydride	78
Unconventional Hierarchically Porous Niobium-Titanium Oxide Monoliths for the Catalytic Dehydration of Xylose to Furfural under Continuous Flow.....	79
Lactic Acid from Glycerol by Pt and Ir Nanoparticles	81
Sustainable Production of Plga-Peg Microparticles by Membrane Emulsification/ Solvent Diffusion-Evaporation Method.....	82
Novel and “Safe” Inorganic Antibacterial Coatings for Cotton Fabrics.....	84
Effect of Ionic Liquids on the Activity and Conformation of Formate Dehydrogenase from Pseudomonas Sp. 101 in the Presence of Lyoprotectants	85
Project 65: Strengthening Chemical and Biological Waste Management in Central Asia Countries for Improved Security and Safety Risk Mitigation	87
Carbon Nanomaterials as Efficient Catalysts for Organic Reactions	88

CHEMISTRY AND ENERGY

Hydrogen and Acrylate Generation by Electrochemical Reforming of Bioalcohols.....	89
First-Principles High-Throughput-Screening Catalyst Design for Ammonia Synthesis.....	90
Synthesis of Ceramic Powders for Energy Applications.....	92
Synthesis of Nanoparticle Oxides via Flame Spray Pyrolysis.....	93
Anion Exchange Membrane Fuel Cells: Enhanced Alkaline Hydrogen Oxidation Activity for Ceria-Palladium Nanoparticle Catalysts.....	94
3D Engineered Photoanodes for Dye-Sensitized Solar Cells.....	95
Platinum-free Dye-Sensitized Solar Cells.....	97
RM@Schools 3.0: A Wider Society Learning Project.....	98

CHEMISTRY FOR LIFE SCIENCES

Semax, a Copper Chelator that Influences the Cu(II) Induced Aggregation, Ros Production and Cytotoxicity of A β by Metal Ion Stripping and Redox Silencing.....	99
Data-Matrix Technology for Multiparameter Monitoring of Cell Cultures.....	100
Glial Interface: Engineering Tools for Brain Study and Health by Using Materials, Device and Approaches Targeting Astrocytes Physiology and Biophysics.....	102
Combined HS-SPME-GC-MS and HPLC Analysis of Saliva Metabolites after the Assumption of Rifaximin, Prebiotics and Probiotics as an Indirect Assessment of Gut Microbiota.....	103
Protective Effects of Punicalagin Against UVA-induced Damage in Retinal Pigment Epithelial.....	105
Drug Discovery Research Using Virtual Screening with Homology Models.....	106
3D Eumelanin Electrospun MicroFibers as Tool to Guide Dopaminergic System Regeneration.....	107
Synthetic Model of Nanostructured, Functionalized Peptide Matrix.....	108
Nanoencapsulation of Biologically Active Compounds in a Biocompatible Polymer for Potential Food Applications.....	109
Donepezil-like Compounds as Acetylcholinesterase and β -Secretase-1 Inhibitors.....	111
Multiple Target Detection of Circulating MiRNA in Coeliac Disease.....	113
Detection of Germline Mutations in Sardinian Patients with Breast and Ovarian Carcinoma using Next-generation sequencing (NGS).....	114
Eucaryotic-like Ser/Thr kinase from <i>S. Pneumoniae</i> : <i>in Silico</i> Structural Characterization of a New Target for Alternative Antipneumonal Drugs.....	116
The Life of Extremophiles from Polar Regions to Volcanic and Hypersaline Area: Surviving in Hostile Habitats by Exopolysaccharide Production.....	117
Do Size, Coating, and Composition of Magnetic Nanoparticles Really Affect Interaction with Living Systems? A Tightly Controlled Systematic Approach.....	118
Hyaluronic Acid-Based Nanocomposite Hydrogels Obtained by Sol-Gel Method for Tissue Engineering Applications.....	120
Gas Permeable Membrane Bioreactor for Engineering a Liver Construct by using Human Skin Derived Mesenchymal Stem Cells with Hepatocytes and Endothelial Cells.....	122
Zeolites as Chameleon Biomaterials: Assessment of the Zeolite Scaffold Physical-Chemical Characteristics on Interactions with Human Cells.....	124
Synthesis of Hydantoin-based Universal Peptidomimetics as potential Inhibitors of Protein-Protein Interactions.....	125

