Piero Ugliengo

europass

Date of birth: 22/05/1957 **Nationality:** Italian **Gender:** Male

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Dipartimento di Chimica, Via P. Giuria 7, 10125, Torino, Italy

About me:

I am a computational chemist who adopts ab initio molecular modeling techniques to address chemical problems at the interfaces between inorganic materials and (bio)organic molecules. Because simulation alone is somewhat of an end, I have maintained close collaboration with experimental groups to provide an interpretation of phenomena at the surface/molecule interface through an atomistic view.

My interests are in systems and properties, all of which have, as a common basis, the interactions between molecules and surfaces. The most relevant are: i) adsorption on metal oxide surfaces; ii) catalysis by microporous materials; iii) drug interaction/diffusion by amorphous/mesoporous silica-based materials; iv) ceramic biomaterials and their interaction with (bio)organic matter; v) prebiotic chemistry on mineral surfaces; vi) modeling of interstellar grains.

More specifically, I have contributed to: (i) develop a method to predict the structures and energy of molecular crystals and molecules at surfaces, accurately assessing the contribution of dispersive interactions (London); (ii) define realistic, yet computable, models of amorphous and mesoporous silica; (iii) elucidate the interaction of hydroxyapatite, a basic ceramic biomaterial of bone and teeth, with amino acids and peptides; (iv) understand molecular interactions at hydroxylated crystalline silica surfaces; (v) study the role of aluminosilicates and amorphous silica in catalyzing peptide bond formation in the prebiotic domain; (vi) model realistic interstellar ice grains. (vii) To understand the mechanism of formation of complex organic molecules at interstellar grain surfaces in an astrochemical context.

WORK EXPERIENCE

01/11/1982 – 30/10/1983 – Torino, Italy

SYSTEM ANALYST – CSI PIEMONTE

Developing computer programs for the public administration

01/11/1983 – 30/10/1992 – Torino, Italy

ASSISTANT PROFESSOR (CHIM02) – (DIP. CHIMICA) UNIVERSITÀ DEGLI STUDI DI TORINO

Research: quantum mechanical modeling of molecular crystal structures, modeling of silica and zeolites
Teaching: support for the physical chemistry courses (mainly Laboratory experiences)

01/11/1992 – 30/10/2015 – Torino, Italy

ASSOCIATE PROFESSOR (CHIM02) – (DIP. CHIMICA) UNIVERSITÀ DEGLI STUDI DI TORINO

Research: quantum modeling of interfaces between inorganic solids and soft-matter
Teaching: Physical Chemistry, Structural Chemistry, Chemistry on the WEB, Molecular Modeling

01/11/2015 – CURRENT – Torino, Italy
FULL PROFESSOR (CHIM02) – (DIP. CHIMICA) UNIVERSITÀ DEGLI STUDI DI TORINO

Research: quantum mechanical modeling of astrochemical and prebiotic chemistry. Modeling of ceramic biomaterials
Teaching: Physical Chemistry, Structural Chemistry, Chemistry on the WEB, Molecular Modeling

EDUCATION AND TRAINING

01/11/1971 – 30/07/1976 – Corso De Gasperi 30, Cuneo, Italy
BACHELOR IN INDUSTRIAL CHEMISTRY – Istituto Tecnico Industriale Statale "Mario Delpozzo"

01/11/1976 – 30/07/1981 – Dipartimento di Chimica, Via P. Giuria 7, Torino, Italy
MASTER IN CHEMISTRY – Università degli Studi di Torino

LANGUAGE SKILLS

Mother tongue(s): **ITALIAN**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH B1		B1	B2	B2	B2
SPANISH B1		B2	B2	B1	B1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

DIGITAL SKILLS

Microsoft Office | Zoom | Skype | Fortran Language | Visual Studio - Visual Basic | Linux, user level; | Microsoft Windows | Mac OSx |

SOFTWARE DEVELOPMENT

MOLDRAW: a program to display and manipulate molecular and crystalline structures

A public domain available software apt to display and manipulate molecules and crystals on a personal computer.

