FEDERICO LAZZARI

PROFESSIONAL SUMMARY

Highly experienced postdoctoral researcher with a robust academic background in chemistry and a strong foundation in software development, specifically C++, python and AR/VR development. My research interests focus on the application of computational techniques, algorithm development, and mathematical modeling to understand and simulate natural phenomena, driving my passion for physical chemistry. I am deeply intrigued by the potential of emerging technologies, including machine learning and mixed reality, to push the boundaries of scientific discovery, with a particular focus on the interdisciplinary fusion of science, cultural heritage, and liberal arts. I am a firm believer in the power of multidisciplinary approaches and collaborative teamwork as essential components in solving complex scientific problems. I am equally passionate about public speaking and education, valuing the exchange of ideas as a means to sustain and evolve knowledge.

RESEARCH EXPERIENCE

- VISITING SCIENTIST - SCUOLA NORMALE SUPERIORE (PISA) - 01/03/2025 -
- RESEARCH FELLOW - SCUOLA SUPERIORE MERIDIONALE (NAPLES) - 01/03/2025

The project aims to build chemically interpretable, continuous feature spaces that capture key topological and electronic characteristics of molecules—first for main-group elements and then for transition-metal centers—to power Δ-machine-learning models that refine low-level quantum-chemical calculations into high-accuracy predictions. These descriptors will enable accurate identification of conformers and transition states on potential-energy surfaces, bridging the gap between physical interpretability and ML efficiency even when molecular bonding patterns change during reactions. Extending the framework to metals will incorporate factors such as crystal-field splitting and spin states, while a reactive variant will treat evolving "atom types" as trajectories through feature space, allowing force-field-level molecular dynamics with ab-initio quality. The project will also develop ML-driven exploration tools—ranging from genetic algorithms to stable-diffusion-based generative models—to map energy minima and higher-order saddle points, and will pair these capabilities with immersive VR/AR visualizations that help researchers intuitively navigate both hypersurfaces and feature spaces. The ultimate deliverable is robust, user-friendly software that accelerates spectroscopy, thermochemistry, and kinetics studies across diverse chemical systems.

- RESEARCH FELLOW - SCUOLA NORMALE SUPERIORE (PISA) - 01/03/2023 - 01/03/2025

The primary focus of my research has been on Molecular Perception (MP), an emerging field that develops methods and algorithms to describe chemical systems from minimal information, such as nuclear coordinates. The goal was to create heuristic-based descriptors for building robust Feature Spaces applicable in Machine Learning (ML). A key achievement has been the development of a continuous atomic type, a novel feature space representation for clustering similar atoms in chemical systems. This approach, as published, offers a more precise tool for understanding atomic similarities and behaviors in complex systems. The automatic perception of these molecular properties is also crucial for data pre- and post-processing and visualization. Another significant result is the development of web tools for composite schemes applied to molecular geometries (the PCS/Bonds tool), which provide interactive graphical interfaces, making them accessible even to non-experts. These tools also support Virtual Reality (VR) and Augmented Reality (AR) platforms via WebXR, simplifying data interpretation and enhancing usability.

- VISITING SCIENTIST - GAUSSIAN, INC. - WALLINGFORD (CT) - 15/01/2024 - 06/02/2024

Visiting Scientist at Gaussian Inc. collaborating on the development of a C++ version of the Gauopen tool.

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EDUCATION

- SCUOLA NORMALE SUPERIORE (PISA), PHD - 01/11/2018 - 31/01/2023

Ph.D. in Methods and Models for Molecular Sciences, *cum laude*. (15/09/2023)

As an extension of my undergraduate and master's work on *Molecular Perception*, my PhD focused on developing *Proxima*, a C++ software with Python bindings, designed to automate the perception of molecular features. The software computes key topological descriptors, including atomic charges, continuous bond orders, and ring structures, directly from Cartesian coordinates (XYZ). The goal was to create a system that could link microscopic molecular data with interpretable chemical features for use in machine learning and computational chemistry. This allowed for efficient, automated analysis of molecular systems, enhancing the accuracy of predictive models while preserving chemical meaning.

- SCUOLA NORMALE SUPERIORE (PISA), DIPLOMA OF STUDENT - 01/10/2013 - 01/03/2019

Awarded for completion of the prestigious higher education program, with a focus on advanced research and academic excellence.