ADVANCED MATERIALS

Tuning Polymorphism in 2,3-Thienoimide Capped Oligothiophene Based Field-Effect Transistors by Implementing Vacuum and Solution Deposition.....	127
Ecosustainable MgO-based Cements: Unravelling the Role of Phosphate Additives by Means of Solid State NMR Spectroscopy.....	128

Photoluminescence and evolution of polar order in Eu:BaZr _x Ti _{1-x} O ₃ ceramics	129
Engineered Ferroelectric PVDF Composites Containing BaTiO ₃ -based Core-shell Inclusions: Dielectric Properties and 3D FEM Modelling of Field Distribution	130
Environmental Applications of Electrospun Keratin Nanofibers.....	131
ANFISOL - amphiphobic coatings with self-cleaning properties for photovoltaic panels.....	132
Self-cleaning Photocatalytic Paints: Efficiency Under Indoor Lighting Systems	133
Reactivity of Silane Compounds with few-layerBlack Phosphorus	135
Interfacial Properties of Binary Dispersions of Titania and Silica Nanoparticles and Applications to Foams and Solid Foams....	136
Synthesis of Sulfur-Rich Polymers: Copolymerization of Cyclohexene Sulfide and Carbon Disulfide Using Chromium Complexes.....	138
Investigation of the Modulation of the Non-Covalent Interaction Between 2D Bp and Fluorescent Pyrene Derivatives Endowed with Different Functional Substituents	139
Interfacial Phenomena in Ni Alloys-Oxides systems of Interest for Investment Casting of Superalloys	140
Recent Progresses in Catalyzed Butadiene and Isoprene Polymerization	141
The P-Sc Structure in Phosphorus: Bringing Order to the High Pressure Phases of Group 15 Elements.....	143
Hi-Tech Ceramics and Composites for Severe Environments.....	144
Lightweight Composites with Hollow Glass Microspheres for Rotational Molding Technology	146
Aziridine Functionalized Carbon Nanotubes as Highly Efficient Electrocatalysts for the Selective CO ₂ Reduction to CO	148
Polypyrrole Nanoparticles Synthesis and Deposition by “Throwing Stones” for Antibacterial Textiles.....	149
Thermo-Mechanical Characterization of NiMnGa Melt Spun Ribbons	150
Solid-Gas Biocatalysis Using PVDF Enzyme-Loaded Membrane	151

COMPUTATIONAL MODELING

Ab Initio Study of the Insulating Power of Defective Magnesium Oxide Ultrathin Films in Ag/Mgo/Ag Tunnel Junctions	153
An Accurate High-Throughput Framework for Materials Discovery.....	154
Correlation between Creep and Relaxation Behaviour in a Cr Martensitic Steel.....	155
Pushing the Limits of Solving Crystal Structures by Powder Diffraction Data	156
Dft Calculations and Raman Spectroscopy of as(Iii) Complexation with Thiol Ligands	157
Exploring the Boundary of 3D Perovskites Domain: The Case of Fapb _{1-x} sn _x br ₃ Perovskites	158
Charge Traps in Lead-halide Perovskites: a Computational Study	159
Conformational Dynamics of Non Visual Arrestin Subtypes	160
First Principles Modeling of Mixed 2D/3D Organohalide Perovskites.....	161
Vibrationally Excited Hydrogen Molecules Formation on a Cesiated Surface	163
Theoretical Investigations on the Solution Chemistry of Organohalide Perovskite Precursors.....	164
A Theoretical and Experimental Investigation of the Mechanism Underlying Response Enhancement of CNT-Si Based Devices upon No ₂ Exposure	165

CHEMISTRY FOR CULTURAL HERITAGE

Temperature Behaviour of PEG Treated Historic Wood by FTIR and Raman Investigations	166
Analysis of Trehalose Treated Wood Fines by Portable Raman and Infrared Spectrometers	167
The “Scream” by Edvard Munch: An Exemplary Case Study of Synergism Between Chemistry and Conservation	168
Corrosion of archaeological bronzes and modern steel artworks: Surface and Electrochemical Investigations.....	170
Innovative and Sustainable Approaches to Inhibit Corrosion Processes in Cultural Heritage Artefacts and Monuments.....	171
SERS Substrates for Pigments Detection in Works of Art: a Combined DFT and Experimental Study	173
X-Ray Analysis <i>in situ</i> : The Importance of Adaptive Instrumentation	174