Ugliengo, P; Viterbo, D; Chiari, G, MOLDRAW - Molecular Graphics on a Personal-Computer, *Zeitschrift Fur Kristallographie*, (1993), 207, 9-23, DOI: 10.1524/zkri.1993.207.Part-1.9

ANHARM: A Program to solve the nuclear Schrodinger equation for an anharmonic A-H oscillator

FORTRAN Files and instructions available on ResearchGate at DOI: 10.13140/RG.2.1.3367.8884

PUBLICATIONS & BIBLIOMETRIC SCORE

All the bibliometrics indicator (number of published papers, h-index, citations etc.) can be found at the following links:

ORCID **PUBLONS** **SCOPUS** **Google Scholar** **ResearchGate**

ACADEMIC COORDINATION AND ORGANIZATION

2009 – 2012
President of the Master's degree in Metodologie Chimiche Avanzate

2015 – 2020
President of the Master's degree in Chimica

2016 – 2021
Deputy Director with responsibility for the teaching organization of the Chemistry department

2015 – 2021
Member of the PhD Doctoral School

PROJECTS

2022 – 2024
Astrochemistry beyond the second period elements

Funding organism: MUR (PRIN 2020, Prot. 2020AFB3FX). National PI: N. Balucani. Local PI: P. Ugliengo

2019 – 2022
Astro-Chemical Origins (ACO)

Funding organism: European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 811312, website: Astro-Chemical Origins" (ACO) (Project PI: C. Ceccarelli, local PI and deputy network coordinator: P. Ugliengo)

2019 – 2022
Life in Space Project

Funding organism: Italian Space Agency (ASI N. 2019-3-U.O), website: "Life in Space Project". National PI: N. Balucani. Local responsabile: P. Ugliengo

2015 – 2018
STARS in the CAOS "Simulation Tools for Astrochemical Reactivity and Spectroscopy in the Cyberinfrastructure for Astrochemical Organic Species"

Funding organism: MIUR (PRIN 2015, Prot. 2015F59J3R_003). National PI: E. Barone, local PI: P. Ugliengo

2014 – 2016
METABIO "METhod to elaborate bioinspired stable Antibacterial surface on metallic BIOmaterials for dental implants"

Funding organism: European M-ERA.NET Call 2013 Project. PI: P. Choquet, Luxembourg Institute of Science and Technology LIST, Lussemburgo

2012 – 2013
MATERA: Elaboration of bioactive surfaces by combining Dielectric Barrier Discharge and site-specific attachment of biomolecules

Funding organism: M-Era-Net subcontracted with the Centre de Recherche Public - Gabriel Lippmann (http://www.crpgl.lu/) – Luxembourg. Local PI: P. Ugliengo

2011 – 2013

Advances in nanostructured materials and interfaces for key technologies

Funding organism: Progetti di Ricerca di Ateneo, Compagnia di San Paolo-Linea 1A, (ID: ORTO11RRT5). PI: M. Baricco

2009 – 2012

FLYHY - Fluorine Substituted High Capacity Hydrides for Hydrogen Storage at low Working Temperatures

Funding organism: EU-FP7, Grant agreement N° 226943-2. Local PI: M. Baricco

2006 – 2009

Interface phenomena in silica-based nanostructured biocompatible materials contacted with biological systems

Funding Organism: Italian Ministry of Research and University (MIUR). PI: C. Morterra

2004 – 2007

Study of physical and chemical surface features of silica powder in relationships with the response elicited in cellular systems

Funding Organism: Italian Ministry of Research and University (MIUR). National PI: D. Ghigo, Local PI: P. Ugliengo

2004 – 2007

Nanostructured biocompatible materials for biomedical applications

Funding Organism: Piedmont Regional Scientific Council. PI: C. Morterra

2003 – 2005

The interface between silica-based materials and biomolecules and/or cell models

Funding Organism: National consortium of Materials Science and Technology (INSTM). PI: C. Morterra

2002 – 2004

Nanostructured oxidic materials for adsorption and catalysis

Funding Organism: National consortium of Materials Science and Technology (INSTM). PI: C. Morterra

