

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.

Expertise

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

Education

- **Ph.D. in Chemical Sciences**, *Curriculum*: Theoretical Chemistry and Computational Modelling — Università degli Studi di Perugia (2022–Present). Expected defence date: Jan 12, 2026.

Thesis title: Expanding the Astrochemical Canvas: a Computational Exploration of Chemistry Beyond the Second Period of the Periodic Table of Elements.

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, Prof. 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.

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 Albert Rimola on the characterization of structures, and energetics, of interstellar grains.

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

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

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

During this period, I worked with 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 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 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.

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 (*Poster*), Helsinki, Finland — *Aug 5–8, 2025*.
- Europlanet Science Congress 2024 (*Contributed talk*), Berlin, Germany — *Sep 8–13, 2024*.
- IMAMPC'2024 (*Contributed talk*), Warsaw, Poland — *Jul 9–12, 2024*.
- QuantumGrain Workshop (*Contributed talk*), Barcelona, Spain — *Jun 9–12, 2024*.
- XIX Congresso Nazionale di Scienze Planetarie (*Contributed talk*), Bormio, Italy — *Feb 5–9, 2024*.
- School of Scientific Communication in Astronomy, Bertinoro, Italy — *Oct 2–6, 2023*.
- SECSmol (*Contributed talk*), Perugia, Italy — *Sep 27–29, 2023*.
- DCTC (*Contributed talk*), Pisa, Italy — *Sep 20–22, 2023*.
- ACO – Chemical Processes in Solar-type SFR (*Poster*), Toulouse, France — *Jun 5–9, 2023*.

Publications

1. **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*.
2. Rosi, M., Campisi, D., **Di Genova, G.**, Gervasi, O., Ceccarelli, C., & Balucani, N. **(2025)**. Formation Routes of Interstellar Metal Oxides: A Computational Chemistry Approach. In *International Conference on Computational Science and Its Applications* (pp. 289–299). Cham: Springer Nature Switzerland.
3. 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. In *International Conference on Computational Science and Its Applications* (pp. 261–271). Cham: Springer Nature Switzerland.
4. **Di Genova, G.**, Balucani, N., Mancini, L., Rosi, M., Skouteris, D., & Ceccarelli, C. **(2025)**. Gas-phase formation routes of dimethyl sulfide in the interstellar medium. *arXiv preprint arXiv:2504.16236*. (accepted for publication in *Astronomy & Astrophysics*)
5. 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.
6. **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.

- 7.** 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).
- 8.** 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. In *International Conference on Computational Science and Its Applications* (pp. 274-282). Cham: Springer Nature Switzerland.
- 9.** 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.
- *Tools:* Presentation software, Spreadsheets, Word processors, Data modelling tools.
- *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),
- Rimola (UAB, Barcelona, Spain),
- G. Nyman & M. Šimsová (GU, Gothenburg, Sweden),
- D. Ascenzi & M. Michielan (UNITN, Trento, Italy),
- A. Simon (LCPQ, Toulouse, France).
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Perugia, 14 Nov 2025

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