Curriculum Vitae et Studiorum of Dr. Mariagrazia Fortino

I Personal details

Mariagrazia Fortino, born on September 24, 1988 in Cosenza (I), Italian nationality.
Email: mariagrazia.fortino@gmail.com

II Education

December 22, 2016: Abilitation for the chemistry profession at Università della Calabria, Cosenza (Italy).

December 11, 2015: PhD in Inorganic Metodology at Università della Calabria, Cosenza (Italy). Thesis title: Theoretical investigation of Bioinorganic compounds: biomimetic catalysts and metal-mediated mismatched DNA base-pairs (supervisor Prof. Nino Russo).

October 05, 2012: Master's degree in Chemistry at Università della Calabria, Cosenza (Italy). Evaluation 110/110 with honors. Thesis title: Interazioni tra nucleobasi mediate da metalli: strutture e proprietà (supervisor Prof. Nino Russo).

December 14, 2010: Bachelor's degree in Chemistry at Università della Calabria, Cosenza (Italy). Evaluation 110/110. Thesis title: Complessi curcuminoidi di $Zn(II)$: problemi e promesse. (supervisor Prof. Daniela Pucci).

July, 2007: Scientific secondary school at Liceo Scientifico Statale G. Scorza of Cosenza (Italy). Evaluation 100/100.

III Academic experience

October 22, 2018-October 21, 2019: Postdoc at Scuola Normale Superiore, Pisa, (Italy).

Research Object: Application and validation of new theoretical models for the study of electronic properties of chromophores (supervisor Prof. Julien Bloino).

June 15, 2017-June 14, 2018: Postdoc at Università di Modena e Reggio Emilia, Modena (Italy).

Research Object: Theoretical investigation of spectroscopic properties of organic molecules used in photovoltaic hybrid cells (supervisor Prof. Alfonso Pedone).

IV Teaching activities

October 2016 - March 2017: Teacher of general chemistry - Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Cosenza (Italy).

October 2016 - September 2017: Teacher of general and inorganic chemistry - Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Cosenza (Italy).

October 2014 - December 2014: Teacher of organic chemistry and laboratory- Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Cosenza (Italy).

V Laboratory and Experimental activities

October 2013 - April 2014: PhD student at Institute for biocomplexity and informatics and Department of Chemistry, University of Calgary, Alberta (Canada). Research line: Computational study of reaction mechanism for new biomimetic compounds (supervisor Prof. Nino Russo and co-supervisor Prof. Dennis R. H. Salahub).

May 2012 - October 2012: Master's graduand at theoretical and computational chemistry laboratory, Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Cosenza (Italy). Research line: Theoretical and computational investigation of interactions between DNA nucleobases and transition metals (supervisor Prof. Nino Russo).

July 2010 - December 2010: Bachelor's graduand at Inorganic Chemistry Laboratory. Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Cosenza (italy). Research line: Synthesis of organometallic compounds containing $Zn(II)$ and curcumin and their characterization using IR, NMR, UV-vis, XR technics (supervisor Prof. Daniela Pucci).

VI Details on research activity

My interest for computational chemistry started during the training period for the master's degree: the research activity had its main focus on the investigation of the structural and electronic properties of new systems of technological interest, characterized by the presence of DNA bais pairs interacting with metal ions. To reach this goal I have used Quantum Mechanic (QM) methods, based on density functional theory (DFT). Using the same computational approach, during the PhD period I have deeply investigated the working mechanism followed by some biomimetic catalysts, for which both the regioselectivity factor and the experimentally activity have been rationalized. During my post-doctoral experience, I have computationally investigated the photophysical properties of medium-large systems in condensed phase, at TD-DFT level of theory, simulating vibrationally resolved electronic spectra and, more recently, in order to investigate the complex relaxation mechanism following the photoexcitation, also 2D Electronic Spectra simulations and and Excited State Molecular Dynamics investigations have bee involved into the theoretical study.

VII Publications

- "Non-radiative relaxation process within Q-band of Cholorophyll a: a dynamic theoretical investigation" M.Fortino, E. Collini, A. Pedone, J.Bloino, Work in progress.

- "The role of specific solute-solvent interactions on the photophysical properties of Distyryl Substituted BODIPY derivatives" M. Fortino, E. Collini, A.Pedone, J.Bloino, Phys. Chem. Chem. Phys., 2020, Accepted Manuscript: doi:/10.1039/DOCP00034E.

- "Computational Mechanistic Insights on the NO Oxidation Reaction Catalyzed by Non-Heme Biomimetic Cr-N-Tetramethylated Cyclam Complexes", T. Marino, M. Fortino, N. Russo, M. Toscano, M. E. Alberto, Int. J. Mol. Sci. 2019, 20(16), 3955.

