

Gabriella Di Genova

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Research Interests

My interdisciplinary work combines the fields of chemistry, theoretical chemistry and astrophysics to tackle some of the open questions of astrochemistry with the ultimate goal to learn about fundamental chemical processes in our Universe. My Ph.D. was funded by the Italian MUR PRIN2020 project *Astrochemistry beyond the second period elements* (PI: Prof. Nadia Balucani) and by the ERC Advanced Grant project *The Dawn of Organic Chemistry* (PI: Prof. Cecilia Ceccarelli).

Expertise

Theoretical study of gas-phase reactions; Chemical kinetics; Chemistry and physics of the interstellar medium (ISM); Star formation; Astrochemistry; Astrochemical modelling; Radiative association reactions; Interstellar ice.

Education

- **Ph.D. in Chemical Sciences, Curriculum: Theoretical Chemistry and Computational Modelling** — Università degli Studi di Perugia (Nov. 2022– Jan. 2026). Defence date: Jan 15, 2026.

Thesis title: Expanding the Astrochemical Canvas: a Computational Exploration of Chemistry Beyond the Second Period of the Periodic Table of Elements. *Grade:* Excellent Cum Laude.

Advisors: Prof. Nadia Balucani, Prof. Cecilia Ceccarelli, Prof. Marzio Rosi.

- **Master's degree - LM-54 2nd level degree in Chemical Sciences** — Università degli Studi di Perugia (2020–2022).

Thesis title: Theoretical study of the impact of metals on (Star)dust formation: focus on Ag-PAH clusters. *Grade:* 110/110 Cum Laude.

Advisors: Prof. Nadia Balucani, Dr. Aude Simon.

- **Master (TCCM) in Theoretical Chemistry & Computational Modelling** — Université Toulouse III – Paul Sabatier (2020–2022).

- **Bachelors's degree - L27 1st level degree in Chemistry** — Università degli Studi di Perugia (2017–2020).

Thesis title: Reaction of N(²D) with cyanoacetylene and implications for Titan's atmospheric chemistry. *Grade:* 102/110.

Advisors: Prof. Nadia Balucani, Dr. Gianmarco Vanuzzo.

Research Abroad

- **Universitat Autònoma de Barcelona, Departament de Química** — *Jan 7–31, 2025.*

During this period, I worked with Prof. Albert Rimola on the characterization of structures, and energetics, of interstellar ice.

- **Institut de Planétologie et d'Astrophysique de Grenoble (IPAG)** — *Jun 1–Sep 30, 2024.*

During this period, I worked with Dr. Cecilia Ceccarelli on the theoretical modeling for reactions of astrochemical relevance.

- **Universitat Autònoma de Barcelona, Departament de Química** — *Nov 1–30, 2023.*

During this period, I worked with Prof. Albert Rimola on the characterization of structures, and energetics, of interstellar ice.

- **University of Gothenburg, Department of Chemistry** — *Apr 11–Jul 15, 2023.*

During this period, I worked with Prof. Gunnar Nyman on the investigation of astrochemical relevant molecules formation by radiative association.

- **Institut de Planétologie et d'Astrophysique de Grenoble (IPAG)** — *Feb 19–Mar 20, 2023.*

During this period, I worked with Dr. Cecilia Ceccarelli on the theoretical modeling for reactions of astrochemical relevance.

- **Université Toulouse III - Paul Sabatier, Quantum Chemistry and Physics Laboratory LCPQ** — *Feb 1–Apr 30, 2022.*

During this period, I worked on my Master's degree with Dr. Aude Simon on the study of the impact of metals in stardust formation.

Work Experience

- **Università degli Studi di Perugia** — Student Support (2022–2025). Teaching support for Chimica Generale e Inorganica I (60 h). Buddy for Erasmus students (150 h).
- **A.Di.S.U. Perugia** — Secretary, Student Welcome Desk (Mar–Aug 2021). Reception and orientation for Italian and foreign students.
- **Master-Up S.r.l.** — Undergraduate Internship (2020). Contributed to software improvements for online tests.

Academic Positions – Eligibility

Eligible candidate (idonea) in the final ranking of the public competition for Researcher, Third Level (fixed-term position), in January 2026, INAF – Osservatorio Astrofisico di Arcetri, Project iSEEDs: “Data Mining, Machine Learning, and astrochemistry for studying young planet-forming systems” (Code: 2025INAFRIC-OAA-iSEEDs3-009).

Scholarships

- **Erasmus+ Traineeship** — IPAG, Grenoble (Supervisor: C. Ceccarelli), *Jun–Sep 2024*.
- **Erasmus+ Traineeship** — University of Gothenburg (Supervisor: G. Nyman), *May–Jul 2023*.
- **Erasmus+ Traineeship** — IPAG, Grenoble (Supervisor: C. Ceccarelli), *Feb–Mar 2023*.
- **Erasmus+** — Université Toulouse III – Paul Sabatier, *Sep 2021–Apr 2022*.
- **A.Di.S.U.** — Scholarship for University education, *2017–2022*; International mobility, *2021–2022*.