HPC COMPUTATIONAL RESOURCES

2007 – 2008

Ab-initio simulation of Hench bioglass

Funding organism: Distributed European Infrastructure for Super Computing Applications (http://www.deisa.eu/). 200000 HPC hrs (PI : P. Ugliengo)

2007 – 2008

Simulation of peptide folding induced by inorganic materials

Funding organism: Barcelona Supercomputing Center (http://www.bsc.es/) (BCV-2008-2-0013). 400000 HPC hrs Mare Nostrum. PI: P. Ugliengo

2010 – 2011

SILDRUG: Large Scale B3LYP-D simulation of silica-based carriers for drug delivery

Funding organism: CINECA. ISCRA-B (HP10A7WAF8). 553000 HPC hrs on IBM/sp6. PI: P. Ugliengo

2011 – 2013

IBUMCM: Quantum mechanical modeling of the interaction of ibuprofen with the mesoporous MCM-41 material

Funding organism: CINECA. ISCRA-B(HP10AN1YJ1), 800000 HPC hrs on the IBM BluGene/Q-Fermi. PI: P. Ugliengo

2012 – 2013

Mesoporous silica for drug delivery: a quantum mechanical simulation

Funding organism: Partnership for Advanced Computing in Europe (PRACE) (2011050810). 20000000 HPC hrs SuperMUC Petascale system at Leibniz-Rechenzentrum. PI: P. Ugliengo

2013 – 2014

IBUEXCP: Static and dynamic DFT-D2 simulations of microsolvated excipient/drugs systems

Funding organism: CINECA. ISCRA-B (HP10BC33PV). I500000 HPC hrs on the IBM BluGene/Q-Fermi CINECA. PI: P. Ugliengo

2014 – 2015

SIL4SKIN: Drug delivery by mesoporous silica for skin applications: static and dynamic DFT-D2 simulations of anti-fungal drugs on amorphous silica surfaces

Funding organism: CINECA. ISCRA-B (HP10BDV8WS). 3500000 HPC hrs on the IBM BluGene/Q-Fermi CINECA. PI: P. Ugliengo

2016 – 2017

BONECOLL: Ab initio investigation of bone constituents: the case of collagen on hydroxyapatite surfaces

Funding organism: CINECA. ISCRA-B (HP10BPE1K6). 125000 HPC hrs on the MARCONI1 CINECA. PI: P. Ugliengo

2018 – 2019

DUSTQM. Ab Initio Quantum Mechanical Simulations of Interstellar Silicate Dust Grains: A Nanocluster Approach

Funding organism: CINECA. ISCRA-B (HP10BWRHU4). 500000 HPC hrs on the MARCONI1 and 186664 on MARCONI2. PI: P. Ugliengo

2019 – 2021

ASTROMD. Ab-initio molecular dynamic simulations on astrochemical reactions occurring on interstellar icy mantles

Funding organism: CINECA. ISCRA-B (HP10BQJLHZ).1000000 HPC hrs on the MARCON2 and 149000 on M100 CINECA. PI: P. Ugliengo

2020 – 2021

ROCK4LIFE. Ab-initio investigations of meteor surfaces as vehicles of molecules of prebiotic interest

Funding organism: CINECA. ISCRA-B (HP10BRR0SE). 510000 HPC hrs on M100 CINECA. PI: P. Ugliengo

NATIONAL & INTERNATIONAL COLLABORATIONS

Prof. Joachim Sauer, Humboldt University in Berlin (DE)

Modeling zeolites and silica surfaces

Dr. V. R. Saunders, Daresbury Laboratory (UK)

Molecular modeling of adsorbates on amorphous silica surfaces

Prof. Alfonso Pedone, Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia (IT)

Simulation of bioglasses and mesoporous silica

Prof. Barbara Onida, Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino (IT)

Drug delivery by mesoporous silica materials

Prof. Giovanni Valdrè, Dipartimento di Scienze Biologiche, Geologiche e Ambientali, Univeristy of Bologna (IT)

