# Laura Grazioli

## Curriculum Vitae

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**Nationality**: Italian, German
**Date of birth**: 14/05/1996

## Education

FROM 09.2024 **École des ponts et chaussées**, Marne-la-Vallée, and **INRIA**, Paris – *Postdoc, Mathematics applied to theoretical chemistry.*
Postdoc on the description of excited states of molecular systems through saddle-point search approaches. Funding provided by the ERC Synergy Grant EMC2, under the supervision of Prof. Eric Cancès.

10.2020-08.2024 **Johannes Gutenberg-Universität**, Mainz, Germany – *PhD, Theoretical Chemistry.*
PhD position under the direct supervision of Prof. Stella Stopkowicz (Universität des Saarlandes, Saarbrücken) and Prof. Jürgen Gauss (Johannes Gutenberg-Universität, Mainz). Thesis with the title *Challenges in the Calculation of Molecular Energies and Properties in a Magnetic Field using Unitary Coupled-Cluster Theory.* Final grade: magna cum laude.

10.2015-09.2020 **Scuola Normale Superiore**, Pisa, Italy – *Honours College, Chemistry.*
Bachelor and Master studies in theoretical chemistry.

09.2018-09.2020 **University of Pisa**, Italy – Master Student in *Theoretical Chemistry.*
Master dissertation thesis: *Strong light-matter coupling in chiral cavities: signatures of enantiomers in rotational spectra* Supervisor: Prof. Henrik Koch (SNS), Co-supervisor: Dott. Enrico Ronca (CNR). Final Grade: 110/110 summa cum laude (maximum score, first class honours)

10.2015–10.2018 **University of Pisa**, Italy – Bachelor Student in *Chemistry.*
Bachelor dissertation thesis: *'A novel theoretical approach to accurately model infrared spectra of flexible molecules in aqueous solution'.* Supervisor: Prof. Chiara Cappelli (SNS). Final Grade: 110/110 summa cum laude (maximum score, first class honours)

## Publications

- Grazioli, L., Hu, Y., Nottoli, T., Lipparini, F., Cancès, E. (2026), *Critical point search and linear response theory for computing electronic excitation energies of molecular systems. Part II: CASSCF*, arXiv:2604.13753.
- Hu, Y., Grazioli, L., (2026), *Constrained dynamics for searching saddle points on general Riemannian manifolds*, arXiv preprint arXiv:2601.03931.
- Grazioli, L., Hu, Y., Cancès, E. (2026), *Critical point search and linear response theory for computing electronic excitation energies of molecular systems. Part I: General framework, application to Hartree-Fock and DFT*, J. Chem. Phys. 164, 064101.
- Grazioli, L., Kitsaras, M.-P., Stopkowicz, S. (2025), *Unitary Coupled-Cluster theory for the treatment of molecules in strong magnetic fields*, J. Chem. Theory Comput. 21 (24): 12634–12651.
- Kitsaras, M.-P., Grazioli, L., Stopkowicz, S. (2024). *The approximate Coupled-Cluster methods CC2 and CC3 in a finite magnetic field*, J. Chem. Phys. 160, 094112.

- Hampe, F., Stopkowicz, S., Gross, N., Kitsaras, M.-P., Grazioli, L., Blaschke, S., Monzel, L., Yergün, Ü. P., *QCUMBRE, Quantum Chemical Utility enabling Magnetic-field dependent investigations Benefitting from Rigorous Electron-correlation treatment*, https://www.qcumbre.org for more information.
- Grazioli, L., Schleicher, L. T., Stopkowicz, S., Gauss, J. (2024) *Theoretical Prediction of Closed-Shell Paramagnetism for Scandium and Yttrium Hydride*, J. Comput. Chem. (Special Issue for Elfi Kraka), 45(15), 1215-1223.
- Riso, R. R., Grazioli, L., Ronca, E., Giovannini, T., Koch, H. (2023). *Strong coupling in chiral cavities: nonperturbative framework for enantiomer discrimination*, Phys. Rev. X, 13(3), 031002.
- Giovannini, T., Grazioli, L., Ambrosetti, M., Cappelli, C. (2019). *Calculation of IR spectra with a fully polarizable QM/MM approach based on fluctuating charges and fluctuating dipoles*, J. Chem. Theory Comput., 15(10), 5495-5507.

