



Present Position: Full Professor in Physical Chemistry

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EDUCATION

- 1983 Degree in Chemistry at the University of Modena
- 1988 Ph. D. in Chemistry at University of Modena
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PREVIOUS POSITIONS AND FELLOSHIPS

- **From October 1987 to October 1988.** PhD Fellowship: Physical Chemistry Laboratory, Oxford University (U.K.)
- **From 1992 to 2002** Researcher of Physical-Chemistry Chemistry Department, Modena University
- **From 2002 to 2016** Associate Professor of Physical Chemistry, Chemistry Department, Modena and Reggio Emilia University.

ACADEMIC DUTIES

- 2021-2024 Coordinator of the Nucleo di valutazione UNIMORE
- Vice-Director of the Department of Chemical and Geological Sciences Unimore 2019-2021
- 2017-2020 Member of “Nucleo di valutazione di Ateneo” UNIMORE
- 2013-2016 Member of “Presidio di Qualità di Ateneo” UNIMORE
- 2007-2010 Member of the National University Council (Area 03-Chemistry)
- 2014- Member of Faculty of the Doctorate Course “Models and Methods for Material and Environmental Sciences”
- 2006-2013 - Director of the School of Graduated Studies “Multiscale Modelling, Computational Simulations and Characterization in Material and Life Sciences”
- 2000 - present Erasmus Coordinator

MEMBERSHIPS AND APPOINTMENTS

- 2021 Fellow of the European Academy of Sciences
- 2020 - 2021 President of the Division of Theoretical and Computational Chemistry of the Italian Chemistry Society
- 2017 - 2019 Elected member of the Board of the “Theoretical and Computational Chemistry Division” (Italian Chemical Society)
- 2014-2015 Member of the Scientific Committee of the Italian Chemical Society.
- 2001- 2009, member of the "Centre of Excellence in New Functional Materials, their Design, Diagnostics and Exploitation” Institute of Physics, University of Tartu, Estonia
- 2003 – 2009, Elected member of the Board of the “Physical Chemistry Division” (Italian Chemical Society)
- 2000-2005, Associate Director of the Virtual Centre for rational drug Design (National Foundation for Cancer Research, USA)

VISITS AND STAYS

- **September 1990** Visiting scientist at Physical Chemistry Laboratory, Oxford University (U.K.)
- **June 2002** Visiting scientist at the Institute of Chemistry, University of Tartu (Estonia)
- **May 2013** Visiting scientist at the Interdisciplinary Department on Molecular Systems and Materials of the IRAMIS Institute at the Commissariat à l'énergie atomique et aux énergies alternatives (CEA) in Saclay, France

BRIEF DESCRIPTION OF THE RESEARCH ACTIVITY

My research is aimed at rationalizing and interpreting experimental observed behavior of bio-molecular systems, biomaterials, nanoparticle-biomolecule interactions, by using computational simulation techniques. Many projects are carried out in close collaboration with experimentalists and emphasis on lead/material discovery is given.

- **Domain of competence:**

Computational Spectroscopy

Molecular dynamics (classical & CP), Parametrization

Molecular Simulation Protocols and computational tools for analysis

Protein-ligand and Protein-protein interaction

Homology Modelling, Docking, Drug Design

Quantitative Structure-Activity Relationships (QSPR).

- **Application fields:**

Computational strategies for the study of the structural, dynamics, elastic and spectroscopic properties of crystalline and amorphous inorganic materials, organic molecules and molecular crystals, nanomaterials, interaction between nanoparticle-biological environment, protein-protein, protein-ligand recognition. Development of theoretical molecular descriptors for simple and efficient quantitative structure-properties relationships.

List of Publications

<http://www.researcherid.com/rid/H-2585-2012>

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FUNDING AND PROJECTS**MAJOR RESEARCH GRANTS:**

- **Principal Investigator** FAR2015, *Rational design of curcumin-based bifunctional ligands for early diagnosis and therapy of Alzheimer's disease* (80.000 euro, 18 mesi) Bando UNIMORE su base competitiva.
- **Principal Investigator** del progetto 2010PA3244 *Insight into Silver Nanocube-protein interactions by computational simulations* finanziato con 150.000 core-hours da PRACE Preparatory Access da utilizzarsi sul supercalcolatore Fermi, CINECA, Italy e Marenostrom, BSC, Spain
- **Local Coordinator** PRIN2010-2011, Prot. 2010C4R8M8_002 coordinatore nazionale Prof. A. Agostiano, UniBa, "*Organizzazione Funzionale a Livello Nanoscopico di (Bio)Molecole e Ibridi per Applicazioni nel Campo della Sensoristica, della medicina e delle Biotecnologie*". (88000 euro, 36 mesi)
- **Local Coordinator** Progetto Regionale Emilia Romagna SPINNER 2013 per i dottorati di Ricerca. Titolo del progetto: 'Ottimizzazione delle forme cristalline di farmaci in relazione all'attività, la biodisponibilità, brevettabilità e alla progettazione di polimorfi solvatati e co-cristalli con metodi a basso impatto ambientale'. (45.000, 36 mesi)