Biomaterials based on hydroxyapatites

Prof. Nadia Balucani, Dipartimento di Chimica, Biologia e Biotecnologie, University of Perugia (IT)

Astrochemistry of molecules of prebiotic interest

Dr. Albert Rimola, Department of Chemistry, Autonomous University of Barcelona UAB (ES)

Prebiotic and astrochemistry chemistry related problems

Prof. Mariona Sodupe, Department of Chemistry, Autonomous University of Barcelona UAB (ES)

Modeling of biomaterials and prebiotic chemistry (regular visit by 1 month/year)

Prof. Cecilia Ceccarelli, IPAG, Observatoire de Grenoble, Universitè J. Fourier de Grenoble

Astrochemistry

Prof. Jean-Francois Lambert, Universite' de Pierre et Marie Curie, Paris (FR)

Modeling and experiments on the silica based materials

Prof. Dominique Costa, Institut de Recherches de Chimie de Paris UMR 8247 ENSCP Chimie Paristech (FR)

Modeling adsorption at silica and hydroxyapatites surfaces

Dr. Stefan Bromley, ICREA Universitat de Barcelona (UB).

Computer modeling of the interstellar grains

- **VISITING SCIENTIST**

01/05/2004 – 01/08/2004
Universitat Autonoma de Barcelona (Prof. Mariona Sodupe)

Funding organism: High-Performance-Europe network. The role of mineral surfaces in the origin of life: an ab-initio approach.

01/05/2005 – 01/08/2005

Universitat Autonoma de Barcelona (Prof. Mariona Sodupe)

Funding organism: Agencia de Gestio d'Aiuts Universitaris i de Recerca della Generalita' di Catalunia, invited professorship. Role of aluminosilicates as catalysts of the peptide bond formation in the prebiotic.

01/07/2009 – 30/07/2009

Universite' de Pierre et Marie Curie, Paris (Prof. Jean-Francois Lambert)

Funding organism: Universite' de Pierre et Marie Curie, Paris. Invited professorship. Special issue of the Chemical Society Review devoted to prebiotic chemistry (Chem. Soc. Rev. 41, 5365-5568, 2012).

01/05/2011 – 30/07/2011

Universitat Autonoma de Barcelona (Prof. Mariona Sodupe)

Funding organism: Universitat Autonoma de Barcelona. Invited professorship.Simulation of crystalline silica surfaces.

CONFERENCES AND SEMINARS

Conferences and Seminars (only the most relevant of more than 60)

09/05/2011 – 11/05/2011 – Lausanne, Switzerland

CECAM Workshop: ProSurf - Modeling Protein Interactions with Solid Surfaces and Nanoparticles

Invited lecture: Molecular Recognition at the Surfaces of Hydroxyapatite Modeled by Periodic DFT Methods Based on Localized Orbitals
http://www.cecam.org/workshop-2-548.html

19/09/2011 – 23/09/2011 – Leiden, Lorentz Center, International Center for workshops in the Sciences, The Netherland

Challenges in modelling the reaction chemistry of interstellar dust

Invited lecture: Ab initio modeling of the adsorption at silica surfaces

17/07/2011 – 22/07/2011 – Santiago de Compostela, Spain

Ninth Triennial Congress of the WORLD ASSOCIATION OF THEORETICAL AND COMPUTATIONAL CHEMISTS WATOC

Iinvited lecture: Molecular Recognition at the surfaces of hydroxyapatite modeled by periodic DFT methods based on localized orbitals
http://www.watoc.net/pdf/WATOC-2011_Programm.pdf]

19/09/2012 – 21/09/2012 – Perugia, Italy

IV Workshop Italian Astrobiology Society "From Astrophysics to Astrochemistry towards Astrobiology"

Invited lecture: Interstellar Prebiotic Formation of Glycine, Delivery to Earth and Polymerization on Feldspars

26/06/2012 – 30/06/2012 – Vlissingen, The Netherlands

14th International Conference on Theoretical Aspects of Catalysis

Invited lecture: Interstellar prebiotic formation of glycine delivery to Earth and polymerization on feldspars

