

## PERSONAL INFORMATION

## Giovanna Bruno



## WORK EXPERIENCE

From 01/06/2022 to 31/05/2023

## Postdoctoral research fellow

Science and High Technology Department (DiSAT), University of Insubria, 9, Valleggio St., Como (CO), 22100, Italy (website:<https://www.uninsubria.it/siti-tematici-o-federati/siti-dei-dipartimenti/dipartimento-di-scienza-e-alta-tecnologia-disat>).

- Lead researcher for the project entitled “Theoretical study of the surface reactivity of silicon dioxide and zinc oxide with silanes and sulfur compounds” supervised by Prof. Massimo Mella and funded by Prometeon Tyre Group, 222, Sarca Av., Milan (MI), 20126, Italy (website:[https://www.prometeon.com/IT/it\\_IT](https://www.prometeon.com/IT/it_IT))
- Supervising activity of a master student’s internship entitled: “TR-DFT simulations to investigate the role of intra and intermolecular hydrogen bonds in the generation of radical oxidant curcuminoids and spectrofluorimetry measurements to determine the latter’s capacity of photosensibilizing the production of oxidant radicals ”

Official internship tutors: Dr. Luca Nardo  
Prof. Massimo Mella

Sector Physical-chemistry (CHIM/02)

From March to June 2019

## Laboratory assistant

Course: Chemistry Laboratory with prevention and safety of the bachelor degree program in Biological Sciences of University of Milan, 26, Giovanni Celoria St., Milano (MI), 20133, Italy (website: <https://www.unimi.it/en/education/biological-sciences>).

Course leader: Prof. Silvia Rizzato (Chemistry Department of University of Milan)

Sector Organic and inorganic chemistry (CHIM/06, CHIM/03)

## EDUCATION AND TRAINING

From 01/10/2018 to 16/09/2022

## Ph.D in Chemistry

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Department of Chemistry, University of Milan, 19, Camillo Golgi St., Milan (MI), 20133, Italy (website: <https://eng.chimica.unimi.it/ecm/home>).

Project title: "Quantum observables of open-shell systems: a theoretical study"

Supervisor: Prof. Leonardo Lo Presti (Chemistry Department of University of Milan)

Co-supervisor: Dr. Carlo Gatti (Istituto di Scienze e Tecnologie Chimiche "Giulio Natta" (SCITEC) of the Consiglio Nazionale delle Ricerche (National Research Council - CNR))

Research fields: Theoretical Chemistry, Quantum Chemistry, Mathematical Chemistry, Quantum Chemical Topology, Differential Topology, Morse Theory, Theoretical Photochemistry, Open-Shell Systems and Materials, Spin Properties of Matter.

Main competences acquired: Development of theoretical methods and computational methodologies (codes implementation in Fortran 90/95) to predict and characterize quantum observables of open-shell systems; use and implementation of codes in AIMPAC and Multiwfn programs; use of Gaussian and ORCA programs.

- Development of the theory of *Electron Spin Density Topology*
- Development of highly accurate computational protocols to predict phosphorescence and related observables of aromatic chromophores of technological interest
- Development of theoretical models of aromaticity(anti) in excited states

From 01/09/2020 to 31/05/2021

#### Ph.D. visiting student

Department of Molecular Theory and Spectroscopy, Max-Planck-Institut für Kohlenforschung, 1, Kaiser-Wilhelm-Platz, Mülheim an der Ruhr, 45470, Germany (website: <https://www.kofo.mpg.de/>).

Project title: "Towards a quantitative framework in which to discuss experimental observables: aromaticity(anti) of planar organic molecules"

Supervisors: Dr. Giovanni Bistoni (now Assistant Professor (RTDB) at the Chemistry, Biology and Biotechnology Department of University of Perugia)

Prof. Frank Neese (Max-Planck-Institut für Kohlenforschung)

Main competences acquired: Development of computational protocols to predict photophysical and photochemical properties of aromatic chromophores, development of theoretical models of aromaticity(anti) in excited states, use of advanced quantum chemistry methods (e.g. DLPNO-CCSD(T)), use of ORCA program package.