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## Conferences, Talks and Summerschools

07.2026 Invited talk at the ERC-EMC2 annual meeting and workshop, Roscoff. Talk with title *Differential geometry for excited states: a unified framework.*

05.2026 Invited talk in *Analysis and Simulation of Quantum and Molecular System* Workshop, Aachen. Title of the talk *A geometric picture of excited states in variational theories.*

03.2026 Invited talk in the group of Prof. Gaspard Kemlin, LAMFA, Amiens. Talk with title *A geometric picture of excited states in variational theories.*

03.2026 GAMM (Gesellschaft für Angewandte Mathematik und Mechanik) 2026, Stuttgart. Talk with title *A geometric picture of linear response theory for variational methods.*

02.2026 Invited talk in the group of Prof. Pierre-François Loos, LCPQ, Toulouse. Talk with title *A geometric picture of excited states in variational theories.*

12.2025 Invited talk in the group of Prof. Benjamin Stamm, Universität Stuttgart. Talk with title *A geometric picture of excited states in variational theories.*

09.2025 STC (Symposium of Theoretical Chemistry) 2025, Berlin. Presentation of a contributed talk with title *Excited States as Critical Points of the Potential Energy Surface.*

09.2025 MWM (Modern Wavefunction Methods) summer school 2025, Pisa - tutor for exercise sessions on the topics of second quantization, mathematics, Coupled Cluster Theory, Stochastics and Quantum Monte Carlo, Response properties.

07.2025 Roscoff seminar: ERC-EMC2 annual meeting and workshop

06.2025 WATOC (World Association of Theoretical and Computational Chemists) Conference 2025, Oslo. Presentation of a talk with title *Excited states as critical points of the potential energy surface.*

05.2025 Attendee at the 7th edition of the Mini-school on mathematics for theoretical chemistry and physics, Paris. Courses on *(Un)supervised learning with applications to molecular dynamics* and *From machine-learned wavefunctions to interatomic potentials.*

06.2025 Invitation to talks at Johannes Gutenberg University, Mainz, and at Universität des Saarlandes, Saarbrücken. Presentations given with title *Excited states as critical points of the potential energy surface.*

03.2025 Mathematical Methods in Quantum Chemistry, Oberwolfach institute, Germany. Presentation of a talk with title *Unitary Coupled-Cluster theory in strong magnetic fields.*

09.2024 MANUEL (Mathematical and Numerical Analysis of Electronic Structure Models) Conference, Stuttgart. Presentation of a poster with the title *Challenges in the Calculation of Molecular Energies and Properties in a Magnetic Field using Unitary Coupled-Cluster Theory.*

06.2024 Söllerhaus Seminar 2024, Hirschegg, Austria: internal retreat organised by the universities of Mainz, Saarbrücken, Karlsruhe and Stuttgart. Presentation of a talk with title *Unitary Coupled-Cluster Theory: energies and properties.*

10.2023 TRR 306 QuCoLiMa (Quantum Cooperativity of Light and Matter) Conference, Erlangen.

09.2023 Talk with the title *Challenges in the Calculation of Properties in a Magnetic Field, using Coupled-Cluster and Unitary Coupled-Cluster Theory* at NTNU, Trondheim, following the invitation by Prof. Henrik Koch.

09.2023 MWM (Modern Wavefunction Methods) Summer school, Pisa: week of lectures and exercise sessions on the most important issues in wavefunction methods, given by highly qualified Professors. Presentation of a poster with title *From Magnetic Circular Dichroism to Magnetic White Dwarfs: Challenges in the Calculation of Properties in a Magnetic Field, using Coupled-Cluster and Unitary Coupled-Cluster Theory.*

07.2023 Söllerhaus Seminar 2023, Hirschegg, Austria: internal retreat organised by the universities of Mainz, Saarbrücken, Karlsruhe and Stuttgart. Presentation of a talk with title *Challenges in the Calculation of Properties in a Magnetic Field, using Coupled-Cluster and Unitary Coupled-Cluster Theory.*

06.2023 ICQC (International Conference in Quantum Chemistry), Bratislava. Presentation of a poster with title *From Magnetic Circular Dichroism to Magnetic White Dwarfs: Challenges in the Calculation of Properties in a Magnetic Field, using Coupled-Cluster and Unitary Coupled-Cluster Theory* and winner of poster prize.

