Gabriella Di Genova, Ph.D.

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Dip. di Chimica, Biologia e Biotecnologie, Via Elce di Sotto 8, 06123, Perugia - Italy thtps://gabrielladigenova.github.io/gabrielladigenova/

Academic 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.

Education

2022 - 2025

Ph.D. in Chemical Sciences

Università degli Studi di Perugia - Dipartimento di Chimica, Biologia e Biotecnologie

Curriculum: Theoretical Chemistry and Computational Modelling. Ph.D Supervisors: Prof. Nadia Balucani, Prof. Cecilia Ceccarelli, Prof. Marzio Rosi

09/2021 - 04/2022

Master in Theoretical Chemistry and Computational Modeling - TCCM Université Toulouse III - Paul Sabatier, Department of Chemistry

09/2020 - 07/2022

Master's degree - LM-54 2nd level degree

Università degli Studi di Perugia - Dipartimento di Chimica, Biologia e Biotecnologie

Thesis title: Theoretical study of the impact of metals on (Star)dust formation: focus on Ag-PAH clusters.

2017 - 2020

\blacksquare Bachelors's degree - L27 1 st level degree

Università degli Studi di Perugia - Dipartimento di Chimica, Biologia e Biotecnologie

Thesis title: An experimental study of the reaction between atomic nitrogen in the excited 2D state with cyanoacetylene and implication for the atmospheric chemistry of Titan.

Research Abroad

07/01/2025 - 31/01/2025

Universitat Autònoma de Barcelona, Departament de Química.

Faculty of Sciences 08193 - Barcelona, Spain.

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

01/06/2024 - 30/09/2024

Institut de Planetologie et d'Astrophysique de Grenoble (IPAG).

122 rue de la Piscine, 38041 Grenoble - France.

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

Research Abroad (continued)

01/11/2023 - 30/11/2023

Universitat Autònoma de Barcelona, Departament de Química.

Faculty of Sciences 08193 - Barcelona, Spain.

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

11/04/2023 - 15/07/2023

■ University of Gothenburg, Department of Chemistry.

Kemigården 4, 412 96 Göteborg, Sweden.

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

19/02/2023 - 20/03/2023

Institut de Planetologie et d'Astrophysique de Grenoble (IPAG).

122 rue de la Piscine, 38041 Grenoble - France.

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

01/02/2022 - 30/04/2022

Université Toulouse III - Paul Sabatier, Quantum Chemistry and Physics Laboratory - LCPQ.

118 Route de Narbonne, 31062 Toulouse, France.

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

Scholarships

01/06/2024 - 30/09/2024

Erasmus+ Traineeship

Institut de Planetologie et d'Astrophysique de Grenoble (IPAG). Grenoble,

France

Supervisor: Cecilia Ceccarelli

15/05/2023 - 15/07/2023

Erasmus+ Traineeship

University of Gothenburg - Department of Chemistry. Gothenburg, Sweden Supervisor: Gunnar Nyman

19/02/2023 - 20/03/2023

Erasmus+ Traineeship

Institut de Planetologie et d'Astrophysique de Grenoble (IPAG). Grenoble,

France

Supervisor: Cecilia Ceccarelli

01/09/2021 - 30/04/2022

Erasmus+

Université Tolouse III - Paul Sabatier. Toulouse, France

2017 - 2022

A.Di.S.U.

Scholarship for University education

2021 - 2022

A.Di.S.U.

For international mobility

Employment History

2022 - 2025

Student support, Università degli Studi di Perugia, Via Elce di Sotto 8 - Perugia 06123, Italy.

Provided teaching support for first-year bachelor's students for the "Chimica Generale e Inorganica I" course (60 hours) and served as a Buddy for Erasmus outgoing and incoming students (150 hours).

03/2021 - 08/2021

Secretary at student's welcome desk, A.Di.S.U. Perugia, Via Benedetta, 14 - 06123 Perugia, Italy.

Support to the offices of the agency in charge of reception and orientation for Italian and foreign students.

2020

Undergraduate Internship. Master-Up S.r.l., Via Elce di Sotto 8 - Perugia 06123, Italy.

Contribution to the improvement of a computer software useful for the purposes of online tests.

