Curriculum Vitae

Dr. Marios-Petros Kitsaras
Postdoctoral researcher
Laboratoire de Chimie et Physique Quantiques (UMR 5626)
Université de Toulouse, CNRS
Toulouse, France

📧 kitsaras@irsamc.ups-tlse.fr

🌐 https://mpkitsaras.com,
https://orcid.org/0000-0002-9549-3674

Personal information

First Name	Marios-Petros
Last Name	Kitsaras
Birthday	20th April 1993
Nationalities	Greek, German
Languages	Greek (native), English (C2), German (C1), Italian (B2), French (B1)
Address	Bat. 3R1b4 - 118 route de Narbonne, 31062 Toulouse Cedex 09, France

Education

- 2019–2023 | Ph.D. in Chemistry, Johannes-Gutenberg University of Mainz, Germany (summa cum laude)
- 2016–2019 | M.Sc. in Chemistry, Free University of Berlin, Germany (very good)
- 2011–2015 | B.Sc. in Chemistry, University of Athens, Greece (excellent)
- 2025 | Mini-school on mathematics for theoretical chemistry and physics (Machine Learning), GDR NBODY, Paris, France
- 2021 | Molecular response properties summer school (MRPSS 2021), Stockholm, Sweden
- 2019 | European summer school in quantum chemistry (ESQC 2019), Sicely, Italy

Professional and Academic Experience

- 2024–present | Postdoctoral researcher in the group of Dr. Pierre-François Loos
  University of Toulouse, CNRS, Toulouse, France
- 2023–2024 | Postdoctoral researcher in the group of Prof. Dr. Stella Stopkowicz
  Saarland University, Saarbrucken, Germany
- 2019–2023 | Scientific staff member in the Theoretical Chemistry group
  (PhD student supervised by Prof. Dr. Jürgen Gauss and Prof. Dr. Stella Stopkowicz)
  Johannes-Gutenberg University Mainz, Mainz, Germany

Teaching Experience

- 2025 | Tutor in the Modern Wavefunction Based Methods in Electronic Structure Theory Summer School (MWM 2025), Pisa, Italy
- 2024 | Tutor in the European Summer school in Quantum Chemistry (ESQC 2024), Sicely, Italy
- 2023 | Tutor in the Modern Wavefunction Based Methods in Electronic Structure Theory Summer School (MWM 2023), Pisa, Italy
- 2023-2024 | Tutorials and Practica for Theoretical Chemistry 1, Theoretical Chemistry 2, Chemistry in the Computer, Introduction to Quantum Mechanics, Physical Chemistry (Thermodynamics and Kinetic Gas theory)
  Saarland University, Saarbrucken, Germany
- 2019-2023 | Tutorials and Practica for Theoretical Chemistry 1, Theoretical Chemistry 2
  Johannes-Gutenberg University Mainz, Mainz, Germany
- 2019-2023 | Co-supervision of Bachelor Theses and research projects
  Johannes-Gutenberg University Mainz, Mainz, Germany
  - "Hochgenaue Equation-of-motion Coupled Cluster Methoden für Moleküle in starken Magnetfeldern", 2022 (Bachelor thesis)
  - "Anregungen von Ethen und Ethin im magnetischen Feld", 2020 (research project)
  - "Moleküle in starken Magnetfeldern mit Coupled-Cluster Methoden", 2020 (Bachelor thesis)

Presentations and Invited Talks

- 2025 | Poster presentation "Analytic G_0W_0 gradients: An IP/EA-EOM-λ-rCCD reformulation" in the 61st Symposium on Theoretical Chemistry (STC 2025), Berlin, Germany
- 2025 | Invited communication "Towards Bethe-Salpeter equation excited-state gradients" in the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025), Oslo, Norway
- 2025 | Contributed talk "Analytic G_0W_0 gradients: An IP/EA-EOM-λ-rCCD reformulation" in the Interdisciplinary conference on many-body theory (NBODY 2025), Nancy, France
- 2025 | Poster presentation "Analytic G_0W_0 gradients: An IP/EA-EOM-λ-rCCD reformulation" in the Emerging Excited-State Methods in Electronic Structure 2025, Toulouse, France
- 2024 | Invited talk "Geometry optimizations for ground and excited states using finite magnetic field coupled-cluster theory" in the workshop New Developments in Coupled-Cluster Theory 2024 (Telluride science research center), Telluride, USA
- 2024 | Poster presentation "Geometry optimizations in the presence of strong magnetic fields: Rotational energy dependence of CH and C_2 via Coupled-Cluster theory" in the European Seminar on Computational Methods in Quantum Chemistry (Strasbourg Seminar) (ESCMQC 2024), Copenhagen, Denmark
- 2023 | Poster presentation "Atoms and molecules in the atmospheres of magnetic White Dwarfs" in the 17th International Congress for Quantum Chemistry (ICQC 2023), Bratislava, Slovakia

- 2021 | Poster presentation “CC2 and CC3 methods in finite magnetic-field calculations” in the 57th Symposium on Theoretical Chemistry (STC 2021), Wurzburg, Germany

Awards and Honors

- 2016 | Deutscher Akademischer Austauschdienst (DAAD) Scholarship - Master Studies for All Academic Disciplines, 2016/17
- 2011 | State Scholarships Greece (IKY), Monetary award for the highest entry grade in the bachelor program of the chemistry department

Technical / Research Skills

- Extensive experience in programming in C/C++, Fortran, Python
- Experience in Linux/Unix environments

Quantum Chemical Programs

- QCUMBRE (https://www.qcumbre.org/) Maintainer/Developer
- CFOUR (https://cfour.uni-mainz.de) Developer
- COrbit19, Complex Orbital visualization (https://gitlab.com/mariospeterkits/corbit19) Creator

Other skills and interests

- Diplomas in piano and classical music theory
- Former member of the Greek scouts movement (2012-2015)