Cv Maria Montagna

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Education

2014: PhD in Engineering and Physical-Mathematical Modeling, Department of Information Engineering, Computer Science and Informatics, University of L'Aquila (Italy)

2009: Master's Degree in Physics, Department of Physics, Sapienza-University of Rome (Italy)

2006: Bachelor's Degree in Physics, Department of Physics, Sapienza-University of Rome (Italy)

Experience

January 2020 - April 2020: Hpc-Europa3 Visiting Scientist at the Chemistry Department, Sapienza-University of Rome (Italy) (Prof. M. D'Abramo)

- I am using classical MD simulation and advanced molecular theories (essential dynamic sampling) approaches to study the main conformational paths of important protein kinases

October 2017 - Present: Post-Doc at the Institute for Materials Science and Nanotechnology TU Dresden (Germany) (Prof. G. Cuniberti, Dr. R. Gutierrez)

- I am studying the molecular mechanisms involved in biomineralization processes, that is, the living organisms ability to produce mineral nanostructures.
- I use classical atomistic molecular dynamics to understand the interaction mechanism between organic molecules and inorganic surfaces as well as determining the aggregation behaviour of these organic components at different biological conditions.

October 2016 - September 2017: Post-Doc at Leibniz Institute of Polymer Research Dresden (Germany) (Prof. J.U. Sommer, Dr. O. Guskova)

- I used density functional theory and classical molecular dynamics simulations to look into the structural, spectroscopic and energetic properties of photosensitive-polymer complexes.

February 2015 - January 2016: Post-Doc at Department of Chemistry, Sapienza - University of Rome (Italy) (Prof. E. Bodo)

- We combined theoretical and experimental approaches to investigate structural, energetic and dynamical properties of a series of room temperature ionic liquids made by amino acids and choline.

- I performed molecular dynamics simulations of Actinoids and Lanthanoids in aqueous and non-aqueous solvents by using an accurate potential polarizable force field.

December 2013 - November 2014: Research Fellow at Department of Pharmaceutical Chemistry and Technologies, Sapienza - University of Rome (Italy) (Emeritus Prof. M. Speranza, Prof. A. Filippi, Dr. C. Fraschetti)

- I used classical and ab-initio approaches to interpret experimental results coming from an Infrared MultiPhoton Dissociation technique for structural analysis of biomolecules and their interactions with metals, acids or chiral guest.

November 2010 - November 2013: PhD in Engineering and Physical-Mathematical Modeling, Department of Information Engineering, Computer Science and Informatics, University of L'Aquila (Italy) (Supervisor: Prof. L. Guidoni)

- I studied transition metal complexes involved in polymerization processes of dienes using classical and first principle simulations methods. These complexes are an important class of catalysts capable of generating regular polymeric structures with several applications in industry (e.g. plastic and rubber production).

June 2010 - October 2010: Post-Master Research Fellow associated to the ERC grant "Ideas" – "Multiscale Modelling with Electron Correlation". Department of Chemistry, Chemical and Materials Engineering, University of L'Aquila (Prof. L. Guidoni)

- I carried on classical and ab initio dynamics simulations to analyse structural, dynamic and vibrational properties of water molecules in the first hydration shell of small hydrophobic solute.

Research Interests (Associated to the corresponding publications)

Protein Modeling: Structural and dynamical characterization of protein evolutionary pathway.

Organic/Inorganic Interactions in Bioinspired Systems and Industrial Catalytic Complexes: Interactions between organic molecules and inorganic surfaces. Self-assembly driving-force characterizations. Geometric and energetic investigations of non-covalent (organic-inorganic) molecular complexes. Reaction pathways in polymeric processes catalysed by transition metal complexes (**[1], [15], [11], [10], [7], [4], [13]**)

Hybrid and Complex Materials: Characterization of complex systems (*i.e.* ionic liquids, functionalized materials) to understand their structural, energetic and dynamical properties **([8], [6], [2])**

Hydration Processes: Geometrical, dynamical and energetic properties of solvation shells in hydrophobic molecules and ions in solution (aqueous and non-aqueous solvents) **([14], [9], [5], [3])**

Vibrational BioSpectroscopy: Calculations of vibrational properties of molecules in explicit solvent and/ or specific environment including finite temperature effects (**[14], [12])**

Selected Oral Contributions in Conferences and Workshops

12-14/3/2018 *"Atomistic Modeling of Organic-Inorganic Interfaces"*; Scientific Symposium: Nanopatterned Organic Matrices in Biological Silica Mineralization Wernigerode/Harz (Germany)

19-24/3/2017*"Azobenzene-containing surfactants and their association with poly(methacrylic acid) at nanometer scale";* DPG (German Physical Society) Spring Meeting-2017, Dresden, (Germany)

20-23/2/2017 *"Computer Simulations of Azobenzene-based Photosensibilisers of Polymers";* Scientific Symposium, Leibniz Institute of Polymer Research, Binz, (Germany)

2-5/09/2013 *"Pathways for polymerization of 1,3-butadiene catalyzed by Cp2TiCl2/MAO";* International Conference on the Reaction Engineering of Polyolefins (Incorep2013) Ferrara (Italy)

6-9/7/2011*"Spectroscopic fingerprint of water around small hydrophobic solutes";* Workshop: Spectroscopic characterization of liquid water from electronic structure CECAM-EPFL, Lausanne, (Switzerland)

Short-Time Stays

October 2015 – One month at the **Laboratoire de Chimie Physique d'Orsay, Universitat de Paris Sud,** Saclay**, (**France) (with Prof. Debora Scuderi)

2011-2013 – Periodic visiting at **CNR-ISMAC**, Milano, (Italy) (with Dr. G. Ricci, Dr. G. Leone, Dr. Francesco Masi)

(27/6-1)/7/2011 - (14-17)/12/2011 – Stay at the **Institut de Biologie Physico-Chimique Laboratoire de Biochimie Théorique**, Paris, (France) (with Dr. F. Sterpone)

Individual Funding and Computational Resources

June 2020 - Iscra C - COVID-19 Fast access to HPC supercomputing facilities time grants issued by CINECA & Associazione Big Data. Project: "*Conformational characterization of Spike glycoprotein in SARS-CoV 2*" (**Principal Investigator**)

(January-April 2020) Hpc-Europa3 fellowship at Chemistry Department, Sapienza-University of Rome. Project: "*Modelling Lck conformational transitions by means of classical molecular dynamics and essential dynamic sampling*". (**Principal Investigator**)

One year Post-Doc scholarship at Leibniz Institute of Polymer Research Dresden, Institute Theory of Polymer. Project: "*Computer simulations of azobenzene-based photosensibilisers of polymers*"

Cost Action, Short Term Scientific Mission (COST-STSM-MP1306-28979) at Laboratoire de Chimie-Physique d'Orsay, Universitat de Paris-Sud**.** Project: "*Experimental and computational characterization of oxidation products of methionine peptides*." **(Principal Investigator)**

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