09.2022 OPERA Symposium in honour of Jürgen Gauss.

07.2022 Söllerhaus Seminar 2022, Hirschegg, Austria: internal retreat organised by the universities of Mainz, Karlsruhe and Stuttgart. Presentation of a talk with title *Unitary Coupled Cluster Theory: Energies and Properties in Strong Magnetic Fields.*

09.2021 STC (Symposium of Theoretical Chemistry), online: conference of the German Chemistry community; attendance of talks and presentation of a poster with the title *Unitary Coupled Cluster Theory in Finite Magnetic Fields as a Solution to Complex Energies.*

09.2021 MRPSS (Molecular Response Properties Summer School), Stockholm: intensive week of lectures and exercise sessions on advanced matters in response theory and spectroscopy, held by the highly-praised Professors of Scandinavian countries.

07.2021 Telluride Conference on Coupled Cluster Theory, online.

09.2019 ESQC (European Summerschool of Quantum Chemistry), Altavilla Milicia, Sicily: two weeks of lectures and exercise sessions on the most important issues in quantum chemistry, trained by highly qualified Professors.

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## Fellowships and awards

07.2023 Winner of Poster Prize at ICQC (International Conference in Quantum Chemistry), Bratislava, with funding from PCCP and Digital Discovery.

09.2019 Funding by SNS for participating in the *European Summerschool in Quantum Chemistry (ESQC)* (2000 euros).

08.2015 Winner of a five-year full residential scholarship at Scuola Normale Superiore, Pisa (value: about 50000 euros).

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## Teaching experience

09.2026 Teaching at the ESQC (European Summerschool for Quantum Chemistry) 2026, Palermo - tutor for exercise sessions.

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| 01.2026-06.2026 | Teaching of two first-year projects at Ecole nationale de Ponts et Chaussées, named *Foundations of Quantum Chemistry : Manifold Structures in Wavefunction Methods* and *Information quantique*. |
| 09.2025 | Teaching at the MWM (Modern Wavefunction Methods) summer school 2025, Pisa - tutor for exercise sessions on the topics of second quantization, mathematics, Coupled Cluster Theory, Stochastics and Quantum Monte Carlo, Response properties. |
| 10.2021-08.2024 | Responsible for teaching the exercise sessions and programming laboratories (six semesters) of the courses *Theoretical chemistry 1* and *Theoretical chemistry 2*, held by Prof. Jürgen Gauss, JGU, Mainz. |
| 01.2023-05.2023 | Supervisor of the Bachelor Thesis of Luca T. Schleicher at JGU, concerning paramagnetism in hydrides. |
| 10.2022-04.2023 | Supervisor of research project of the master student Zahra Mamadli at JGU, concerning the calculation of MCD spectra. |
| 05.2022 | Supervisor of research project of the master student Maximilian M. Braun at JGU, concerning the implementation and calculation of MCD spectra. |
| 04.2021-10.2023 | Speaker and organiser in the project *A Choice for Life - Giulio Deangeli*, an orienteering and coaching conference for high school students taking part from all over Italy, with the aim of giving help and suggestion in the choice of university subjects. |
| 10.2019-10.2020 | Mentoring activity for academic help to all younger chemistry students at SNS, with particular attention to first-year students as regards classical mechanics. |

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## Language Knowledge

- **Italian**: Mother-tongue
- **German**: Mother-tongue
- **English**: Fluent (Cambridge FCE passed with C1 level)
- **French**: Intermediate (C1 level)
- **Chinese**: Intermediate (B2 level)
- **Latin**: Understanding, translation and interpretation
- **Greek**: Basic (A1 level)

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## Computer Skills

- Markup, graphics and editing: Office Softwares and Internet Browsers, LaTeX
- Programming: C++, Fortran 77, Fortran 90, Bash, Matlab, Python, Mathematica