30/06/2013 – 05/07/2013 – Granada, Spain
QUITEL2013, XXXIX Theoretical Chemists of Latin Expression

Keynote lecture: Can dispersion overcome H-bond interactions? The case of drugs adsorbed on silicas modeled at DFT-D2 level

06/07/2014 – 11/07/2014 – Nara, Japan
ORIGINS 2014 International Conference – 2nd ISSOL – The international Astrobiology Society and Bioastronomy, Joint International Conference

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Oral talk: Peptide Bond Formation Catalyzed by Silica Surfaces. Insights from DFT calculations

08/04/2015 – 10/04/2015 – CECAM-EPFL, Lausanne, Switzerland
CECAM workshop: Emergent structural and electronic phenomena at interfaces of nanoscale oxides

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Invited lecture: Can Dispersion Overcome H-bond Interactions? The Case of Drugs Adsorbed on Amorphous Silica Surfaces and in Mesoporous Silica Pores as Modeled by DFT-D

20/06/2016 – 22/06/2016 – CECAM-FR-IDF, Paris, France
CECAM workshop: Atomistic simulations in prebiotic chemistry: a dialog between experiment and theory

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Invited lecture: The rôle of interstellar icy grain surfaces in prebiotic chemistry

05/09/2016 – 09/09/2016 – Kutná Hora, Czech Republic
VI International Workshop on Layered Materials

Invited talk: Amide Bond Formation by Condensation between Unactivated Reagents at Silica Surfaces: Role in Prebiotic Chemistry

10/09/2017 – 14/09/2017 – Paestum, Italy
XXVI Congresso Nazionale della Società Chimica Italiana

Oral talk: Amide Bond Formation by Condensation between Unactivated Reagents at Silica Surfaces: Role in Prebiotic Chemistry

15/02/2018 – 16/02/2018 – Bologna, Italy
Astro-Winter Modeling – Advances in Computational & Experimental Modeling: Applications to Astrochemistry

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Invited talk: Amide Bond Formation by Condensation between Un-activated Reagents at Silica Surfaces: Role in Prebiotic Chemistry

01/07/2019 – 03/07/2019 – CECAM-FR-IDF, Paris, France
CECAM workshop: Atomistic simulations in prebiotic chemistry – a dialog between experiment and theory

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Invited lecture: Interplay Between Experiment and Computer Simulation to Elucidate the Amide Bond Formation at Silica (TiO_2) Surfaces in a Prebiotic Context

25/10/2019 – 30/10/2019 – Montreal, Canada
QUITEL2019 - Congreso Internacional de Químicos Teóricos de Expresión Latina

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Plenary lecture: From Astrochemistry to Prebiotic Chemistry through the Eyes of Computer Molecular Modeling

MEMBERSHIP

2011 – 2021
International advisory board of the Horizons in Hydrogen Bond Research

2018 – 2021
Advisory board of Royal Society Journal CrystEngChem

Physical chemistry division of the Italian Chemical Society

Association of Italian Crystallography

European Crystallographic Association

2018 – 2020
American Chemical Society (Physical Chemistry +Astrochemistry).

2013 – 2016
Management Committee of the [CM1401 IT] COST Action CM1401 "Our Astro-Chemical History"

2020 – CURRENT
Associate editor for Astrochemistry of Frontiers in Astronomy and Space Science Journal

Member of the "Italian Society of Astrobiology"

National Consortium of Materials Science and Technology (INSTM)

Nanostructured Interfaces and Surfaces (NIS) center of Excellence of the University of Torino

International Society for the Study of the Origin of Life – The International Astrobiology Society

EDITORIAL & REFEREE ACTIVITIES

Referee of Scientific Journals

Journal of Physical Chemistry (A, C)
ACS Earth & Space Chemistry Journal
Chemistry of Materials
Langmuir
Journal of American Chemical Society
Journal of Molecular Structure (THEOCHEM)
Journal of Chemical Physics
Chemical Physics Letters
Surface Science
Physical Chemistry Chemical Physics
Journal of Catalysis
CrystEngComm
Proceeding of the National Academy of Science
Minerals
Molecules

