Curriculum Vitae for publication

Marco Micciarelli

Personal data

Date of birth July 29^{th} 1982

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Present work position

Post doctoral fellow at Università degli studi di Milano, in the group of prof Michele Ceotto at the chemistry department within the ERC project SEMICOMPLEX . The research project I am involved in aims at developing and testing novel methodologies based on new semiclassical approaches for the calculation of vibrational properties of materials and molecules including quantum and anharmonicity effects.

Professional experience

2014-2016 **Post doctoral fellow**

Scuola Internazionale Superiore di Studi Avanzati, (**SISSA**) Trieste, Italy

Condensed matter sector

Within the group of prof. Stefano Baroni, the research project I've been involved in was aimed at developing and testing novel methodologies for the computational modeling of the

color optical properties of complex molecular dyes in solution. The project was carried in collaboration with industrial partners working to the identification of most suitable natural dyes expressing custom-designated hues of colors.

Education

2010-2013 **Ph.D. in fundamental and applied physics**

Università degli studi di Napoli Federico II, Italy

PHD THESIS TITLE:

Model systems approach to the study of UV light induced DNA-proteins interaction

ADVISORS: Prof. Carlo Altucci, Dr. Ivano Tavernelli

2006-2009 **Master in physics**

Università degli studi di Napoli Federico II, Italy

NOTE: 110/110 cum laude

MASTER THESIS TITLE:

Ab Initio study of a model system for light induced DNA-proteins interaction

ADVISOR: Prof. Carlo Altucci

2001-2006 **Bachelor degree in physics**

Università degli studi di Napoli Federico II, Italy

NOTE: 110/110

THESIS TITLE:

An experiment for thermodynamics didactics: a measure for the Stirling engine thermal efficiency

ADVISOR: Dr. Emilio Balzano

Scholarships

2010 **European Science Foundation (ESF) Grant in the framework activity Molecular Simulations in Biosystems and Material Science (SimBioMa)**

GRANTED PROJECT TITLE:

DNA-proteins crosslink reactions simulation with QMMM techniques

2008 **ERASUM Placement grant**

Training period in the molecular physics group at the NIRDIMT, at Cluj Napoca, Romania

Internships periods

2011- 2014 GCI computational group, Università degli studi La Sapienza, Roma, Italy

2010 - 2011 Laboratory of Computational Chemistry and Biochemistry (Rothlisberger group), EPFL, Lausanne, Switzerland

International scientific schools

Dec. 2015 **Python for computational science** at CINECA, Rome, Italy

Jun. 2013 **Ab initio molecular dynamics for biomolecules** Santo Stefano di Sessanio, Italy

April 2013 **Rome school on Open Systems and the Quantum-Classical Boundary**Rome, Italy

Jan. 2012 **Time-Dependent Density-Functional Theory: Prospects and Applications** Benasque, Spain

May 2012 **Non adiabatic quantum dynamics with MCTDH and CPMD** at CECAM, Lausanne, Switzerland

Teaching experience

2013 Teaching assistance in the course "Laboratorio di calcolo 1" for the first year bachelor degree in physics at La Sapienza university in Rome

Languages

Italian: Native

English: Fluent

French: Basic

Computational skills

Programming and scripting:

C, Fortran: Good level

MPI and OpenMP: Basic

Python, Bash: Good level

Computational physics packages:

Classical MD: LAMMPS, Gromacs, Amber, Gromos

Electronic structure: QUANTUM ESPRESSO, CPMD, Gaussian09

Graphics: VMD, X-crysden, Molden

Pubblications

Characterization of the Photochemical Properties of 5-Benzyluracil via Time-Dependent Density Functional Theory. *Marco Micciarelli, Basile Curchod, Sara Bonella, Carlo Altucci, Mohammadhassan Valadan, Ursula Rothlisberger, and Ivano Tavernelli*; J. Phys. Chem. A, 2017, 121 (20), 3909?3917

Sampling molecular conformers in solution with quantum mechanical accuracy at a nearly molecular mechanics cost. *Marta Rosa, Marco Micciarelli, Alessandro Laio, and Stefano Baroni,* J. Chem. Theory Comput. 2016, 12, 4385?4389

Multi-model approach to the optical properties of molecular dyes in solution. *Iurii Timrov, Marco Micciarelli, Marta Rosa, Arrigo Calzolari, and Stefano Baroni* J. Chem. Theory Comput. 2016, 12, 4423?4429

Photophysics and photochemistry of a DNA-protein cross-linking model: a synergistic approach combining experiments and theory *Marco Micciarelli, Mohammadhassan Valadan, Bartolomeo Della Ventura, Giovanni Di Fabio, Lorenzo De Napoli, Sara Bonella, Ursula Rothlisberger, Ivano Tavernelli, Carlo Altucci, Raffaele Velotta*; J Phys Chem B. 2014, 118(19), 4983-92.

Low-lying excited-states of 5-benzyluracil *Marco Micciarelli, Carlo Altucci, Bartolomeo Della Ventura, Raffaele Velotta, Valer Tosa, Adan B. Gonzalez Perez, Martin Perez, Angel R. de Lera and Attila Bende*; Phys Chem Chem Phys. 2013, 15(19), 7161-73.

Nonlinear protein-nucleic acid crosslinking induced by femtosecond UV laser pulses in living cells, *C. Altucci, A. Nebbioso, R. Benedetti, R. Esposito, V. Carafa, M. Conte, M. Micciarelli, L. Altucci, and R. Velotta*; Laser Physics Letters, Volume: **9** Issue: **3** Pages: 234-239 (2012)

Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems, *E. Brunk, N. Ashari, P. Athri, P. Campomanes, F.F. de Carvalho, B. Curchod, P. Diamantis, M. Doemer, J. Garrec, A. Laktionov, M. Micciarelli, M. Neri, G. Palermo,T.J. Penfold, S. Vanni, I. Tavernelli, U. Rothlisberger*; CHIMIA Volume: 65 Issue: **9** Pages: 667-671 (2011)