Conferences and Schools

Attended

- "ACO Chemical Processes in Solar-type Star-Forming Regions," Tolouse, France 5-9/06/2023, **Poster contribution**. OURL: https://aco-conference2023.sciencesconf.org/.
- "DCTC VIII Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della SCI," Pisa, Italy 20-22/09/2023, **Selected Oral contribution**. URL: https://www.skies-village.it/dctc2023/.
- "EGU General Assembly 2024," Vienna, Austria 14-19/04/2024, **Selected Oral contribution.** Ourl: https://www.egu24.eu/.
- "EPSC, Europlanet Science Congress 2024," Berlin, Germany 8-13/09/2024, **Selected Oral contribution.** OURL: https://www.epsc2024.eu/.
- "IMAMPC'2024 13th International Meeting on Atomic and Molecular Physics and Chemistry," Warsaw, Poland 9-12/07/2024, **Selected Oral contribution.** OURL: https://www.imampc2024.pl/.
- "Quantumgrain Workshop: Emerging Horizons in the Chemistry of the Universe," Barcelona, Spain 9-12/06/2024, **Selected Oral contribution.** § URL: https://workshop.quantumgrain.eu/.
- 7 "School of Scientific Communication in Astronomy," Bertinoro, Italy 2-6/10/2023. ♥ URL: https://andymelandri.wixsite.com/scia2023.
- "SECSmol Southern European Conference on the Science of Molecules," Perugia, Italy 27-29/09/2023, **Selected Oral contribution.** Ourl: http://www.dcbb.unipg.it/en/secsmol.
- 9 "XIX Congresso Nazionale di Scienze Planetarie," Bormio, Italy 5-9/02/2024, **Selected Oral contribution.** 9 URL: https://www.scienzeplanetarie.it/congresso-nazionale-bormio-2024/.

Research Production

Publications

R. Dahmani, C. Alauzet, **Di Genova, Gabriella**, F. Spiegelman, and A. Simon, "Adsorption of silver clusters on naphthalene: Theoretical insights into structural, energetic, electronic, and infrared properties," ACS Publications, 2025. URL: https://doi.org/10.1021/acs.jpca.5c00436.

- **Di Genova, Gabriella**, N. Balucani, L. Mancini, M. Rosi, S. Dimitrios, and C. Ceccarelli, "Gas-phase formation routes of dimethyl sulfide in the interstellar medium.," in *Astronomy and Astrophysics (in press)*, 2025. **O** URL: https://doi.org/10.48550/arXiv.2504.16236.
- Di Genova, Gabriella, J. Perrero, M. Rosi, C. Ceccarelli, A. Rimola, and N. Balucani, "Hot Sulfur on the Rocks: The Reaction of Electronically Excited Sulfur Atoms with Water in an Ice-Surface Model," in ACS Earth and Space Chemistry, 2025. URL: https://pubs.acs.org/doi/10.1021/acsearthspacechem.4c00351.
- M. Rosi, D. Capisi, **Di Genova, Gabriella**, O. Gervasi, C. Ceccarelli, and N. Balucani, "Formation routes of interstellar metal oxides: A computational chemistry approach," in *International Conference on Computational Science and Its Applications (accepted)*, Springer, 2025.
- L. Giani, M. Šimsová née Zámečníková, **Di Genova, Gabriella**, C. Ceccarelli, N. Balucani, and G. Nyman, "Isotope effect on the formation of CN by radiative association reactions," in *AIP Advances*, vol. 14, 2024. URL: https://pubs.aip.org/aip/adv/article-lookup/doi/10.1063/5.0192682.
- A. Giustini, **Di Genova, Gabriella**, N. Balucani, C. Ceccarelli, M. Rosi, and A. Lombardi, "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, Springer, 2024, pp. 274–282. URL: https://doi.org/10.1007/978-3-031-65343-8_19.

Skills

Languages

Native: Italian. Strong reading, writing and speaking competencies for: English, Catalan, Romanian. Basic reading, writing and speaking competencies for Spanish and French.

Coding

Fortran77, Python, R, LATEX,

Misc.

Presentation Software (advanced), Spreadsheets (advanced), Word processors (advanced), Network architecture (basic), Operating systems (advanced), Data modeling tools (intermediate).

References

Prof. Nadia Balucani

University of Perugia, Via Elce di Sotto, 8 - 06123 Perugia - Italy https://nadiabalucani.weebly.com/

Prof. Marzio Rosi

Università degli Studi di Perugia Dipartimento di Ingegneria Civile ed Ambientale Via G. Duranti, 93 - 06125 - Perugia, Italy https://www.unipg.it/personale/marzio.rosi

Prof. Gunnar Nyman

University of Gothenburg Department of Chemistry Kemigården 4, 412 96 Göteborg, Sweden https://www.gu.se/en/about/findstaff/gunnarnyman

Prof. Cecilia Ceccarelli

Université Grenoble Alpes Institut de Planétologie et d'Astrophysique de Grenoble 122 rue de la Piscine, 38041 Grenoble - France https://ipag.osug.fr/french/recherche/equipes/interstellaire/

Prof. Aude Simon

Université Toulouse III - Paul Sabatier Quantum Chemistry and Physics Laboratory - LCPQ 118 Route de Narbonne, 31062 Toulouse, France https://www.lcpq.ups-tlse.fr/spip.php?article1130

Prof. Albert Rimola

Universitat Autònoma de Barcelona Departament de Química Faculty of Sciences 08193 - Barcelona, Spain https://www.quantumgrain.eu/