Referee of National/International Projects

Agència de Gestió d'Ajuts Universitaris i de Recerca, (Barcelona). 2011, 2013, 2017, 2018
ANR – The French National Research Agency 50, avenue Daumesnil - 75012 Paris – France. 2010, 2021
Austrian Science Fund, 1090 Vienna, Sensengasse 1, Austria. 2018
Barcelona Supercomputing Center- Centro Nacional de Supercomputación, 2013-2017
Canada Foundation for Innovation | Fondation canadienne pour l'innovation, 2019
Czech Science Foundation, 2010, 2019
Deutsche Forschungsgemeinschaft (German Research Foundation), 2016
ERC European Research Council, 2009, 2010, 2011, 2015, 2017, 2020
ETH Zurich Research Commission, 2014
Chilean National Science and Technology Commission, 2016, 2017, 2019, 2020
Bando Galileo, Università Italo-Francesi, 2017
Bando Vinci, Università Italo-Francesi, 2020
Premio Giovedì Scienza, 2018, 2019, 2020
National Science Centre (Narodowe Centrum Nauki - NCN; www.ncn.gov.pl), 2017
Research Council KU Leuven, 2020
National Science Foundation (NSF), 2014
Scuola Normale Superiore, Pisa, 2018
Italian SuperComputing Resource Allocation - ISCRA, CINECA, 2016, 2018

PHD SUPERVISOR ACTIVITY

1998 – 2000

PhD: Bartolomeo Civalleri. Il legame ad idrogeno in sistemi molecolari e cristallini: studio computazionale ab initio.

Chemical Science PhD School, University of Torino

2000 – 2003

PhD: Claudia Busco. Study of Lewis/Bronsted acidity in zeolites by the combined use of computational and experimental techniques

Chemical Science PhD School, University of Torino

2003 – 2006

PhD: Sergio Tosoni. Intermolecular interactions between inorganic solid surfaces and small organic molecules. An ab-inito study

Chemical Science PhD School, University of Torino.

2004 – 2007

PhD: Marta Corno. Ab-initio modelling of biomaterials: the cases of hydroxyapatite and 45S5 bioglass

Chemical Science PhD School, University of Torino.

2008 – 2011

PhD: Federico Musso. Theoretical Study of the Surface Properties of Crystalline and Amorphous Silica Polymorphs

Co-tutoring: Programa de Doctorado en Quimica Teorica y Computacional, Autonomous University of Barcelona (UAB).

2010 – 2013

PhD: Fabio Chiatti. Ab initio simulation of ceramic biomaterials and their interaction with biomolecules

Chemical and Material Sciences. University of Torino.

2011 – 2014

PhD: Massimo Delle Piane. Quantum Mechanical Simulation of Biomolecules at the Interface with Inorganic Oxides

Chemical and Material Sciences. University of Torino.

2015 – 2018

PhD: Michele Cutini. Large-scale ab initio simulations of electronic and structural features of ceramic biomaterial surfaces and their interactions with biomolecules

Chemical and Material Sciences. University of Torino

2017 – 2019

PhD: Lorenzo Zamirri. Ab initio Computer Simulations of the Cores and Mantles of Interstellar Dust Grains

Chemical and Material Sciences. University of Torino.

2019 – 2022

PhD: Aurele Roger Germain. Quantum chemistry computations of analogues of water amorphous ice covering interstellar grains, and binding energies of important interstellar molecules plus IR spectra

Chemical and Material Sciences - University of Torino

2020 – 2023

PhD: Jessica Perrero. Phenomena at Interstellar Core and Mantle Grains: a Quantum Mechanical Approach

Co-tutoring Chemical and Material Sciences - University of Torino and in Chemistry – Universitat Autonoma de Barcelona

2019 – 2022

PhD: Lorenzo Tinacci. Gas-grain models and artificial intelligence application to improve astrochemical reactions

Co-tutoring. Chemical and Material Sciences - University of Torino University of Torino and Physics - l'Université Grenoble Alpes.

