

# Antoine Marie

PHD STUDENT

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## Education

### Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier

Toulouse, France

PHD IN THEORETICAL CHEMISTRY

Oct. 2022 - Today

- Supervisor: Pierre-François Loos

### École Normale Supérieure de Lyon

Lyon, France

MSC IN COMPUTATIONAL PHYSICS AND CHEMISTRY

Sep. 2019 - Jul. 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

### Laboratoire de Chimie et Physique Quantique, Université Toulouse Paul Sabatier

Toulouse, France

PHD IN PIERRE-FRANÇOIS LOOS' GROUP

Oct. 2022 - Today

- Derived a new  $qsGW$  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.

### 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 Physique et Chimie Quantique

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 Physique et Chimie Quantique

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.

## Skills

**Programming** Fortran, Mathematica, Python, Rust, Bash  
**Software** Linux, LaTeX  
**Languages** French (native), English (Cambridge C1 certification)

## Publications

### Anomalous propagators and the particle-particle channel: Bethe-Salpeter equation

Preprint at arXiv:2411.13167

A. MARIE, P. ROMANIELLO, X. BLASE AND P.F. LOOS.

(2024)

### 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

P.F. LOOS, **A. MARIE** AND A. AMMAR.

*Faraday Discuss.*

**254**, 240 (2024)

## Reference energies for valence ionizations and satellite transitions

**A. MARIE** AND P.F. LOOS.

*J. Chem. Theo. Comput.*

**20**, 4751 (2024)

## Can *GW* handle multireference systems?

A. AMMAR, **A. MARIE**, M. RODRIGUEZ-MAYORGA, H.G.A. BURTON AND P.F. LOOS.

*J. Chem. Phys.*

**160**, 114101 (2024)

## The *GW* Approximation: A Quantum Chemistry Perspective

**A. MARIE**, A. AMMAR AND P.F. LOOS.

*Adv. Quant. Chem.*

**90**, 157 (2024)

## A similarity renormalization group approach to Green's function methods

**A. MARIE** AND P.F. LOOS.

*J. Chem. Theory Comput.*

**19**, 3943 (2023)

## Excited states, symmetry breaking, and unphysical solutions in state-specific CASSCF theory

**A. MARIE** AND H.G.A. BURTON.

*J. Phys. Chem. A*

**127**, 4538 (2023)

## Connections between many-body perturbation and coupled-cluster theories

R. QUINTERO-MONSEBAIZ, E. MONINO, **A. MARIE** AND P.F.L. LOOS.

*J. Chem. Phys.*

**157**, 231102 (2022)

## Real space Mott-Anderson electron localization with long-range interactions: exact and approximate descriptions

**A. MARIE**, D.P. KOOI, M. SEIDL, Z.H. MUSSIMANI, K. GIESBERTZ AND P. GORI-GIORGI.

*Phys. Rev. Res.*

*Editors' suggestion*

**4**, 043192 (2022)

## Variational coupled cluster for ground and excited states

**A. MARIE**, F. KOSSOSKI, AND P.F. LOOS.

*J. Chem. Phys.*

**155**, 104105 (2021)

## Excited states from state specific orbital optimized pair coupled cluster

F. KOSSOSKI, **A. MARIE**, A. SCEMAMA, M. CAFFAREL, AND P.F. LOOS.

*J. Chem. Theory Comput.*

**17**, 4756 (2021)

## Perturbation theory in the complex plane: Exceptional points and where to find them

**A. MARIE**, H.G.A. BURTON, P.F. LOOS.

*J. Phys. Cond. Mat.*

**33**, 283001 (2021)

## Talks

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### ETSF Correlation meetings

BETHE-SALPETER EQUATION FOR THE PARTICLE-PARTICLE PROPAGATOR

*Palaiseau, France*

Dec. 2024

### 6<sup>th</sup> Workshop on "Green's function methods: the next generation"

ANOMALOUS PROPAGATORS AND THE PARTICLE-PARTICLE CORRELATION CHANNEL OF MANY-BODY PERTURBATION THEORY

*Toulouse, France*

Oct. 2024

### Lennard-Jones Center (LJC) seminar series

ANOMALOUS PROPAGATORS AND THE PARTICLE-PARTICLE CORRELATION CHANNEL OF MANY-BODY PERTURBATION THEORY: HEDIN'S EQUATIONS

*Cambridge, United Kingdom*

Jul. 2024

### Journée "Théorie, Modélisation et Simulation"

REFERENCE ENERGIES FOR VALENCE IONIZATIONS AND SATELLITE TRANSITIONS

*Strasbourg, France*

Oct. 2023

## Teaching/mentoring

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**Bachelor** Introduction to Python and algorithmic (2022-2024)

**Master** Supervised two first-year master internships (2024)