- UNIVERSITY OF PISA, MASTER'S DEGREE IN CHEMISTRY, PHYSICAL CHEMISTRY TRACK - 23/12/2016 - 26/10/2018

Graduated with 110/110 *cum laude*.

- UNIVERSITY OF PISA, BACHELOR'S DEGREE IN CHEMISTRY - 20/09/2013 - 20/12/2016

Graduated with 110/110 *cum laude*.

CONFERENCES AND PRESENTATIONS

- STSM (COSY NETWORK) (WROCŁAW, PL.) 06/10/2025 - 23/10/2025.

Short-Term Scientific Mission (STSM, COSY network) at the University of Wrocław (Prof. Małgorzata Biczysko) entitled: "Toward a Unified Platform for High-Accuracy Molecular Geometry and Spectral Prediction".

- STC (BERLIN, DE) 20/09/2025 - 27/09/2025.

Attending the 61st Theoretical Chemistry Symposium with a 15-minute oral presentation

- ICCS (NOORDWIJKERHOUT, NL.) 01/06/2025 - 06/06/2025

Participation in the ICCS international conference on chemical structure (https://iccs-nl.org) was accompanied by the presentation of a poster.

- TEACHING ACTIVITY - SCUOLA SUPERIORE MERIDIONALE (NAPLES) - 2025

Taught chemical kinetics within the "Complements of Chemistry II" course to second-year students at the Scuola Superiore Meridionale.

- PEER REVIEWER ACTIVITY - 2025
- GUEST LECTURER - WINTER MODELING 2025 (NAPLES)

Guest Lecturer with a presentation on the refinement of molecular geometries through custom-designed feature spaces for atoms and bonds in molecules.

- ATTENDANT - QUANTUM CHEMISTRY AND CHEMINFORMATICS - ACCADEMIA NAZIONALE DEI LINCEI (ROMA) - 2024

Participant at a workshop organised in Rome by Accademia dei Lincei on Quantum Chemistry and Cheminformatics.

- GUEST LECTURER - MOLECULAR ELECTRONIC STRUCTURE (MES) - PESCARA - 2024

Guest Lecturer with a presentation on the refinement of molecular geometries through correction of geomerical parameters such as covalent bond lengths.

- ORGANIZING COMMITTEE AND ORAL SPEAKER - SUMMER MODELING - CASTIGLIONE DELLA PESCAIA - 2024

With an contribution titled: *Quantum Chemistry Meets Machine Learning for Accurate Molecular Structures*

- GUEST LECTURER - SOCIETÀ CHIMICA ITALIANA (SCI) - MILANO - 2024

Invited talk in parallel sessions titled: *The Virtual Laboratory Framework: Blending Computation, Representation and Visualization from Quantum Chemistry, through Machine-Learning, to Virtual Reality*.

- PEER REVIEWER ACTIVITY - 2024
- SEMINAR SPEAKER - SCUOLA SUPERIORE MERIDIONALE - NAPOLI - 2024

Presentation of a seminar as part of the MOSES PhD cycle at the Scuola Superiore Meridionale titled: From Perception, through Computation, to Interpretation: The Virtual Laboratory.

- PEER REVIEWER ACTIVITY - 2023
- POSTER PRESENTATION AND CHAIRPERSON - DCTC - PISA - 2023

Poster presentation of an interactive website capable of refining molecular geometries at the VIII National Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society (SCI).

- SCIENTIFIC COMMITTEE AND ORAL SPEAKER - SUMMER MODELING - CASTIGLIONE DELLA PESCAIA - 2023

Oral contribution titled: *The construction of chemically based feature spaces for Machine-Learning: The Synthon.*

- GUEST LECTURER - ACCADEMIA DELLE SCIENZE DELL'ISTITUTO DI BOLOGNA - 2023

Oral contribution titled:: *La ricerca dei mattoni della vita con l'aiuto di teoria, esperimenti e realtà virtuale*.

- SEMINAR SPEAKER - SCUOLA SUPERIORE MERIDIONALE - NAPOLI - 2022

Speaker at the seminars dedicated to the 1st year MOSES PhD students, 38th Cycle, that are part of the Astrochemistry Course, introducing the most recent advancements in Molecular Perception.