2002 – 2011

Hosting foreign PhD

The Piero Ugliengo group hosted 6 PhD students from abroad for short (three months) periods:
Xavier Solans-Monfort, 2002 e 2003, Universitad Autonoma di Barcellona
David Hugas, 2004, Universitad de Girona
Albert Rimola, 2005, Universitad Autonoma de Barcelona
Flora Elisabeth Imrie, 2011, University of Aberdeen
Elisa Jimenez Izal, 2011, Euskal Herriko Unibertsitatea.

POST-DOC SUPERVISOR ACTIVITY

2007 – 2017

Dr. Marta Corno

2007-2009. PRIN2006: Interface phenomena in silica-based nanostructured biocompatible materials contacted with biological systems
2009-2011. European project FP7 "Fluorine Substituted High Capacity Hydrides for Hydrogen Storage at low Working Temperatures" – FLYHY

2012. European project FP6 MATERA/BBM-2563 "Elaboration of bioactive surfaces by combining Dielectric Barrier Discharge and site-specific attachment of biomolecules" – BioADBD
2013-2014. Progetto di Ricerca di Ateneo-Compagnia di San Paolo-2011-Linea 1A "Advances in nanostructured materials and interfaces for key technologies" (Progetto ORTO11RRT5)
2014-2015. Italian Ministry of Education, University and Research (MIUR), research activity based on static and dynamic modelling of adsorption processes at the interphase of ceramic biomaterials
2015-2017. European project M-ERA.NET Call 2013 METABIO "METhod to elaborate bioinspired stable Antibacterial surface on metallic BIOmaterials for dental implants

2018 – 2019
Dott. Michele Cutini

2018. UNITO: Quantum-mechanical simulation of collagen-hydroxyapatite interaction as a model of bone
2019. UNITO: Quantum-mechanical simulation of the structure-property relationship in the collagen protein

2008 – 2009
Dr. Albert Rimola

2008-2009. Spanish Ramón Areces Foundation (http://www.fundacionareces.es/)

2012 – 2012
Hosting foreign Post-Doc

The Piero Ugliengo group hosted for 2 months in 2012 Dr. Jamieson Keir Christie of the London University College as a PostDoc to work on the simulation of phosphorous based bioglasses as granted by HPC-Europa2 Transnational Access programme.

INSTITUTIONAL TEACHING COURSES

1995 – CURRENT
Physical Chemistry (Bachelor degree in Chimica e Tecnologie Chimche)

The course provides foundations on intermolecular interactions and phenomenological chemical kinetics with some hints on transport phenomena.

01/01/1998 – CURRENT
Chemistry on the World Wide Web (Bachelor degree in Chimica e Tecnologie Chimiche)

Basic concepts of HTML language and of standard molecular visualization program on the web (Jmol program). To be able to get chemically relevant data on the web and to handle structural data base. To be able to establish the quality of the chemical information available on the web. Usage of the molecular visualization program (MOLDRAW, WebLabViewer, ArgusLab). To be able to construct a web site based on chemical concepts. To be able to present a web site to a wide audience.

01/01/1995 – CURRENT
Structural Chemistry (Master in Chemistry)

To show to the student what is the modern approach for the detrmination of the molecular structure with atomic resolution. The student will acquire the basic concepts on matter in the crystalline state and on the interaction between crystals and x-ray radiation. The student should be able to understand the modern literature in which structural information is the key factor (biochemistry, material science, catalysis, etc.). He/she will also be able to visualize with proper graphical tools the structural data from crystallographic databases.

01/01/2004 – CURRENT
Molecular Simulation by Computers (Master in Biotecnologie Industriali)

Both for scientific aspects and for those applications the module entitled "Molecular simulation by computers" gives the background of methods apt to study the conformation and dynamic behaviour of

biological macromolecules like proteins and nucleic acids by means of suitable algorithms and computer codes. The student will learn basic concepts like molecular mechanics and molecular dynamics, mathematical methods to locate structures which are minima on the mechanical energy, techniques based on the Metropolis Monte Carlo method to explore the potential energy surface and molecular dynamics to study the molecular mobility. The student should be able to understand modern literature based on molecular simulation to study biochemical mechanism and protein structure mobility.

