

# Curriculum Vitae et Studiorum of Dr. Mariagrazia Fortino

## I Personal details

Mariagrazia Fortino, born on [REDACTED]

Email: [REDACTED]

## II Education

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

**December 11, 2015:** PhD in Inorganic Methodology 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

**July 01, 2020-present:** Postdoc at Università Magna Graecia di Catanzaro, Catanzaro, (Italy).

Research Object: Development of Density Functional Theory based methods for designing photoactive molecules" (supervisor Prof. Adriana Pietropaolo).

**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 Publications

- "Multi-replica biased sampling for photoswitchable  $\pi$ -conjugated polymers" M. Fortino, C. Cozza, M. Bonomi, A. Pietropaolo, J. Chem. Phys. Accepted Manuscript
- "Unrevealing the internal conversion process within the Q-bands of a chlorophyll-like-system through Surface-Hopping Molecular Dynamics Simulations " M.Fortino, E. Collini, J.Bloino, A. Pedone, J. Chem. Phys. 2021, 154, 094110.
- "Combined Experimental and Computational Approach toward the Structural Design of Borosilicate-Based Bioactive Glasses" N. Stone-Weiss, H. Bradtmuller, M. Fortino, M.Bertani, R. E. Youngman, A. Pedone, H. Eckert, A. Goel, J. Phys. Chem. C, 2020,124, 32, 17655-17674.
- "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, 22, 10981-10994.
- "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; 102, 7225-7243.
- "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-Driven Inertial 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, *Chem. Eur. J.*, 2015, 21, 8554-8560.

## VII Contributions to Conferences and Workshops

- Hamiltonian excited state Replica Exchange for photoisomerization processes in conjugated polymers, *Virtual Sumposium on Chemical Theory and Computation, SCI*, December 2020. (Talk)
- 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 Iodothyronine Deiodinase enzymes, University of Calgary- AB (Canada), October 2013. (Talk)

## VIII 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.

## **IX Informatic skills**

- Excellent knowledges of toolkit: Gaussian16, Turbomole, Spectron, SoS-NMR, NewtonX, GROMACS MD, PLUMED.
- Excellent knowledges of the visualization softwares Gaussview, ArgusLab, XYZViewer, Molden, Mercury, Avogadro, VMS-draw, VMD.
- 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).

April 26, 2021

Mariagrazia Fortino