Matteo Castagnola, Ph.D.

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Employment History

Nov. 2022 – Present **Ph.D., Norges teknisk-naturvitenskapelige universitet (NTNU)**
Theoretical and Computational Chemistry – Molecular Polaritons – *Ab Initio* Quantum Electrodynamics

Education

2017 – 2022 **Second-level university Master in Chemistry and Geology, Scuola Normale Superiore (SNS)**
Final Grade 100/100 cum Laude. Awarded with a 5-year full scholarship.

2020 – 2022 **Master's degree in chemistry, Pisa University** Final Grade 110/110 cum Laude
Thesis title: *Ab initio response methods for entangled light-matter systems in the strong coupling regime.*

2017– 2020 **Bachelor's degree in chemistry, Pisa University** Final Grade 110/110 cum Laude
Thesis title: *Optical response properties of metal nanoparticles: fully atomistic classical model.*

List of Publications

Journal Articles

1. **M. Castagnola**, M. T. Lexander, and H. Koch, "Realistic ab initio predictions of excimer behavior under collective light-matter strong coupling," *Physical Review X*, vol. 15, no. 2, p. 021 040, 2025.
2. **M. Castagnola**, R. R. Riso, Y. El Moutaoukal, E. Ronca, and H. Koch, "Strong coupling quantum electrodynamics hartree–fock response theory," *The Journal of Physical Chemistry A*, 2025.
3. Y. El Moutaoukal, R. R. Riso, **M. Castagnola**, E. Ronca, and H. Koch, "Strong coupling møller–plesset perturbation theory," *Journal of Chemical Theory and Computation*, 2025.
4. R. R. Riso, **M. Castagnola**, E. Ronca, and H. Koch, "Chiral polaritonics: Cavity-mediated enantioselective excitation condensation," *Reports on Progress in Physics*, vol. 88, no. 2, p. 027 901, 2025.
5. **M. Castagnola**, M. T. Lexander, E. Ronca, and H. Koch, "Strong coupling electron-photon dynamics: A real-time investigation of energy redistribution in molecular polaritons," *Physical Review Research*, vol. 6, no. 3, p. 033 283, 2024.
6. Y. El Moutaoukal, R. R. Riso, **M. Castagnola**, and H. Koch, "Toward polaritonic molecular orbitals for large molecular systems," *Journal of Chemical Theory and Computation*, vol. 20, no. 20, pp. 8911–8920, 2024.
7. **M. Castagnola**, T. S. Haugland, E. Ronca, H. Koch, and C. Schäfer, "Collective strong coupling modifies aggregation and solvation," *The Journal of Physical Chemistry Letters*, vol. 15, pp. 1428–1434, 2023.
8. **M. Castagnola**, R. R. Riso, A. Barlini, E. Ronca, and H. Koch, "Polaritonic response theory for exact and approximate wave functions," *Wiley Interdisciplinary Reviews: Computational Molecular Science*, e1684, 2023.
9. T. Giovannini, L. Bonatti, P. Lafiosca, *et al.*, "Do we really need quantum mechanics to describe plasmonic properties of metal nanostructures?" *ACS photonics*, vol. 9, no. 9, pp. 3025–3034, 2022.

Miscellaneous Experience

International Conferences

2025 **Oral presentation** at the "Symposium on Polaritonic Effects in Molecular Systems" at the Annual Conference of the DPG and DPG Spring Meeting, Bonn (Germany)

Oral presentation at the American Physical Society (APS) Global Physics Summit, Los Angeles (California, USA)

2024 **Oral presentation** at the Quantum Chemistry and Modelling meeting of the Norwegian Chemical Society (NKS), Trondheim (Norway)

Poster at the European Materials Research Society (EMRS) Meeting, Strasbourg (France)

International Schools

Ab Initio Quantum Electrodynamics for Quantum Materials Engineering, Lausanne (Switzerland)

2023 **Modern Wavefunction Methods (MWM)**, Pisa (Italy)

2019 **International Summer School on Vibrational Spectroscopy (VISPEC)**, Perugia (Italy)

Program Developing

eT Program Developer, an open source electronic structure program

Experience with **Python**, **Fortran**, **Git**, **Linux**, **Latex**

Courses

ACS Reviewer Lab course for peer review; Focus on Peer Review: A Nature Masterclasses course; IOP Peer Review Excellence training course.

References

Prof. Henrik Koch
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Norwegian University of Science and Technology,
Høgskoleringen 5, 7034, Trondheim.
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Prof. Enrico Ronca
Associate Professor
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