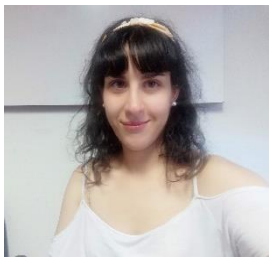
Silvia Alessandrini



Nationality: Italian

Date of birth: 07/05/1993

Sex: Female

(+39) 3492906604

E-mail address: silvia.alessandrini7@unibo.it

Address: Via A. Fioravanti 9, 40129 Bologna (Italy)

EDUCATION AND TRAINING

High-School Diploma in Industrial Chemistry

ITIS E. Mattei [01/09/2007 – 15/07/2012]
Address: Via L. Pacioli 22, 61029 Urbino (Italy)
Final grade: 100/100 – **EQF Level: EQF Level** 4

Bachelor's degree in chemistry and chemistry of materials

Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna
[01/09/2012 – 10/12/2015]
Address: Via F. Selmi 2, 40126 Bologna (Italy)
Fields of study: Natural Sciences, Mathematics and Statistics: *Chemistry*
Final grade: 110/110 laude – **EQF Level: EQF Level** 6
Thesis: Energetic and Structural Characterization of a prebiotic molecule: formamide and its dimer
Supervisor: Professor C. Puzzarini

Master's degree in chemistry (Curriculum B: Methodologies of Analysis and Characterization)

Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna
[16/12/2015 – 12/10/2017]
Address: Via F. Selmi 2, 40126 Bologna (Italy)
Fields of study: Natural Sciences, Mathematics and Statistics: *Chemistry*
Final grade: 110/110 laude – **EQF Level: EQF Level** 7
Thesis: Spectroscopic Characterization of New Sulfur-containing Molecules for Astrochemical Purposes
Supervisor: Professor C. Puzzarini Co-supervisors: Professor J. Gauss and Dr. Lorenzo Spada

PhD in "Methods and Models for Molecular Sciences"

Scuola Normale Superiore di Pisa [01/11/2017 – 12/05/2022]
Address: Piazza dei Cavalieri 7, 56126 Pisa (Italy)
Grade: Passed with honors – EQF **Level: Level 8 EQF** – SSD: **CHIM/02**
Thesis: Modelling Weak Interactions in the Gas Phase: From Rotational Spectroscopy to Reaction Rates Using Accurate Quantum-Chemical Approaches
Supervisor: Professor C. Puzzarini Co-supervisor: Professor V. Barone

Research Fellow

Scuola Normale Superiore di Pisa [10/01/2022 – 09/01/2023]
Address: Piazza dei Cavalieri 7, 56126 Pisa (Italy)

Topic*: Theoretical-computational analysis of complex intermolecular interactions (Duration 1 year) within the project "LCFA – Local charge flux analysis: a new scheme for the analysis of intermolecular interaction"*
SSD: CHIM/02
Advisor: Dr. Sergio Rampino
Co-advisor: Professor V. Barone

Research Fellow

Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna
[01/02/2023 – to present]
Address: Via F. Selmi 2, 40126 Bologna (Italy)
Topic*: Computational study of gas-phase reactivity in the interstellar medium (Duration: 2 years)*
SSD: CHIM/02
Advisor: Professor C. Puzzarini

LANGUAGE SKILLS

Mother tongue: **Italian**
Other languages: **English**

LISTENING	C2	**READING**	C2	**WRITING**	C1
ORAL PRODUCTION	C1	**ORAL INTERACTION**	C1		

DIGITAL SKILLS

Software
Software AutoCAD / Google suite (Gmail, Google Drive, Google Slide, Google Docs, Google Sheets, Google Forms, Google) / Office Suite

Quantum Mechanics Programs
High skill in the use of CFour and Gaussian16
Moderate ability to use MolPro, Turbomole, MESS, Automekin, Crest

Spectroscopy Programs
PGOPHER / SPFIT and SPCAT modules of H. Pickett / Virtual Multifrequency Spectrometer (VMS) - Comp and Rot modules

PUBLICATIONS (January 2024)

*Corresponding author; †Both authors contributed equally

1) S. Alessandrini and C. Puzzarini*, *Structural and Energetic Characterization of Prebiotic Molecules: The Case Study of Formamide and Its Dimer.* J. Phys. Chem. A, *120*, 5257 (2016).