- "Assessment of B-O interatomic parameters for the reproduction of borosilicate glass structures through DFT-GIPAW calculations", M. Fortino, A. Berselli, L. Deng, A. Goel, J. Du, A. Pedone, J. Am. Ceram. Soc. 2019; 00, 1-19.

- "The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics", D. Cesario, M. Fortino, T. Marino, F. Nunzi, E. Sicilia, J. Comp. Chem., 2019, 40, 8, 944-951.

- "On the simulation of vibrationally resolved electronic spectra of medium-size molecules: the case of styryl substituted BODIPYs", M. Fortino, J. Bloino, E. Collini, L. Bolzonello, M. Trapani, F. Faglioni, A. Pedone, Phys. Chem. Chem. Phys., 2019, 21, 3512-3526.

- "Two-Dimensional Electronic Spectroscopy Discloses Dynamics and Mechanisms of Solvent-DrivenInertial Relaxation in Polar BODIPY Dyes", L. Bolzonello, A. Polo, A. Volpato, E. Meneghin, M. Cordaro, M. Trapani, M. Fortino, A. Pedone, M. Castriciano, E. Collini, J. Phys. Chem. Letters 9 (5), 2018, 1079-1085.

- "A DFT investigation of a bulky biomimetic model catalyzing the 5'-outer ring deiodination of thyroxine", M. Fortino, T. Marino, N. Russo, E. Sicilia J.Mol. Model, 2016, 22, 287.

- "Mechanistic investigation of the reduction of trimethylamine-N-oxide catalysed by biomimetic molybdenum enzyme models", M. Fortino, T. Marino, N. Russo, E. Sicilia, Phys. Chem. Chem. Phys., 2016, 18, 8428-8436.

- "Theoretical study of silver-ion-mediated Base Pairs: The case of C-Ag-C and C-Ag-A systems", M. Fortino, T. Marino, N. Russo, J Phys, Chem. A, 2015, 119, 5153-5157.

- "Mechanism of Thyroxine Deiodination by Naphtyl-Based Iodothyronine Deiodinase Mimics and the Halogen Bonding Role: a DFT Investigation", M. Fortino, T. Marino, N. Russo, E. Sicilia, Phys, Chem. Eur. J., 2015, 21, 8554-8560.

VIII Contributions to Conferences and Workshops

- Theoretical Spectroscopic Investigation of Specific Solute-Solvent Interactions: Distyryl Substituted BODIPYs as Test Cases, *VI Congresso DCTC, SCI*, Arcavacata di Rende (Italia), September 2019. (Talk)

- Simulation of vibrationally resolved electronic spectra: the case of styryl substituted BODIPYs,*Winter Modeling 2019*, Napoli (Italy), February 2019. (Talk)

- On the simulation of vibrationally resolved electronic spectra of medium-size molecules: the case of styryl substituted BODIPYs,*V Congresso della Divisione di Chimica Teorica e Computazionale della Societa' Chimica Italiana*, Trieste (Italy), September 2018. (Poster)

- Vibrationally resolved electronic spectra of styryl-substituted bodipys:benchmark of new computational protocols for the simulation,*ERC AdG-Barone DREAMS:Final Meeting Advances in computational modelling: from isolated molecules to soft matter*, Pisa (Italy), December 2017. (Talk)

- Mechanism of Thyroxine Deiodination by Naphthyl-Based Iodothyronine Deiodinase Mimics and the Halogen Bonding Role: A DFT Investigation,*7th International theoretical biophysics symposium TheoBio*, Cagliari (Italy), June 2015. (Poster)

- Computational study of thyroid hormones deiodination by bio-inspired iodothyronine deiodinase complexes *XXV Congresso Nazionale della societa' Chimica Italiana*, Cosenza (Italy), September 2014. (Poster)

- *Seminario:* Selenium Naphtyl-Based compounds as mimics of Todothyronine Deiodinase enzymes, University of Calgary- AB (Canada), October 2013. (Talk)

IX Languages

- Italian: Native
- English: Excellent, with Certifications:

  [November, 2006:] Trinity Grade 8 at Trinity College, London, UK.

  [July, 2005:] Preliminary English Test at University of Cambridge, Cambridge, UK.

  [July, 2004:] Key English Test at University of Cambridge, Cambridge, UK.

X Informatic skills

- Excellent knowledges of toolkit: Gaussian16, Turbomole, Spectron, xtb/CREST, SoS-NMR, NewtonX.
- Excellent knowledges of the visualization softwares Gaussview, ArgusLab, XYZViewer, Molden, Mercury, Avogadro, VMS-draw.
- Excellent knowledges of the operative systems MacOSX, Unix, Linux and Windows and their tools.
- Good knowledges of the text editing (LaTeX).
- Excellent knowledges of the main internet clients (browser, research engines and email programs).

May 06, 2020

Mariagrazia Fortino