

CV - Luigi Crisci

Personal Information

Born on July 29, 1995. Italian Citizen.

Scuola Superiore Meridionale

Ph. D. in Astrochemistry

Largo S. Marcellino, 10, 80138 Napoli NA

e-mail (work): l.crisci@ssmeridionale.it

ORCID: 0000-0002-8140-5397

Education

02/2025-present	POST DOCTORAL position at Scuola Superiore Meridionale. Advisors Professor Vincenzo Barone and Professor Nicola Tasinato
11/2020-01/2025	PH.D. cum laude in Astrochemistry, Scuola Normale Superiore di Pisa. Advisors Professor Nicola Tasinato and Vincenzo Barone
10/2020	M. SC. cum laude in Chemical Sciences, Università di Napoli <i>Federico II</i> . <i>Dissertation</i> : Photophysics of Tetracene derivatives in monomeric and dimeric forms through ab-initio methods. Advisor Professor Nadia Rega and Dr. Alessio Petrone
07/2018	B. SC. cum laude in Chemistry, Università di Napoli <i>Federico II</i> . <i>Dissertation</i> : Tuning the dispersion correction in DFT-D for metal molecule interfaces. Advisor Professor Michele Pavone and Professor Ana Belen Muñoz-García

Research Interests

- Theoretical and computational chemistry. Single- and multireference electronic structure theory
- Modeling reactions of astrochemical interest
- Monte Carlo sampling
- Theoretical characterization and methodology development for gas-phase barrierless reactions
- *Ab-Initio* molecular dynamics simulations. Hybrid methods (QM/MM), non-periodic boundary conditions (non-PBCs)

Ph.D. Advanced Courses

- Astrochemistry and Molecular Astrophysics - Prof. Vincenzo Barone, SNS, and Prof. Cristina Puzzarini, UNIBO
- Scientific Programming I: Data Processing and Software Prototyping - Prof. Julien Bloino, SNS
- Computational Spectroscopy - Prof. Nicola Tasinato, SNS
- Scientific Programming II: High Performance Computing - Prof. Julien Bloino, SNS

Teaching Activities

2025	TEACHING Complementi di Chimica II class, Scuola Superiore Meridionale, Napoli, Italy.
12/2022	Seminary by title "Astrochemistry: spectroscopy and kinetics", organized by Scuola Superiore Meridionale
03/2022	Seminary by title "Reattività e cinetica", organized by Scuola Superiore Meridionale

Tutoring and Mentoring Activities

2025	MASTER'S THESIS SUPERVISION - Luca Di Fiore, Università di Pisa, Pisa, Italy. Research projects combining methodological development with applications to biological systems. This mentoring activity resulted in the publication of three peer-reviewed articles. Thesis defense expected: February 2026.
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Honors and Awards

2024	Winner of 1000 Fellowships Programme of Società Chimica Italiana
2023	Winner of fellowship COST Action: CA18212 MD-GAS
2020-present	MIUR (Italian Ministry of Education, University and Research) national scholarship for the Ph.D. program in Astrochemistry

Training experiences

2024	Developer training at Gaussian, Inc. - 340 Quinnpiac St Bldg 40 Wallingford, CT 06492 USA
2022	Internal Training at Professor Carlo Cavallotti's Laboratory

Publication List,(*, Corresponding author)