PUBLIC ENGAGEMENT ACTIVITY

2005 – 2007

Architetture molecolari, spazi nanometrici e computer graphics

Il Domino dello spazio: scienze, tecniche, rappresentazioni, CSI-Piemonte, Torino 20-10-2005
Molecole, Cristalli e Materiali, Università degli Studi del Piemonte Orientale Amedeo Avogadro, 03-05-2007

05/05/2007 – CURRENT

Ipotesi chimica sull'origine della vita: dal Big Bang alla comparsa dei primi organismi viventi

Associazione delle Università della Terza Età, UNITRE, Università delle tre Età, Caluso 05-05-2007
I seminari del Dipartimento di Chimica e Chimica Industriale, Genova 03-03-2009
Orizzonti lontani: alla ricerca della vita extraterrestre, Scuola di Biotecnologie dell'Università degli Studi di Torino, Torino 07-03-2010
Festival della Scienza, Immaginazione, Genova 25-10-2012
La scienza incontra il quotidiano, Istituto di Istruzione Superiore Ada Gobetti Marchesini – Luigi Casale, Torino, 18-01-2016

2013 – CURRENT

Polvere cosmica e origine della vita

NANODAY 2013, Agorà Scienza, Centro Interuniversitario, Centro Incontri Regione Piemonte, Torino 06-03-2013.
5° Festival della Innovazione e della Scienza, Settimo Torinese, 20 October 2017.
Liceo Statale "Vasco Beccaria Govone", Piazza IV Novembre 4, Mondovi', 20-12-2018.
Incontri e opportunità nelle Biblioteche Civiche Torinesi, Biblioteca Centrale di Torino 19 Novembre 2019.

06/06/2017 – 06/06/2017

Le basi chimiche all'origine della vita

Cerimonia di premiazione dei Giochi della Chimica, Università Piemonte Orientale, Alessandria

11/11/2019 – 11/11/2019

COSMIC BRICKS: dagli elementi chimici alle molecole

INFINI*TO, Planetario di Torino, Museo dell'Astronomia e dello Spazio, Pino Torinese

02/07/2019 – 02/07/2019

Siamo Polvere di Stelle? Studio Astrochimico sulle Molecole della Vita

FRIDA: Forum della Ricerca di Ateneo: Racconti

31/08/2020 – 31/08/2020

Siamo Polvere di Stelle? L'incontro di due Atomi nell'Universo

FRIDA: Forum della Ricerca di Ateneo: Racconti

11/11/2021 – 11/11/2021

Nascita ed evoluzione molecolare: dagli atomi alla vita

Ciclo di conferenze della Accademia delle Scienze di Torino: L'origine della vita: dalla nucleosintesi alle molecole.

BACHELOR & MASTER THESIS SUPERVISOR

2010 – CURRENT

Bachelor and Master thesis at the Chemistry Department

More than 45 Bachelor degree thesis
More than 25 Master degree thesis

ORGANIZATION OF NATIONAL/INTERNATIONAL CONFERENCES

2001 – 2001

XV conference on "Horizons in Hydrogen Bond Research", Torino

Local Organizing committee

2003 – 2003

XXI Italian Chemistry Society Conference, Torino

Local Organizing committee and webmaster of the website conference

2010 – 2010

International NIS Colloquium "First chemical steps towards the origin of life", Torino

Chair of the Local Organizing committee

2015 – 2015

Congress of Theoretical Chemists of Latin Expression CHITEL2015, Torino

Vice chair of the Scientific committee (website)

2020 – 2020

International colloquium "Machine Learning Meets Chemistry", Torino

Chair of the local organizing committee (website)

2021 – 2021

International Conference on "Chemical processes in Solar-type star forming regions", Torino

Chair of the scientific and organization committee (website)