From 18/12/2015 to 24/10/2018

#### M.Sc. in Chemical Sciences, degree mark 110/110 with honours

Department of Chemistry, University of Milan, 19, Camillo Golgi St., Milan (MI), 20133, Italy

Master thesis title: "Electron spin density topology: a preliminary study"

Supervisors: Prof. Leonardo Lo Presti

Dr. Carlo Gatti

Main competences acquired: Fundamentals of Bader's "Quantum Theory of Atoms in Molecules" (QTAIM) and of Quantum Chemical Topology (QTC) in order to apply such tools to the special case of electron spin density; use of Gaussian, AIMPAC and Multiwfn programs.

From 01/10/2012 to 18/12/2015

#### B.Sc. in Chemistry, degree mark 100/110 (top marks)

Department of Chemistry, University of Milan, 19, Camillo Golgi St., Milan (MI), 20133, Italy

Bachelor thesis title: "Effect of the anharmonicity of the potential energy surface in tunnelling processes"

Supervisors: Prof. Michele Ceotto

Prof. Leonardo Lo Presti

Main competences acquired: Fundamentals of classical, semiclassical and quantum dynamics, theory of harmonic oscillators and statistical thermodynamics to apply these tools for the calculation of the thermal rate constants associated with exchange reactions at different temperatures. Implementation of codes in Fortran 90/95 and use of Gaussian program.

From 2007 to 2012

#### Classical lyceum (high school) diploma, final mark 100/100

Liceo Classico e Artistico "Pitagora", Bachelet St., Nova Siri (MT), 75020, Italy.

PERSONAL SKILLS

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Mother tongue(s) Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
	English	Proficient user	Proficient user	Proficient user	
French	Basic user	Basic user	Basic user	Basic user	Basic user
Spanish	Basic user	Basic user	Basic user	Basic user	Basic user
German	Basic user	Basic user	Basic user	Basic user	Basic user

Communication skills

- good communication skills gained through my experience as students representative at Chemistry Department of University of Milan from 2013 to 2018.
- good science communication skills in the fields of both academic and industrial research, gained by presenting my research work in conferences (oral and poster session presentations) and in meetings with the Research and Development (R&D) team of the company Prometeon Tyre Group

Organisational / managerial skills

good leadership skills gained by being, from 2016 to 2018, one the members of the steering committee of the student union "Lista Aperta Obiettivo Studenti" of the Sciences and Technologies Faculty of University of Milan. The committee coordinated all activities of the association in the scientific departments of University of Milan and kept relations with corresponding committees of Faculty of Humanities of University of Milan and of Politecnico of Milan.

Job-related skills

- good teamwork skills gained by collaborating to research projects which involved researchers affiliated to different research institutes, universities or companies and having different scientific backgrounds (e.g. theoretical and computational chemists, experimental chemists and physicists, organic chemists and engineers)
- good critical thinking and problem solving skills gained working on topics which were initially far from my scientific background as a chemist (e.g. working on differential topology problems at the beginning of my PhD or on engineering problems related to tyres production during my first postdoctoral fellowship)

Computer skills

- good command of Windows and Linux operating systems
- good programming skills with Fortran, C, Python and bash languages
- good skills with markup languages (e.g. LaTeX)
- good skills with quantum chemistry program packages (Gaussian, ORCA, Multiwfn, AIMPAC)
- good skills with molecular and crystal structure editors (Molden, Avogadro, Chimera, VESTA, Diamond)