- 2025 26. **L. Crisci**, M. K'allay, V. Barone, J. Phys. Chem. Lett. <https://doi.org/10.1021/acs.jpcclett.5c03312>
- 2025 25. S. Srivastav, V. Barone, A. Vats, A. Pandey, **L. Crisci**, S. Mishra, A. Pathak, L. Majumdar Mon. Not. R. Astron. Soc. <https://doi.org/10.1093/mnras/staf1932>
- 2025 24. L. Uribe, S. Mato, **L. Crisci**, S. Municio, E. R. Alonso, J. L. Alonso, I. León, V. Barone, Spectrochim. Acta A Mol. Biomol. Spectrosc. (2025) <https://doi.org/10.1016/j.saa.2025.127250>
- 2025 23. F. Lazzari, **L. Crisci***, V. Barone, Small Structures (2025) <https://onlinelibrary.wiley.com/doi/10.1002/ssstr.202500557>
- 2025 22. **L. Crisci**, F. Lazzari, V. Barone, J. Phys. Chem. A (2025) <https://pubs.acs.org/doi/full/10.1021/acs.jpca.5c06530>
- 2025 21. F. Lazzari, **L. Crisci**, S. Di Grande, V. Barone, J. Chem. Theory Comput. (2025). <https://pubs.acs.org/doi/full/10.1021/acs.jctc.5c01428>
- 2025 20. **L. Crisci**, F. Lazzari, L. Di Fiore, M. Mendolicchio, V. Barone, J. Phys. Chem. A (2025) <https://doi.org/10.1021/acs.jpca.5c07251>
- 2025 19. F. Lazzari, **L. Crisci**, V. Barone, J. Chem. Theory Comput. (2025). <https://pubs.acs.org/doi/full/10.1021/acs.jctc.5c01188>
- 2025 18. L. Di Fiore, **L. Crisci***, F. Lazzari, and V. Barone, J. Phys. Chem. A, (2025). <https://pubs.acs.org/doi/full/10.1021/acs.jpca.5c04369>
- 2025 17. L. Di Fiore, **L. Crisci***, F. Lazzari, and V. Barone, J. Phys. Chem. A (2025). <https://doi.org/10.1021/acs.jpca.5c05292>
- 2025 16. **L. Crisci***, F. Lazzari, and V. Barone, J. Phys. Chem. Lett. (2025). <https://pubs.acs.org/doi/full/10.1021/acs.jpcclett.5c02292>
- 2025 15. **L. Crisci***, F. Lazzari, and V. Barone, J. Chem. Theory Comput (2025). <https://doi.org/10.1021/acs.jctc.5c00797>
- 2025 14. **L. Crisci***, F. Lazzari, and V. Barone, J. Phys. Chem. Lett. (2025). <https://doi.org/10.1021/acs.jpcclett.5c01823>
- 2025 13. M. Mendolicchio, L. Uribe, F. Lazzari, **L. Crisci**, G. Scalmani, M.J. Frisch, and V. Barone, Phys. Chem. Chem. Phys. (2025). <https://doi.org/10.1039/d5cp01611h>
- 2025 12. F. Lazzari, S. Di Grande, **L. Crisci**, M. Mendolicchio, and V. Barone, J. Chem. Phys. (2025). <https://doi.org/10.1063/5.0255564>
- 2025 11. F. Lazzari, L. Uribe, S. Di Grande, **L. Crisci**, M. Mendolicchio, and V. Barone, J. Phys. Chem. A (2025). <https://doi.org/10.1021/acs.jpca.4c07181>
- 2025 10. V. Barone, F. Lazzari, S. Di Grande, **L. Crisci** Chem. Phys. Lett. (2025). <https://doi.org/10.1016/j.cplett.2025.141956>
- 2024 9. **L. Crisci**, B. Ballotta, M. Mendolicchio and V. Barone, J. Chem. Theory. Comput. **20**(19), 9435-9445, (2024) <https://doi.org/10.1021/acs.jctc.4c01076>
- 2024 8. **L. Crisci*** and Vincenzo Barone, J. Chem. Theory. Comput. **20**(19), 8539–8548, (2024) <https://pubs.acs.org/doi/full/10.1021/acs.jctc.4c00911>
- 2024 7. L. Uribe, F. Lazzari, S. Di Grande, **L. Crisci**, M. Mendolicchio, and V. Barone, J. Chem. Phys. **161**(1), 014307, (2024) <https://doi.org/10.1063/5.0216384>
- 2024 6. L. Uribe, S. Di Grande, **L. Crisci**, F. Lazzari, M. Mendolicchio, and V. Barone, J. Phys. Chem. A **128**(13), 2629–2642, (2024) <https://doi.org/10.1021/acs.jpca.4c00573>
- 2023 5. V. Barone, **L. Crisci**, and S. Di Grande, J. Chem. Theory Comput., **19** (20), 7273–7286, (2023) <https://doi.org/10.1021/acs.jctc.3c00817>
- 2023 4. **L. Crisci**, S. Di Grande, C. Cavallotti and V. Barone - *J. Chem. Theory. Comput.*, **19**, 7626-7639, (2023) <https://doi.org/10.1021/acs.jctc.3c00857>
- 2023 3. **L. Crisci**, F. Coppola, A. Petrone, and N. Rega *J. Comp. Chem.*, 1-12, (2023) <https://doi.org/10.1002/jcc.27231>
- 2022 2. F. Coppola, P. Cimino, F. Perrella, **L. Crisci**, A. Petrone, N. Rega, *J. Phys. Chem. A*, **126** (40), 7179–7192 (2022) <https://doi.org/10.1021/acs.jpca.2c05001>
- 2022 1. A. Petrone, F. Perrella, F. Coppola, **L. Crisci**, G. Donati, P. Cimino, N. Rega, *Chem. Phys. Rev.*, **3**, 021307 (2022) <https://doi.org/10.1063/5.0085512>

Book Chapters

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| 2026 | 2. L. Crisci , “Transition state theory: a step further”, Chapter 28 in <i>Handbook of Electronic Structure Theory</i> , Elsevier (in press, 2026) |
| 2026 | 1. L. Crisci , “Transition state theory: a (quasi)classical perspective”, Chapter 13 in <i>Handbook of Electronic Structure Theory</i> , Elsevier (in press, 2026) |

Training School

2023 | MD-GAS Training School: Theory and modelling of dynamics of molecules and clusters in the gas phase.