- GUEST LECTURER - WINTER MODELING (BIS) - NAPLES - 2022

Speaker at the 2022 second edition of the Winter Modeling workshop in Naples detailing the role of Virtual Reality together with Molecular Perception and Machine-Learning in building the Virtual Laboratory.

- GUEST LECTURER - WINTER MODELING - NAPLES - 2022

Speaker at the Winter Modeling workshop in Naples introducing the research work on Molecular Perception (MP).

- GUEST LECTURER - TUMA - ANCONA - 2019

Speaker at the TUMA convention (XXXVI Convegno Interregionale Tosco Umbro Marchigiano Abruzzese) introducing the work on Molecular Perception.

- ATTENDANT - CECAM-IT-SISSA-SNS WORKSHOP - PISA - 2018

An attendant of the Emerging Technologies in Scientific Data Visualization workshop where new technologies were investigated for better scientific data representations.

- GUEST LECTURER - SENATO DELLA REPUBBLICA (ROMA) - 2017

Speaker at Senato della Repubblica, Roma for a presentation of the Scuola Normale Superiore to new generations of students (Le scuole di eccellenza si raccontano).

- GUEST LECTURER - CORTONA - 2017

Speaker at a presentation event in Cortona on behalf of Scuola Normale for a presentation of the school to new generations of students.

PUBLICATIONS

1. Lazzari, F.; Crisci, L.; Barone, V.
   From molecular bricks to sustainable nanomaterials: an accurate and scalable unsupervised workflow. Small Structures2025.

2. Lazzari, F.*; Crisci, L.; Barone, V.
   High-fidelity ring fragments for molecular design and spectroscopy: the PCS–LCB25–Nano-LEGO framework. Journal of Chemical Theory and Computation 2025, 21, 10617–10632.

3. Lazzari, F.; Uribe, L.; Di Grande, S.; Crisci, L.; Mendolicchio, M.; Barone, V.
   Structures and rotational constants of monocyclic monoterpenes at DFT cost by Pisa composite schemes and vibrational perturbation theory. Journal of Physical Chemistry A 2025, 129, 503–517.

4. Lazzari, F.*; Crisci, L.; Di Grande, S.; Barone, V.
   Cost-effective accuracy in molecular structures via smart databases, topological features, and random forests. Journal of Chemical Theory and Computation 2025, 21, 10633–10644.

5. Lazzari, F.; Di Grande, S.; Crisci, L.; Mendolicchio, M.; Barone, V.
   Molecular structures with spectroscopic accuracy at DFT cost by the templating synthon approach and the PCS141 database. Journal of Chemical Physics 2025, 162, 114310.

6. Barone, V.; Lazzari, F.; Di Grande, S.
   Accurate structures and spectroscopic parameters of CN-substituted polycyclic hydrocarbons at DFT cost. Journal of Physical Chemistry A 2025, 129, 2876–2886.

7. Crisci, L.; Lazzari, F.; Barone, V.
   Composite gradient schemes for accurate molecular geometries: a flexible interface and hierarchical optimization workflow. Journal of Physical Chemistry Letters 2025, 7376–7382.

8. Crisci, L.; Lazzari, F.; Barone, V.
   Accurate yet affordable: an integrated tool for the simulation of Criegee intermediates via Pisa composite schemes and localized corrections. Journal of Chemical Theory and Computation 2025, 21, 7188–7197.

9. Barone, V.; Lazzari, F.; Di Grande, S.; Crisci, L.
   Accurate structures and rotational constants of nitroaromatic explosives and their taggants at DFT cost by Pisa composite schemes and vibrational perturbation theory. Chemical Physics Letters 2025, 866, 141956.

10. Crisci, L.; Lazzari, F.; Barone, V.
    Accurate, affordable, and unsupervised: analytical F12 gradients driven by generalized internal coordinates. Journal of Physical Chemistry Letters 2025, 16, 9985–9992.

11. Crisci, L.; Lazzari, F.*; Barone, V.
    Pushing the boundaries of spectroscopic accuracy: from small sheet to large bowl models of graphene. Journal of Physical Chemistry A 2025, 129, 10529–10539.

12. Di Fiore, L.; Crisci, L.; Lazzari, F.; Barone, V.
    Intramolecular hydrogen bonds and proton transfer: quantum-chemical benchmarks for structural and energetic properties. Journal of Physical Chemistry A 2025, 129, 9011–9018.