2) S. Alessandrini, J. Gauss and C. Puzzarini*, *Accuracy of Rotational Parameters Predicted by HighLevel Quantum-Chemical Calculations: Case Study of Sulfur-Containing Molecules of Astrochemical Interest,* J, Chem. Theory Comput., *14,* 5360 (2018).

3) D. A. Obenchain, L. Spada, S. Alessandrini, S. Rampino, S. Herbers, N. Tasinato, M. Mendolicchio, P. Kraus, J. Gauss, C. Puzzarini, J. -U. Grabow*, V. Barone*, *Unveiling the Sulfur–Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond.* Angew. Chem. Int. ed., *57,* 15822 (2018).

4) J. Wang, L. Spada, J. Chen, S. Gao, S. Alessandrini, G. Feng*, C. Puzzarini*, Q. Gou*, J-U. Grabow, V. Barone*, *The Unexplored World of Cycloalkene–Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy*, Angew. Chem. Int. Ed., *58*, 13935 (2019).

5) S. Alessandrini*, V. Barone*, C. Puzzarini*, *Extension of the "Cheap" Composite Approach to Noncovalent Interactions: The jun-ChS Scheme*, J. Chem. Theory Comput., *16, 988* (2020).

6) S. Alessandrini*, V. Dell'Isola, L. Spada, V. Barone, C. Puzzarini*, *A Computational Journey in the CH2O2S Land: an Accurate Rotational and Ro-vibrational Analysis of the Sulfene Molecule and the O,S-and O,O-Monothiocarbonic Acids,* Mol. Phys., 118*, e1766707 (2020)*

7) C. Puzzarini*, L. Spada, S. Alessandrini, V. Barone, *The challenge of non-covalent interactions: theory meets experiment for reconciling accuracy and interpretation*, J. Phys. Condens. Matter, *32*, 343002 (2020)

8) J. Lei, S. Alessandrini, J. Chen, Y. Zheng, L. Spada*, Q. Gou*, C. Puzzarini, V. Barone*, *Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex,* 25, 4899 (2020)

9) S. Alessandrini*, F. Tonolo, C. Puzzarini, *In search of phosphorus in astronomical environments: The reaction between the CP radical (*X2Σ+*) and methanimine,* J. Chem. Phys.*, 154,* 054306 (2021)

10) V. Barone, S. Alessandrini, M. Biczysko, J. R. Cheeseman, D. C. Clary, A. B. McCoy, R. J. DiRisio, F. Neese, M. Melosso, C. Puzzarini*, *Computational molecular spectroscopy* Nat. Rev. Methods Primers, *1*, 38 (2021)

11) S. Alessandrini*, M. Melosso *Fate of the gas-phase reaction between oxirane and the CN radical in interstellar conditions,* Front. Astron. Space Sci., *8*, 159 (2021)

12) S. Alessandrini*, M. Melosso, N. Jiang, L. Bizzocchi, L. Dore, C. Puzzarini *Conformational stability of cyclopropanecarboxaldehyde is ruled by vibrational effects,* Mol. Phys., *119, e1955988* (2021)

13) J. Lupi†, S. Alessandrini†, C. Puzzarini*, V. Barone* junChS and junChS-F12 models: parameter-free efficient yet accurate composite schemes for energies and structures of non-covalent complexes*, J. Chem. Theory and Comput.,* 17*, 6974 (2021)*