Poster Presentations

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| 2025 | 6. L. Crisci , “Pisa Composite Scheme Meets Generalized Internal Coordinates and Effective Gradients for Accurate Equilibrium Structures of Large Molecules at Reduced Cost”, 61st Symposium on Theoretical Chemistry (STC 2025), Berlin, Germany |
| 2024 | 5. L. Crisci ; International Conference of Molecular Electronic Structure, Villa Maria Hotel in Pescara, IT |
| 2024 | 4. L. Crisci , and V. Barone; 27th International Symposium on Gas Kinetics and Related Phenomena, in Leeds, UK. |
| 2023 | 3. L. Crisci , C. Cavallotti, and V. Barone; International Congress of Quantum Chemistry, in Bratislava, Slovakia. |
| 2023 | 2. L. Crisci , C. Cavallotti, N. Rega and V. Barone; EuChemS CompChem2023, in Thessaloniki, Greece. |
| 2022 | 1. L. Crisci , C. Cavallotti, N. Rega and V. Barone; Unimolecular reactions Faraday Discussion, in Oxford, UK. |

Oral Presentations, ([†], invited speaker)

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| 2025 | 10. L. Crisci [†] , 3rd General Meeting COSY Cost Action, Department of Philosophy, Bologna, (BO), July 2025 |
| 2025 | 9. L. Crisci [†] , Winter Modeling Napoli Edition: From Ab-Initio to Data Driven, Centro Congressi Federico II, Napoli (NA), February 2025 |
| 2024 | 8. L. Crisci and V. Barone, Summer Modeling, Riva Del Sole, Castiglione (GR), September 2024 |
| 2024 | 7. L. Crisci , XXVIII Congresso Nazionale della Società Chimica Italiana, Allianz MiCo Fiera Milano Congressi, Milano (MI), September 2024 |
| 2023 | 6. L. Crisci , C. Cavallotti and V. Barone, VIII congresso nazionale della divisione di chimica teorica e computazionale della società chimica italiana, Scuola Normale Superiore, Pisa (PI), September 2023 |
| 2023 | 5. L. Crisci and V. Barone, Summer Modeling, Riva Del Sole, Castiglione (GR), September 2023 |
| 2023 | 4. L. Crisci [†] , C. Cavallotti, N. Rega, and V. Barone, Centro Congressi Federico II, Napoli (NA), February 2023 |
| 2022 | 3. L. Crisci , C. Cavallotti, N. Rega, and V. Barone, Centro Congressi Federico II, Napoli (NA), November 2022 |
| 2022 | 2. L. Crisci , C. Cavallotti, N. Rega, and V. Barone, Ischia Summer Modeling: Challenges of Molecular Sciences towards 2030, Hotel Continental Terme, Ischia (NA), September 2022 |
| 2022 | 1. L. Crisci , F. Coppola, A. Petrone, and N. Rega, Winter Modeling Largo San Marcellino Napoli (NA), February 2022 |

Invited Seminars

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| 2025 | 3. L. Crisci , “Democratizing High-Accuracy Quantum Chemistry: Code Interoperability and the Pisa Composite Schemes”, Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics, Budapest, Hungary, November 25, 2025 |
| 2025 | 2. L. Crisci , “From Stationary Points to Reaction Rates: A Comprehensive Approach to Kinetic Modeling of Gas-Phase Reactions”, Department of Chemistry, University of Florence, Campus Sesto, Florence, Italy, November 7, 2025 |
| 2025 | 1. L. Crisci , “Modern Computational Approaches to Gas-Phase Kinetics: Barrierless Reactions, Wells, and Beyond”, Department of Chemistry “Giacomo Ciamician”, University of Bologna, Bologna, Italy, October 20, 2025 |

Attendance at Congresses

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| 2022 | 2. F. Coppola, L. Crisci , A. Petrone, R.R. Frontiera, N. Rega; Workshop della Divisione di Chimica Teorica e Computazionale, Aula Magna del Rettorato, Università degli Studi di Firenze, Firenze, April 8 2022 |
| 2021 | 1. F. Coppola, L. Crisci , P. Cimino, A. Petrone, R.R. Frontiera and N. Rega; International Chemical Congress of Pacific Basin Societies (Pacifichem 2020) - December 16-21 2021, Honolulu, Hawaii, USA |

Skills and Competences

Language Skills
Computer Skills

Italian (native). English (intermediate)
Operating Systems: LINUX, WINDOWS-OS, MAC-OS.
Programming Languages: FORTRAN (77, 90, 95, 03, 08), PYTHON, BASH SCRIPT, MAKEFILE.
Markup Languages: LATEX, MARKDOWN.
Ab-initio Quantum Chemistry Software: GAUSSIAN, MOLPRO, MRCC.
Ab-initio Kinetics Software: VARECOF, MESS, ESTOKTP.
Other Scientific Softwares: PACKMOL, VMD, VESTA (molecular graphics), GRACE, ORIGIN-LAB, GIMP (image manipulation).

Il sottoscritto Luigi Crisci dichiara che tutte le informazioni contenute nel curriculum vitae sopra riportato sono veritiere. Autorizza inoltre al trattamento dei propri dati personali, ai sensi del GDPR (Regolamento UE 2016/679) e al Decreto Legislativo n. 196 del 30/06/2003.