13. Di Fiore, L.; Crisci, L.; Lazzari, F.; Mendolicchio, M.; Barone, V.
    Benchmark equilibrium structures of nucleobase tautomers validated against experimental rotational constants. Journal of Physical Chemistry A 2025, 129, 9217–9226.

14. Crisci, L.; Lazzari, F.*; Di Fiore, L.; Mendolicchio, M.; Barone, V.
Canonical and rare tautomers of nucleobases and their taggants in the gas phase: a benchmark computational study. Journal of Physical Chemistry A 2025, 129, 10751–10761.

15. Mendolicchio, M.; Uribe, L.; Lazzari, F.; Crisci, L.; Scalmani, G.; Frisch, M. J.; Barone, V.
Computational efficiency meets spectroscopic accuracy: an unsupervised workflow for equilibrium geometries and vibrational effects in gas-phase prebiotic molecules. Physical Chemistry Chemical Physics 2025, 27, 16383–16397.

16. Barone, V.; Crisci, L.; Lazzari, F.
The road to affordable accuracy beyond small molecules: from energetics toward molecular structures. Accounts of Chemical Research, in press.

17. Lazzari, F.*; Crisci, L.; Mendolicchio, M.; Barone, V.
Toward circular astrochemistry: simulated spectral fingerprints of phenalene and isomeric dihydronaphthalenes for guiding and interpreting laboratory and astronomical observations. ACS Earth and Space Chemistry, under review.

18. Barone, V.; Crisci, L.; Di Grande, S.; Lazzari, F.; Mendolicchio, M.; Uribe, L.
Mechanical and electrical anharmonicity in the infrared spectra of graphene fragments: from planar polycyclic aromatic hydrocarbons to buckybowls. Journal of Chemical Physics, submitted.

19. Crisci, L.; Lazzari, F.; Barone, V.
Accurate and affordable equilibrium geometries of organic radicals enabled by local explicit correlation and embarrassingly parallel numerical gradients. Journal of Physical Chemistry Letters, submitted.

20. Barone, V.; Lazzari, F.; Mendolicchio, M.
Accurate and affordable vibrational spectra of large molecules: primary, auxiliary, and spectator modes in a perturb-then-diagonalize framework. Journal of Chemical Theory and Computation, submitted.

21. Di Grande, S.; Lazzari, F.; Barone, V.
Accurate geometries of large molecules at DFT cost by semiexperimental and coupled-cluster templating fragments. Journal of Chemical Theory and Computation 2024. DOI: 10.1021/acs.jctc.4c00900.

22. Uribe, L.; Lazzari, F.; Di Grande, S.; Crisci, L.; Mendolicchio, M.; Barone, V.
Accurate structures and rotational constants of bicyclic monoterpenes at DFT cost by means of the bond-corrected Pisa composite scheme (BPCS). Journal of Chemical Physics 2024, 161, 014307. DOI: 10.1063/5.0216384.

23. Uribe, L.; Di Grande, S.; Crisci, L.; Lazzari, F.; Mendolicchio, M.; Barone, V.
Accurate structures and rotational constants of steroid hormones at DFT cost. Journal of Physical Chemistry A 2024, 128, 2629–2642. DOI: 10.1021/acs.jpca.4c00573.

24. Lazzari, F.; Mendolicchio, M.; Barone, V.
Accurate geometries of large molecules by integration of the Pisa composite scheme and the templating synthon approach. Journal of Physical Chemistry A 2024, 128, 1385–1395. DOI: 10.1021/acs.jpca.3c08382.

25. Barone, V.; Lazzari, F.
Hunting for complex organic molecules in the interstellar medium: the role of accurate low-cost theoretical geometries and rotational constants. Journal of Physical Chemistry A 2023, 127, 10517–10527. DOI: 10.1021/acs.jpca.3c06649.

26. Barone, V.; Uribe Grajales, L. M.; Di Grande, S.; Lazzari, F.; Mendolicchio, M.
DFT meets wave-function methods for accurate structures and rotational constants of histidine, tryptophan, and proline. Journal of Physical Chemistry A 2023, 127, 7534–7543. DOI: 10.1021/acs.jpca.3c04227.