14) L. Bizzocchi, S. Alessandrini, M. Melosso, V. M. Rivilla, C. Puzzarini* *Ab Initio Study of Fine and Hyperfine Interactions in Triplet POH,* Molecules, *27*, 302 (2022)

15) M. Melosso*, L. Bizzocchi, H. Gazzeh, F. Tonolo, J.-C. Guillemin, S. Alessandrini, V. M. Rivilla, L. Dore, V. Barone, C. Puzzarini*, *Gas-phase identification of (Z)-1,2-ethenediol, a key prebiotic intermediate in the formose reaction*, Chem. Commun., *58*, 2570 (2022)

16) X. Li, L. Spada, S. Alessandrini, Y. Zheng, K. G. Lengsfeld, J.-U. Grabow, G. Feng*, C. Puzzarini, V. Barone*, *Stacked but not Stuck: Unveiling the Role of π→π* Interactions with the Help of the Benzofuran–Formaldehyde Complex* Angew. Chem. Int. Ed., *61*, 264 (2022)

17) F. Tamassia*, L. Bizzocchi*, M. Melosso*, M. A. Martin-Drumel, O. Pirali, A. P. Charmet, E. Canè, L. Dore, I. E Gordon, J.-C. Guillemin, B. M. Giuliano, P. Caselli, S. Alessandrini, V. Barone, C. Puzzarini, *Synchrotron-based far-infrared spectroscopy of HC3N: Extended ro- vibrational analysis and new line list up to 3360 cm-1,* J. Quant. Spectrosc. Radiat., *279*, 108044 (2022)

18) N. Jiang, M. Melosso*, L. Bizzocchi, S. Alessandrini, J.-C. Guillemin, L. Dore, C. Puzzarini*, *Spectroscopic and Computational Characterization of 2-Aza-1,3-butadiene, a Molecule of Astrochemical Significance,* J. Phys. Chem. A, 126*, 1881 (2022)*

19) V. M. Rivilla*, L. Colzi, I. Jimenez-Serra, J. Martìn-Pintado, A. Megìas, M. Melosso, L. Bizzocchi, A. Lòpez-Gallifa, A. Martìnez-Henares, S. Massalkhi, B. Tercero, P. de Vicente, J.-C. Guillemin, J. G. de la Concepcion, F. Rico-Villas, S. Zeng, S. Martìn, M. A. Requena-Torres, F. Tonolo, S. Alessandrini, L. Dore, V. Barone, C. Puzzarini, *Precursors of the RNA-world in space: Detection of (Z)-1,2-ethene-diol in the interstellar medium, a key intermediate in sugar formation* , Astrophys. J. Lett., *929*, L11 (2022)

20) L. Bizzocchi*, S. Alessandrini*, M. Melosso*, C. Puzzarini*, *Dipolar spin-spin coupling as auxiliary tool for structure determination of small isolated molecules*. Phys. Chem. Chem. Phys., *24*, 15173 (2022)

21) A. Melli, M. Melosso*, L. Bizzocchi, S. Alessandrini, N. Jiang, F. Tonolo, S. Boi, G. Castellan, C. Sapienza, J-C. Guillemin, L. Dore, C. Puzzarini*, *Rotational Spectra of Unsaturated Carbon Chains Produced by Pyrolysis: The Case of Propadienone, Cyanovinylacetylene, and Allenylacetylene.*, J. Phys. Chem. A, *126,* 6210, (2022)

22) P. Recio†, S. Alessandrini†, G. Vanuzzo, G. Pannacci, A. Baggioli, D. Marchione, A. Caracciolo, V. J. Murray, P. Casavecchia, N. Balucani*, C. Cavallotti*, C. Puzzarini*, V. Barone*, Intersystem crossing in the entrance channel of the reaction of O (*3P) with pyridine, Nat. Chem.* 14*, 1405 (2022)*

23) H. Ye, S. Alessandrini, M. Melosso, C. Puzzarini*, *Exploiting the "Lego brick" approach to predict accurate molecular structures of PAHs and PANHs*, Phys. Chem. Chem. Phys., 24*, 23254 (2022)*