Conferences & Seminars

- AI in Astrochemistry Training School (*Poster: “Expanding the Astrochemical Canvas: Computational Exploration of Chemistry Beyond the Second Period”*), Helsinki, Finland — *Aug 5–8, 2025*.
- Europlanet Science Congress 2024 (*Contributed talk: “Possible gas-phase formation routes of dimethyl sulfide in extraterrestrial environments”*), Berlin, Germany — *Sep 8–13, 2024*.
- IMAMPC’2024 – 13th International Meeting on Atomic and Molecular Physics and Chemistry (*Contributed talk: “Sulfur reactivity on ice: a theoretical study”*), Warsaw, Poland — *Jul 9–12, 2024*.
- QuantumGrain Workshop (*Contributed talk: “Sulfur reactivity on ice: a theoretical study”*), Barcelona, Spain — *Jun 9–12, 2024*.
- XIX Congresso Nazionale di Scienze Planetarie (*Contributed talk: “Sulfur reactivity on interstellar water ice surface”*), Bormio, Italy — *Feb 5–9, 2024*.
- School of Scientific Communication in Astronomy, Bertinoro, Italy — *Oct 2–6, 2023*.
- SECSmol Southern European Conference on the Science of Molecules (*Contributed talk: “Aluminium monoxide formation by radiative association”*), Perugia, Italy — *Sep 27–29, 2023*.
- DCTC VIII Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della SCI (*Contributed talk: “Theoretical investigation on $S(^1D)$ insertion reactions leading to the formation of S-bearing species in space”*), Pisa, Italy — *Sep 20–22, 2023*.
- ACO – Chemical Processes in Solar-type Star-Forming Regions (*Poster: “ $S(^1D)$ insertion reactions on the surface of ice mantles. An overlooked mechanism to form S-containing organic species?”*), Toulouse, France — *Jun 5–9, 2023*.

Publications

1. **Di Genova, G.**, Pareras, G., Dominguez-Dalmases, C., Balucani, N., Ceccarelli, C., & Rimola, A. (2026). Quantum mechanical atomistic investigation of the H addition to CS on interstellar water ice. *Astronomy & Astrophysics* (in prep.)
2. **Di Genova, G.**, Balucani, N., Mancini, L., Giustini, A., Rosi, M., Skouteris, D., & Ceccarelli, C. (2025). Gas-phase formation routes of dimethyl sulfide in the interstellar medium. *Astronomy & Astrophysics*, 704, A305.
3. **Di Genova, G.**, Zámečníková, M. Š. N., Giani, L., Balucani, N., Ceccarelli, C., Rosi, M., & Nyman, G. (2025). Radiative association formation of AlO, a candidate seed of dust nucleation. *Monthly Notices of the Royal Astronomical Society*.

4. Rosi, M., Campisi, D., **Di Genova, G.**, Gervasi, O., Ceccarelli, C., & Balucani, N. **(2025)**. Formation Routes of Interstellar Metal Oxides: A Computational Chemistry Approach. *Lecture Notes in Computer Science*, 15888, 289–299; doi: 10.1007/978-3-031-97596-7_19.
5. Giustini, A., **Di Genova, G.**, Balucani, N., Ceccarelli, C., Rimola, A., Ugliengo, P., & Rosi, M. **(2025)**. Theoretical study of the NaO + HCl reaction: a potential formation route of NaCl in the interstellar medium. *Lecture Notes in Computer Science*, 15888, 261–271; doi: 10.1007/978-3-031-97596-7_17.
6. Dahmani, R., Alauzet, C., **Di Genova, G.**, Spiegelman, F., & Simon, A. **(2025)**. Adsorption of Silver Clusters on Naphthalene: Theoretical Insights into Structural, Energetic, Electronic, and Infrared Properties. *The Journal of Physical Chemistry A*, 129(17), 3829-3843.
7. **Di Genova, G.**, Perrero, J., Rosi, M., Ceccarelli, C., Rimola, A., & Balucani, N. **(2025)**. Hot Sulfur on the Rocks: The Reaction of Electronically Excited Sulfur Atoms with Water in an Ice-Surface Model. *ACS Earth and Space Chemistry*, 9(4), 844-855.
8. Giani, L., Šimsová née Zámečníková, M., **Di Genova, G.**, Ceccarelli, C., Balucani, N., & Nyman, G. **(2024)**. Isotope effect on the formation of CN by radiative association reactions. *AIP Advances*, 14(3).
9. Giustini, A., **Di Genova, G.**, Balucani, N., Ceccarelli, C., Rosi, M., & Lombardi, A. **(2024)**. Theoretical Insights on the S(¹D) + H₂O Reaction and Implications on the Chemistry at the Surface of Ice in Extraterrestrial Environments. *Lecture Notes in Computer Science*, 14825, 274–282; doi: 10.1007/978-3-031-65343-8_19.
10. Giustini, A., **Di Genova, G.**, Skouteris, D., Ceccarelli, C., Rosi, M., & Balucani, N. **(2024)**. Gas-phase and model ice-surface reactions of S(¹D) with water and methanol: A computational investigation and implications for cosmochemistry/astrochemistry. *ACS Earth and Space Chemistry*, 8(11), 2318-2333.

Skills

- Programming: Python, Fortran, LaTeX, R.
- Operating Systems: macOS, Windows, Linux/UNIX.
- General Tools: Presentation software, Spreadsheets, Word processors, Data modelling tools.
- Computational Chemistry tools: Gaussian, Molpro, Orca, VASP, GaussView, Avogadro, Jmol, Molden, Moldraw, VMD.
- Writing/communication experience: Published and co-published nine academic papers in the last two years on astrochemistry relevant journals. Made presentations at eight national and international conferences.

Languages

- Italian (Mother tongue).
- English (C1).
- Romanian (B2), Catalan (B1), Spanish (A2), French (A2).

Main Collaborators

- N. Balucani, D. Skouteris, L. Mancini (DCBB-UNIPG, Perugia, Italy),
- C. Ceccarelli (IPAG, Grenoble, France),
- M. Rosi (DICA-UNIPG, Perugia, Italy),
- L. Giani (INAF-Arcetri, Firenze, Italy),
- A. Rimola (UAB, Barcelona, Spain),
- G. Nyman & M. Šimsová (GU, Gothenburg, Sweden),
- D. Ascenzi & M. Michielan (UNITN, Trento, Italy),
- A. Simon (LCPQ, Toulouse, France).

Perugia, 29 Jan 2026

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