27. Barone, V.; Di Grande, S.; Lazzari, F.; Mendolicchio, M.
Accurate structures and spectroscopic parameters of guanine tautomers in the gas phase by the Pisa composite schemes. Journal of Physical Chemistry A 2023, 127, 6771–6778. DOI: 10.1021/acs.jpca.3c03999.

28. Barone, V.; Ceselin, G.; Lazzari, F.; Tasinato, N.
Toward spectroscopic accuracy for the structures of large molecules at DFT cost: refinement and extension of the Nano-LEGO approach. Journal of Physical Chemistry A 2023, 127, 5183–5192. DOI: 10.1021/acs.jpca.3c01617.

29. Barone, V.; Fusè, M.; Aguado, R.; et al.
Bringing machine-learning-enhanced quantum chemistry and microwave spectroscopy to conformational landscape exploration: the case of 4-fluoro-threonine. Chemistry – A European Journal 2023, 29, e202203990. DOI: 10.1002/chem.202203990.

30. Barone, V.; Fusè, M.; Lazzari, F.; Mancini, G.
Benchmark structures and conformational landscapes of amino acids in the gas phase. Journal of Chemical Theory and Computation 2023, 19, 1243–1260. DOI: 10.1021/acs.jctc.2c01143.

31. Mancini, G.; Fusè, M.; Lazzari, F.; Barone, V.
Fast exploration of potential-energy surfaces with a joint venture of quantum chemistry, evolutionary algorithms, and unsupervised learning. Digital Discovery 2022, 1, 790–805. DOI: 10.1039/d2dd00070a.

32. Albertini, N.; Baldini, J.; Dal Pino, A.; et al.
PROTEUS: an immersive tool for exploring cultural heritage across space and time scales. Heritage Science 2022, 10, 71. DOI: 10.1186/s40494-022-00708-3.

33. Falbo, E.; Fusè, M.; Lazzari, F.; Mancini, G.; Barone, V.
Integration of quantum chemistry, statistical mechanics, and artificial intelligence for computational spectroscopy. Journal of Chemical Theory and Computation 2022, 18, 6203–6216. DOI: 10.1021/acs.jctc.2c00654.

34. Mancini, G.; Fusè, M.; Lazzari, F.; Chandramouli, B.; Barone, V.
Unsupervised search of low-lying conformers with spectroscopic accuracy. Journal of Chemical Physics 2020, 153, 124110. DOI: 10.1063/5.0018314.

35. Lazzari, F.; Salvadori, A.; Mancini, G.; Barone, V.
Molecular perception for visualization and computation: the Proxima library. Journal of Chemical Information and Modeling 2020, 60, 2668–2672. DOI: 10.1021/acs.jcim.0c00076.

36. Martino, M.; Salvadori, A.; Lazzari, F.; et al.
Chemical promenades: exploring potential-energy surfaces with immersive virtual reality. Journal of Computational Chemistry 2020, 41, 1310–1323. DOI: 10.1002/jcc.26172.

LANGUAGE SKILLS

Italian (native), English (proficient), French (pre-intermediate)

SOFTWARE DEVELOPMENT SKILLS

C++, Fortran, Python, Cython, Swift, C#, C, Javascript, HTML, LaTex, Unity, Blender (basic skills of 3D modeling, fluid and particle simulation), WebGL, WebXR (Web API for the development of VR and AR applications for the browser), Metal (Apple low-overhead API for rich shading language for Apple Silicon GPU), ARKit (Apple API for developing augmented reality applications), SwiftUI (Apple API for developing graphical user interfaces that can be used on major apple platforms from watchOS and iOS/iPadOS to macOS), CreateML/CoreML (Apple API for Machine-Learning algorithms that make use of the neural engine component of apple silicon to run more efficiently), TensorFlow, scikit-learn. Experience in developing VR applications for Oculus VR headsets using the Unity software.

SCIENTIFIC SKILLS

Chemistry, Quantum Chemistry, Computational Chemistry, Molecular Perception, Physical Chemistry, Graph Theory, Statistics and Probability, Cheminformatics, Mathematical Modeling, Data Analysis, Machine-Learning.

PERSONAL SKILLS

Public speaking, problem solving, presentation skills, team work, creative thinking, giving and receiving feedbacks efficiently, self-awareness, avid-learner

Date

Signature