24) D. Alberton*, L. Bizzocchi, N. Jiang, M. Melosso, V. M. Rivilla, A. Pietropolli Charmet, B.M. Giuliano, P. Caselli, C. Puzzarini, S. Alessandrini, L. Dore, I. Jiménez-Serra, J. Martín-Pintado, *Laboratory spectroscopy of allylimine and tentative detection towards the G+0.693-0.027 molecular cloud,* Astron. Astrophys., *669*, A93 (2023)

25) N. Jiang, M. Melosso*, S. Alessandrini, L. Bizzocchi, M.A. Martin-Drumel, O. Pirali, C. Puzzarini*, *Insights into the molecular structure and infrared spectrum of the prebiotic species aminoacetonitrile,* Phys. Chem. Chem. Phys. *25*, 4754 (2023)

26) S. Alessandrini*, L. Bizzocchi, M. Melosso, C. Puzzarini, *Protonation of apolar species: From Cl2H+ to (E)-NCCHCHCNH+ through computational investigations*, Front. Astron. Space Sci., *10*, 1128896 (2023)

27) C. Puzzarini*, S. Alessandrini, L. Bizzocchi*, M. Melosso*, *Hunting for interstellar molecules: Rotational spectra of reactive species,* Faraday Discuss., 245, 309-326 (2023).

28) S. Alessandrini*, M. Melosso, V. M. Rivilla, L. Bizzocchi, C. Puzzarini*, *Computational Protocol for the Identification of Candidates for Radioastronomical Detection and Its Application to the C3H3NO Family of Isomers, Molecules*, 28*, 3226 (2023).*

29) H. Ye, S. Alessandrini*, C. Puzzarini*, *Gas-phase formation route for trans-HC(O)SH and its isomers under interstellar conditions: A state-of-the-art quantum-chemical study,* Mon. Notices Royal Soc., 525, 1158-1166 (2023)

30) C. Puzzarini*, S. Alessandrini, L. Bizzocchi, M. Melosso, *From the laboratory to the interstellar medium: A strategy to search for exotic molecules in space,* Front. Astron. Space Sci., *10*, 1211784 (2023)

31) M. Melosso*, S. Alessandrini, L. Spada*, A. Melli, X. Wang, Y. Zheng, C. Duan, J. Li, W. Du, Q. Gou*, L. Bizzocchi, L. Dore, V. Barone, C. Puzzarini, *Rotational spectra and semi-experimental structures of furonitrile and its water cluster,* Phys. Chem. Chem. Phys. *25*, 31281 (2023)

32) C. Puzzarini*, H. Ye, S. Alessandrini, *Isomerism of CH_2SO: Accurate structural, energetic, and spectroscopic characterization,* J. Comput. Chem., 1 (2024)

33) C. Puzzarini*, S. Alessandrini, Interstellar Ices: A Factory of the Origin-of-Life Molecules, ACS Cent. Sci. 10, 13 (2024)

34) H. Ye, S. Alessandrini*, C. Puzzarini*, *On the General Mechanism for the Gas-phase Reaction of Methanimine with a Radical Species in the Interstellar Medium: Some Failures and an Important Success*. Astrophys. J. *962, 32* (2024).

CONFERENCES

List of Conferences, Seminars and Schools (updated January 2024)

- Poster presentation at the congress "ERC AdG-Barone DREAMS: final meeting", Scuola Normale Superiore, Pisa, 29 November - 2 December 2017.
- Participation in the ASTRO-Winter Modeling congress "Advances in computational and experimental modeling: Application to Astrochemistry", University of Bologna, Bologna, 15-16 February 2018.

