# Antoine **Marie**

Postdoctoral researcher

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## Education

**Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier** — *Toulouse, France*

PhD in Theoretical Chemistry — *Oct. 2022 - Nov. 2025*

- Supervisor: Pierre-François Loos

**École Normale Supérieure de Lyon** — *Lyon, France*

MSc in Computational Physics and Chemistry — *Sep. 2019 - July 2022*

- Two years of master and one year as a research intern abroad

**École Normale Supérieure de Lyon** — *Lyon, France*

BSc in Chemistry — *Sep. 2018 - Jul. 2019*

## Experience

**Department of Physics, University of Warsaw** — *Warsaw, Poland*

Postdoctoral researcher in Dominika Zgid's group — *Feb. 2026 - Today*

- Working on the description of magnetic compounds with strong spin-orbit coupling using the relativistic $GW$ framework.

**Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier** — *Toulouse, France*

PhD student in Pierre-François Loos' group — *Oct. 2022 - Nov. 2025*

- Derived a new qs$GW$ static self-energy using the similarity renormalization group.
- Extended the QUEST database of FCI-quality excitation energies to ionization potentials.
- Worked on development in many-body perturbation theory using anomalous propagators.
- Applied the parquet approximation to chemical systems for the first time.

**Department of Theoretical Chemistry, Vrije Universiteit Amsterdam** — *Amsterdam, the Netherlands*

Internship in Paola Gori-Giorgi's group — *Mar. 2022 - Jul. 2022*

- Studied many-body localization of fermions in disordered systems using the strictly correlated electrons formalism of density functional theory.

**Department of Chemistry, University of Oxford** — *Oxford, United Kingdom*

Internship in Hugh Burton's group — *Sep. 2021 - Feb. 2022*

- Analyzed the multiple solutions on the complete-active-space self-consistent-field energy landscape.

**Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier** — *Toulouse, France*

2nd year MSc internship in Pierre-François Loos' group — *Feb. 2021 - Jul. 2021*

- Worked on variational coupled-cluster for excited states.

**Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier** — *Toulouse, France*

1st year MSc internship in Pierre-François Loos' group — *May 2020 - Jul. 2020*

- Reviewed the connection between singularities in the complex plane and convergence properties of perturbation theory.

## Publications

**Parquet theory for molecular systems: Formalism and static kernel parquet approximation** — *J. Chem. Phys. [Editors' pick]*

**A. Marie** and P.F. Loos. — ***163***, *194115 (2025)*

**Anomalous propagators and the particle-particle channel: Bethe-Salpeter equation**
*J. Chem. Phys.*
**A. Marie**, P. Romaniello, X. Blase and P.F. Loos.
***162***, *134105 (2025)*

**Anomalous propagators and the particle-particle channel: Hedin's equations**
*Phys. Rev. B*
**A. Marie**, P. Romaniello and P.F. Loos.
***110***, *115155 (2024)*

**Cumulant Green's function methods for molecules**
*Faraday Discuss.*
P.F. Loos, **A. Marie** and A. Ammar.
***254***, *240 (2024)*

**Reference energies for valence ionizations and satellite transitions**
*J. Chem. Theo. Comput.*
**A. Marie** and P.F. Loos.
***20***, *4751 (2024)*

**Can $GW$ handle multireference systems?**
*J. Chem. Phys.*
A. Ammar, **A. Marie**, M. Rodriguez-Mayorga, H.G.A. Burton and P.F. Loos.
***160***, *114101 (2024)*

**The $GW$ Approximation: A Quantum Chemistry Perspective**
*Adv. Quant. Chem.*
**A. Marie**, A. Ammar and P.F. Loos.
***90***, *157 (2024)*

**A similarity renormalization group approach to Green's function methods**
*J. Chem. Theory Comput.*
**A. Marie** and P.F. Loos.
***19***, *3943 (2023)*

**Excited states, symmetry breaking, and unphysical solutions in state-specific CASSCF theory**
*J. Phys. Chem. A*
**A. Marie** and H.G.A. Burton.
***127***, *4538 (2023)*

**Connections between many-body perturbation and coupled-cluster theories**
*J. Chem. Phys.*
R. Quintero-Monsebaiz, E. Monino, **A. Marie** and P.F.L. Loos.
***157***, *231102 (2022)*

**Real space Mott-Anderson electron localization with long-range interactions: exact and approximate descriptions**
*Phys. Rev. Res.*
*[Editors' suggestion]*
**A. Marie**, D.P. Kooi, J. Grossi, M. Seidl, Z.H. Musslimani, K. Giesbertz and P. Gori-Giorgi.
***4***, *043192 (2022)*

**Variational coupled cluster for ground and excited states**
*J. Chem. Phys.*
**A. Marie**, F. Kossoski, and P.F. Loos.
***155***, *104105 (2021)*

**Excited states from state specific orbital optimized pair coupled cluster**
*J. Chem. Theory Comput.*
F. Kossoski, **A. Marie**, A. Scemama, M. Caffarel, and P.F. Loos.
***17***, *4756 (2021)*

**Perturbation theory in the complex plane: Exceptional points and where to find them**
*J. Phys. Cond. Mat.*
**A. Marie**, H.G.A. Burton, P.F. Loos.
***33***, *283001 (2021)*

## Talks

**Seminar at Laboratoire de chimie ENS de Lyon**
*Lyon, France*
Single and double ionization potentials of molecular systems with the $GW$ approximation
*Jun. 2025*

**2nd workshop "Emerging excited-state methods in electronic structure"**
*Toulouse, France*
Bethe-Salpeter equation for the particle-particle propagator
*Apr. 2025*

**ETSF Correlation meetings** — *Palaiseau, France*
Bethe-Salpeter equation for the particle-particle propagator — *Dec. 2024*

**6th Workshop on "Green's function methods: the next generation"** — *Toulouse, France*
Anomalous propagators and the particle-particle correlation channel of many-body perturbation theory — *Oct. 2024*

**Lennard-Jones Center (LJC) seminar series** — *Cambridge, United Kingdom*
Anomalous propagators and the particle-particle correlation channel of many-body perturbation theory: Hedin's equations — *Jul. 2024*

**Journée "Théorie, Modélisation et Simulation"** — *Strasbourg, France*
Reference energies for valence ionizations and satellite transitions — *Oct. 2023*

## Posters

**13th WATOC congress** — *Oslo, Norway*
Particle-particle Bethe-Salpeter equation and Parquet theory — *Jun. 2025*

**Third general meeting of the GDR NBODY** — *Nancy, France*
Particle-particle Bethe-Salpeter equation and Parquet theory — *Jun. 2025*

**Faraday Discussion "Correlated electronic structure"** — *London, United Kingdom*
Anomalous propagators and the particle-particle correlation channel — *Jul. 2024*

**Rencontres Théories, Modélisations et Simulations Atomistiques - RCTF** — *Rouen, France*
Anomalous propagators and the particle-particle correlation channel — *Jun. 2024*

**Summer school "Modern Wavefunction Based Methods in Electronic Structure Theory"** — *Pisa, Italy*
A similarity renormalization group approach to Green's function methods — *Sep. 2023*

**Workshop "Emerging excited-state methods in electronic structure"** — *Toulouse, France*
A similarity renormalization group approach to Green's function methods — *Apr. 2023*

## Teaching/mentoring

**Bachelor** Introduction to Python and algorithmic (2022-2024)
**Master** Supervised two first-year master internships (2024)