ADDITIONAL INFORMATION

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Publications	<p><b>Bruno, G.;</b> Macetti, G.; Lo Presti, L.; Gatti, C. Spin Density Topology, <i>Molecules</i> 2020, 25, 3537. DOI: <a href="https://doi.org/10.3390/molecules25153537">https://doi.org/10.3390/molecules25153537</a></p> <p><b>Bruno, G.;</b> de Souza, B.; Neese, F.; Bistoni, G. Can Domain-Based Local Pair Natural Orbitals Approaches Accurately Predict Phosphorescence Energies?, <i>Physical Chemistry Chemical Physics</i>, 2022. DOI: <a href="https://doi.org/10.1039/D2CP01623K">https://doi.org/10.1039/D2CP01623K</a></p> <p>Gatti, C.; <b>Bruno, G.</b> Chemical insights from the Source Function reconstruction of various scalar fields, in J. Anderson; J. Rodriguez and F. Guzman (Eds), <i>Advances in Quantum Chemical Topology Beyond QTAIM</i>, 1st Edition. Paperback ISBN: 9780323908917</p>
Research interest and current projects	<p><b>Spin and magnetic properties of matter</b></p> <ul style="list-style-type: none"> <li>- Spin transport and magnetic properties of prototypical organometallic molecular magnets</li> <li>- Accuracy of spin density distributions as a function of the adopted theoretical method</li> <li>- Topological descriptors of spin density distributions</li> </ul> <p><b>Optical properties of organic chromophores</b></p> <ul style="list-style-type: none"> <li>- Theoretical models of aromaticity-antiaromaticity reversal based on optical observables</li> <li>- Theoretical study of the antioxidant power of curcuminoids in both ground and excited states and its relation with eventual intra and intermolecular H-bonds</li> </ul> <p><b>Material Science</b></p> <ul style="list-style-type: none"> <li>- Theoretical models of hydrogen isotopes separation via quantum sieving on alkali-earth oxides</li> </ul>
Conferences and presentations	<p>Florence, 2023      <b>Oral didactic presentation by invitation</b> at ENERCHEM School organized by Italian Chemical Society</p> <p>Genoa, 2022        <b>Oral presentation</b> at National Congress of Physical Chemistry</p> <p>Amsterdam, 2022   <b>Poster presentation</b> at 28th IUPAC Symposium on Photochemistry</p> <p>Online, 2021        CECAM Workshop: Second discussion Meeting on Quantum Crystallography: expectations and reality</p> <p>Lausanne, 2021    CECAM Workshop: Non-Covalent Interactions in Large Molecules and Extended Materials</p> <p>Muelheim an der Ruhr, 2021   <b>Oral presentation</b> at Summer Symposium of the Department of Molecular Theory and Spectroscopy of the Max-Planck-Institut für Kohlenforschung</p> <p>Online, 2020        <b>Poster presentation</b> at Quantum Crystallography Online Meeting 2020</p> <p>Rome, 2020         <b>Poster presentation</b> at V School of Magnetism organized by Associazione Italiana di Magnetismo</p> <p>Palermo, 2019      <b>Poster presentation</b> at European Summer School in Quantum Chemistry</p> <p>Goettingen, 2018   <b>Oral presentation</b> at Annual Meeting of the Centre for Materials Crystallography</p>
Honours and awards	<p>ENERCHEM School Grant of the Italian Chemical Society (2023)</p> <p>Master Degree Prize of the 'Grazioli' Foundation for Chemistry and Physics (2019) <a href="https://www.fondazionegrazioli.it/cultura/premio-di-laurea-2019">https://www.fondazionegrazioli.it/cultura/premio-di-laurea-2019</a> <a href="https://lastatalenews.unimi.it/listituto-lombardo-premia-nove-laureati-statale">https://lastatalenews.unimi.it/listituto-lombardo-premia-nove-laureati-statale</a></p> <p>PhD Scholarship of Chemistry Department of University of Milan (2018)</p>

Courses and certificates	February, 2019	'Training course for learning support tutors of scientific faculties' Centro di servizio di ateneo per l'orientamento allo studio e alle professioni (COSP), University of Milan, 7, Festa del Perdono St., Milan (MI), 20122, Italy.
	May, 2017	'Introduction to Modern Fortran' CINECA, 4, R. Sanzio St., Segrate (MI), 20090, Italy.
	October, 2015	'Introduction to Scientific and Technical Computing in C' CINECA, 4, R. Sanzio St., Segrate (MI), 20090, Italy.
Extracurricular activities	2021-present	Voluntary activity at "Fondazione Banco Alimentare", 4, Legnone St., Milano (MI), 20158, Italy.
	2015-2018	Voluntary activity at care home for mental disorders patients "Sacra Famiglia", 1, Monsignor Luigi Moneta Square, Cesano Boscone (MI), 20090, Italy.
	2013-2015	Voluntary activity as tutor for chemistry, physics and maths at 'Associazione Portofranco Milano Onlus', 58, Papiniano Av., Milano(MI), 20123, Italy.
	October, 2015	Speaker and representative of the Chemistry Department of University of Milan at the conference <i>OrientaGiovani 2015 'Il mio futuro e la chimica'</i> organized by Federazione Nazionale Industria Chimica (Federchimica).
Memberships	Junior associate of the Physical-chemistry division and of the Interdivisional Group on the Chemistry of Renewable Energies (ENERCHEM) of the Italian Chemical Society.	