- Poster Presentation at AstrochemII – 2nd Italian Workshop on Astrochemistry "Chemical Evolution in our Galaxy: Spectroscopy, Observations and Reactivity", Follonica, 13-16 June 2018.
- Participation in the Summer School "Lake Como School of Advanced Studies - Computational Spectroscopy: Bridging Theory and Experiment", Lake Como, 9-14 September 2018.
- Participation with presentation of a poster at the Summer School "Modern Wavefunctions Methods in Electronic Structure Theory Summer School", Gelsenkirchen, 30 September - 5 October 2018.
- Invited oral contribution to "Winter Modeling 2019 - Special Edition on Valentine's Day", University of Naples Federico II, Naples, 14 February 2019. Title: "Benchmark of quantum-chemical computations for molecules containing second-row atoms."
- Oral contribution at the 4th COST- MOLIM General Meeting, University of Bologna, Bologna, 27 February – 1 March 2019
  Title: "Benchmark of quantum-chemical computations for molecules containing second-row atoms."
- Oral contribution to the conference "Young Reaserchers Meet Molecular Spectroscopy", Scuola Normale Superiore, Pisa, 4-5 April 2019. Title: "Benchmark of quantum-chemical computations for molecules containing second-row atoms."
- Oral contribution to the VI Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society (SCI), University of Calabria, Arcavacata di Rende, 19-20 September 2019. Title: "Noncovalent Interactions: an improved and affordable model chemistry."
- Invited oral contribution to the Virtual Symposium on Chemical Theory and Computation (VS-CTC) of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society (SCI), 21 December 2020. Title: "The junChS composite scheme: an affordable model chemistry for noncovalent interactions."
- Oral contribution in the section "Structure Determination" at the International Symposium on Molecular Spectroscopy, Online Meeting, 21-25 June 2021. Title: "The equilibrium structure of small radicals: the semi-experimental approach at work."
- Participation in the Astrochemical Frontiers 2021 online meeting, Online Meeting, 5-9 July 2021.
- Oral Contribution at the Merck Young Chemists' Symposium (MYCS) organized by the Youth Division of the Italian Chemical Society (SCI), Rimini, 22-24 November 2021. Title: "In search of P-bearing species in astronomical environments: the reaction between CH2NH and the CP radical."
- Oral contribution to "Winter Modeling 2022", University of Naples Federico II, Naples, 14-15 February 2022. Title: "Simulating the gas-phase reaction between oxirane and the CN radical in interstellar conditions."
- Oral contribution to "COSPAR 44th Scientific Assembly, Session F3.1", Athens, Greece 15-19 July 2022. Title: "Ab initio modeling of gas-phase reactions in the interstellar medium."
- Participation (with poster presentation) at the Winter School "Les Houches School of Physics, Laboratory Astrophysics", 5-10 February 2023, Les Houches, France.