Dft Calculations and Raman Spectroscopy of as(III) Complexation with Thiol Ligands

Fausta Giacobello^{a)}, Giuseppe Cassone^{b)}, Donatella Chillè^{c)}, Claudia Foti^{c)}, Ottavia Giuffrè^{c)},
Viviana Mollica Nardo^{a)}, Rosina Celeste Ponterio^{a)}, Franz Saija^{a)}, Sebastiano Trusso^{a)}

e-mail: fausta.giacobello@ipcf.cnr.it

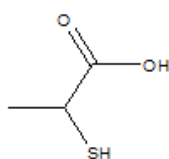
- ^{a)} CNR - Istituto per i Processi Chimico Fisici, Viale Ferdinando Stagno d'Alcontres, 37 –, 98158 Messina;
^{b)} Institute of Biophysics, Czech Academy of Sciences, Brno (Czech Republic);
^{c)} Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali dell'Università degli Studi di Messina, Viale F. Stagno d'Alcontres, 31 – 98166 Messina.

The interest in the chemistry of arsenic complexes has increased in recent years. This metal is a natural pollutant, present in trace in the environment and living organisms [1]. About 60% of arsenic is released by volcanic activity and largely derives from anthropogenic sources. It is well known, indeed, that arsenic compounds have several applications in many industrial fields, such as pesticides and herbicides in agriculture, as chemioterapeutic agent in medicine and as constituent of numerous consumer goods. For these reasons, humans are usually exposed in food, water, air and soil. Accordingly, the extensive arsenic contamination is considered one of the most important toxicological problem.

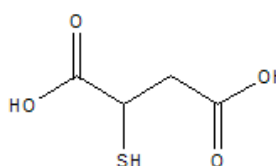
The significance of the metal pollution, as well as its mobility and bioavailability, depends on arsenic speciation, which represents the distribution of the different chemical species in a given system. The predominant species in aqueous solutions are the inorganic As(III) and As(V) ones, derivatives of the arsenous and arsenic acids, respectively. It was found, already in the past, that arsenite(III) compounds are more poisonous than arsenate(V) ones and even more dangerous of its organic species. This toxicity is mainly due to its high affinity for the sulfhydryl groups present in active biomolecules, such as enzymes and proteins [2]. Nevertheless, few data on the As(III) interaction with thiols are reported in the literature.

In the light of these considerations, an investigation on the As³⁺ complexation with S-donor ligand in aqueous solution was performed, in particular with thiolactic (TLA) and thiomalic acids (TMA).

This study is based on a speciation analysis on As³⁺-TLA and As³⁺-TMA systems and a Raman spectroscopic investigation combined with density functional calculations (DFT). Up to now, detailed Raman investigations of thiolactic and thiomalic ligands are missing in the literature.



2-mercaptopropanoic acid or
thiolactic acid (TLA)



2-mercaptosuccinic acid or thiomalic
acid (TMA)

The Raman spectroscopy results combined with DFT calculations shed light on the arsenic chelation mechanisms with these S-donor ligands.

Keywords: Arsenic, Raman spectroscopy, DFT calculations.

References:

- [1] B.K. Mandal, K.T. Suzuki. *Talanta*, (2002), **58**, 201.
[2] T. Kaise, et al. *J. Food, Hygien. Soc. Jpn.* (1996), **37**, 135.

Conferenza di Dipartimento 2018

24-25-26 Settembre, Assisi

Grand Hotel Assisi

DSCCTM



Dipartimento Scienze Chimiche e Tecnologie dei Materiali

Premio YIA2018 - Chimica Verde

Premio YIA2018 - Chimica per l'Energia Rinnovabile

Premio YIA2018 - Chimica per la Salute e le Scienze della Vita

Premio YIA2018 - Materiali Avanzati

Premio YIA2018 - Modellistica Computazionale

Premio YIA2018 - Chimica per i Beni Culturali