- Oral contribution to "Ischia Summer Modeling: Challenges of Molecular Sciences Towards 2030", Ischia, 5-7 September 2022. Title: "Explicit Correlated F12 Composite Schemes for Noncovalent Systems: Interaction Energy and Geometry."
- Invited oral contribution to "Winter Modeling 2022(bis) - NAPLES: A very Special Edition in the Fall", Naples, 10-11 November 2022. Title: "Intersystem crossing in the entrance channel of the reaction between $O(^{3P})$ and pyridine."
- Invited oral contribution to "Winter Modeling 2023 – New frontiers in astrochemistry and astrobiology", Naples, 23-24 February 2023. Title: "Protonation of apolar species: from Cl2H+ to *E-NCCHCHCNH+.*"
- Oral contribution to the "New Methods for the Description of Non-Covalent Interactions - Online meeting of WG1 COSY", 23 May 2023. Title: Explicit correlated F12 composite schemes for noncovalent systems: interaction energy and geometry.
- Oral contribution to the "VII congress of the Italian Society of Astrobiology", Rome, 12-15 June 2023. Title: "In search of P-bearing species in astronomical environments: the reaction between methanimine and the CP radical".
- Oral Contribution to "The 11th OpenMolcas Developers' Workshop", Bologna, 14-16 June 2023. Title: "Explicit Correlated F12 Composite Schemes for Noncovalent Systems: Interaction Energy and Geometry."
- Oral contribution to the congress "The 28th Colloquium on High-Resolution Molecular Spectroscopy", Dijon 28 August-1 September 2023. Title: "Far-infrared spectrum of cyclohexane from soleil synchrotron source".
- Invited oral contribution to "25th International Conference on Horizons in Hydrogen Bond Research and Graduate Research Day (GRD)", Bologna, 11-15 September 2023. Title: "Ab initio modelling of noncovalent System in the gas-phase: Interaction Energy and Geometry."
- Oral contribution to the "Summer Modeling 2023" congress, Castiglione della Pescaia from 23-30 September 2023. Title: "Chemical Evolution of a Molecular Cloud – Step 3: Gas-Phase Reactivity"
- Oral contribution at the National Congress of Astrochemistry (Proto-)Planetaria, Trieste 11-14 September 2023. Title: "Gas-phase interstellar reactivity via computational methodologies"
- Participation in the VIII National Congress of the Division of Theoretical and Computational Chemistry of the SCI as winner of the "Giuseppe del Re" award with oral presentation. Scuola Normale Superiore, Pisa, 20-22 September 2023. Title: "Modelling weak interactions in the gas phase: from non-covalent bond to reactions rates"

SEMINAR AND SUPERVISION ACTIVITIES

Seminar in research group	UCL London's Global University, 23 September 2021	Seminar in the Trove/ExoMol group by Professor Sergei Yurchenko. Seminar title: "*Bites of Astrochemistry and the search for Phosphorus" (30min)*
Master's Thesis Tutor/Co-Supervisor	March 2021-December 2021	Master's Thesis by Giorgia Giusti, at the University of Bologna. Thesis title: "*Investigation of a surface of reactive potential energy of astrochemical interest: the reaction between oxirane and methylidene radical*"

Master's Thesis Tutor/Co-Supervisor	March 2021-October 2021	Master's Thesis by Mattia Ravasio, at the University of Milan Bicocca with internship at the University of Bologna. Thesis title: "*Quantum-chemical modelling of gas-phase reactions in the interstellar medium: the formation of glycolonitrile and methyl isocyanate*"
PhD Tutor	November 2021-present	I am currently supervising PhD student Hexu Ye at the University of Bologna.
Social Media Manager	October 2019 - present	I manage the Twitter account of the Rot&Comp group in Bologna, keeping the account updated with the latest publications of the group. Occasionally I have also managed Facebook and Twitter accounts of congresses, such as the 2022 Winter Modeling.

HONORS AND AWARDS

List of Awards won until January 2024

- Winner of a three-month Erasum Traineeship Scholarship for an internship at the University of Mainz, Germany.
- Winner of the best poster award at AstrochemII - 2 Italian Workshop on Astrochemistry "Chemical Evolution in our Galaxy: Spectroscopy, Observations and Reactivity", Follonica, 13 -16 June 2018
- Winner of the prize for the best publication in the field of methodological development of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society. October 2020.
- Finalist of the ChiMiCapire 2023 competition held on May 23, 2023 in Bari and organized by the Interdivisional Group by the Diffusion of the Chemical Culture of the SCI. Topic: Reactions in astrochemistry.
- Winner of the "Giuseppe del Re" prize for the best doctoral thesis in the field of theoretical and computational chemistry. Motivation "for the development of original models for the treatment of weak interactions and their effective application in the field of rotational spectroscopy and kinetics of reactions in the gas phase". The prize is awarded by the board of directors of the Theoretical and Computational Chemistry Division of the Italian Chemical Society. June 2023.

TEACHING ACTIVITY

Period of development *(start date and end date of activity)*	**Institution and State**	**Brief description of the teaching activity carried out**
from 01/09/2019 to 29/02/2020	University of Bologna, Italy	Laboratory Assistant of the course of "Computational Spectroscopy" of the master's degree "Photochemistry and Molecular Materials" for the year 2019/2020 (2h) CHIM/02
from 01/03/2020 to 31/08/2020	University of Bologna, Italy	Laboratory Assistant of the course of "Thermodynamics and Molecular Modeling" of the master's degree in "Chemistry" for the year 2019/2020 (6h) CHIM/02
from 01/09/2020 to 28/02/2021	University of Bologna, Italy	Laboratory Assistant of the course of "Computational Spectroscopy" of the master's degree "Photochemistry and Molecular Materials" for the year 2020/2021 (4h) CHIM/02
from 19/04/2021 to 30/04/2022	University of Bologna, Italy	Tutor activity for module 2 of the course "Spectroscopic Methods" of the bachelor's degree in "Chemistry and Chemistry of Materials" for the year 2020/2021 (32h) CHIM/02

from 01/03/2021 to 31/08/2021	University of Bologna, Italy	Laboratory Assistant of the course of "Thermodynamics and Molecular Modeling" of the master's degree in "Chemistry" for the year 2020/2021 (12h) CHIM/02
from 01/09/2021 to 28/02/2022	University of Bologna, Italy	Laboratory Assistant of the course of "Computational Spectroscopy" of the master's degree "Photochemistry and Molecular Materials" for the year 2021/2022 (2h) CHIM/02
from 16/02/2022 to 16/02/2022	Southern School of Advanced Studies, University of Naples Federico II, Italy	2h lecture on non-covalent systems for the first year of the PhD course in "Molecular Sciences for Earth and Space" (MOSES) of the Southern School of Advanced Studies
from 04/04/2022 to 22/04/2022	University of Bologna, Italy	Tutor activity for module 2 of the course "Spectroscopic Methods" of the bachelor's degree in "Chemistry and Chemistry of Materials" for the year 2021/2022 (32h) CHIM/02
from 23/05/2022 to 27/05/2022	University of Bologna, Italy	Tutor for the course "Thermodynamics and Molecular Modelling" of the master's degree in "Chemistry" for the year 2021/2022 (16h CHIM/02
From 28/11/2022 to 30/11/2022	University of Bologna, Italy	Tutor for the course "Chemical Properties from High Resolution Spectroscopy" of the master's degree in "Chemistry" for the year 2022/2023 (12h) CHIM/02
From 16/05/2023 to 19/05/2023	University of Bologna, Italy	Tutor for the course "Thermodynamics and Molecular Modelling" of the master's degree in "Chemistry" for the year 2021/2022 (16h) CHIM/02
From 14/11/2023 to 17/11/2023	University of Bologna, Italy	Tutor for the course "Chemical Properties from High Resolution Spectroscopy" of the master's degree in "Chemistry" for the year 2022/2024 (12h) CHIM/02

As a didactic tutor of the course in "Spectroscopic Methods" I learned to independently use Fourier transform IR instruments (FT-IR), UV-Vis and Raman spectrophotometers, together with their respective software.
For the courses of "Thermodynamics and Molecular Modeling" and "Computational Spectroscopy" I developed, in collaboration with Professor C. Puzzarini, exercises and tutorials of the various programs used during the laboratory. Lectures and exercises were held in English for the course of "Photochemistry and Molecular Materials". In 2023/2024, I developed the laboratory experiences for the "Astrobiology" course of the degree in "Photochemistry and Molecular Materials", participating as a volunteer teaching support to the entire computer laboratory.

EXPERIENCES ABROAD AND IN OTHER RESEARCH GROUPS

Three-month internship at Johannes Gutenberg University Mainz, Germany

[06/03/2017 – 06/06/2017]

I did my internship in the theoretical chemistry group of Professor Juergen Gauss thanks to an Erasum Traineeship scholarship (3 months, 6/03/2017-6/06/2017)

Three-month internship at the University of Oxford

[01/07/2021 – 01/10/2021]

Three-month internship for the recognition of the "Doctor Europaeus" certification upon completion of the Italian doctorate. The internship was carried out at the chemistry theory group of Professor David Tew, University of Oxford, UK.

Principal investigator at AILES-A-High Resolution Interferometer

[20/11/2022 – 24/11/2022]

Principal investigator for the project "*From the chair to the boat -- a twisting journey in the conformational land of cyclohexane via ro-vibrational analysis of its excited vibrational states*", held at the soleil synchrotron in Paris in collaboration with the RotComp group of the University of Bologna and the rotational spectroscopy group of the Institut des Sciences Moléculaires d'Orsay (ISMO).

Visiting Post-Doc at Politecnico di Milano

[27/11/2023 – 13/12/2023]

Research period at the group of Professor C. Cavallotti at the Politecnico di Milano to learn the use of the EStokTP program, which is developed by the PoliMI research group.

RESEARCH AND EDITORIAL ACTIVITIES

Research and Editorial Activities in January 2024

Citation Statistics as of July 2023 (SCOPUS)

H-index: 12
Publications: 32, 12 as first author
Citations: 447

Citation Statistics as of January 2024 (Google Scholar)

H-index: 11
Publications: 33, 12 as first author
Citations: 585

Research activities

My research activity is focused on the development and application of very accurate computational methods for the description of small-medium sized molecular systems, whether isolated species or non-covalently linked bi-molecular complexes. The final goal of these analyses is to have an accurate energetic characterization of the species considered and, possibly, their spectroscopic characterization. The latter is mainly focused on obtaining *ab intio* rotational and vibro-rotational spectra for stable and transient species, such as radicals or ions, but also on reactive species such as enolates 1,2 and 1,1 or imines. Energy considerations, on the other hand, can be used for the study of potential energy surfaces (PES) that I use in astrochemistry. In the latter field, the study may involve families of structural isomers or the analysis of portions of reactive potential energy surfaces, where various reaction paths accessible in the conditions of the interstellar medium can be investigated. In these cases, an accurate energetic characterization is essential to have an accurate estimate of the reaction barriers that can strongly influence the final products of the reaction. The accuracy of these energy barriers is obtained in my work thanks to the application of composite schemes, where numerous energy contributions are calculated at the best possible theoretical level considering the size of the system under consideration. When the reaction paths are well computationally characterized, the next step is to derive the kinetic constants of the reaction, which determine the eventual formation of the product of interest and any co-products, under the conditions of the interstellar medium. Considering the time scale in astronomy, kinetic constants are already significant if their value is around $10\text{-}16^{/10\text{-}15}$ cm3 molecule-1 $^{s\text{-}1}$.

Publishing activity

Top Coordinator of the Research Topic *"Chemical Evolution Across Space: the PAH connection from Interstellar Molecules to Prebiotic Processes and Beyond"* for the journals "Frontiers in Astronomy and Space Sciences" (Astrochemistry and Astrobiology Sections) and "Frontiers in Chemistry" (Astrochemistry Section)
Editor: Prof. V. Barone, Prof. M. d'Ischia

Guest Editor together with Professor C. Puzzarini of the Special Issue "Spectroscopic and Theoretical Methods to investigate Interstellar Medium" of the journal Molecules, section "Applied Chemistry". Link: https://www.mdpi.com/journal/molecules/special_issues/B75FD21NLF

Reviewer for journals in the physicochemical field, such as Frontiers in Astronomy and Space Sciences, Journal of Physical Chemistry, ACS Earth and Space Sciences, and Publications of the Astronomical Society of Australia, International Journal of Quantum Chemistry.

DRIVER'S LICENSE

Driver's license: B and A

I authorize the processing of my personal data pursuant to D.L. 196/2003
Bologna, 20/02/2024