

Emmanuel Fromager

Institut de Chimie de Strasbourg, Laboratoire de Chimie Quantique, Université de Strasbourg, Strasbourg, France.

Date of birth: April, 2nd 1979

Nationality: French

Family: married, one child

Current position: Full Professor (Professeur des Universités), University of Strasbourg

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Education and employment

Sept. 2019- ... Full Professor (Professeur des Universités),
Laboratoire de Chimie Quantique, Chemistry Institute (UMR 7177), University of Strasbourg,
France.

Oct. 2013 Habilitation degree (HDR), University of Strasbourg, France.
Thesis title: *"Methods development in quantum chemistry: multi-determinant density-functional theory for ground and excited states"*.

2012-2013 One-year sabbatical at the CNRS ("délégation"),
Laboratoire de Chimie Quantique, Institut de Chimie, University of Strasbourg, France.

2008-2019 Maître de Conférences (Associate Professor),
Laboratoire de Chimie Quantique, Chemistry Institute, University of Strasbourg, France.

2007-2008 Post-doc assistant, Prof. K. Ruud, Center for Theoretical and Computational
Chemistry, Department of Chemistry, University of Tromsø, Norway.
Research project: *development of time-dependent multiconfigurational range-separated
linear response theory*.

2005-2007 Post-doc assistant, Prof. H. J. Aa. Jensen, Department of Physics and Chemistry,
University of Southern Denmark, Denmark.
Research project: *development of multiconfigurational range-separated density-functional
theory*.

2002-2005 Co-supervised PhD (“thèse en cotutelle”) in the Laboratory of Quantum Physics, IRSAMC, Paul Sabatier University, Toulouse, France *and* Albanova University Center, Institute of Physics, Stockholm, Sweden.

Supervisors: Prof. Christian Teichteil (Toulouse), Dr. Laurent Maron (Toulouse), and Prof. Ulf Wahlgren (Stockholm).

Thesis title: *"Treatment of spin-orbit interaction in quantum chemistry and application in actinide chemistry"*.

2002 Master's degree in Physics of matter, Laboratory of Quantum Physics, IRSAMC, Paul Sabatier University, Toulouse, France.

2002 Engineering diploma from the “École Nationale Supérieure de l’Aéronautique et de l’Espace” (SUPAERO), Toulouse, France.

Teaching

I teach theoretical chemistry (192 hours per year) at the University of Strasbourg. I give lectures and/or tutorials on mathematics, quantum mechanics and advanced quantum chemistry (wavefunction and density-functional theories) at both undergraduate and master levels. My lecture notes are available online: <https://lcqs.unistra.fr/teaching/>

Current research topics

- **Ensemble density functional theory** of excited states.
- **Quantum embedding** theories for strongly correlated electrons.

On-going grants

2021-2023: « Initiative d’Excellence » (**IdEx**) grant, Université de Strasbourg (funding for a 18-month postdoc position),
project's title: *"Rewriting density functional theory for ensembles: Towards an in-principle-exact description of density-driven correlations and coupling terms"*.

2023-2026: “Interdisciplinary Thematic Institute in Quantum science & nanoMATERials ” (ITI-QMAT) and “QuantEdu-France” grant, Université de Strasbourg (funding for a 3-year PhD position),
project's title: *"Quantum implementation of a Functional-Free Density-Functional Theory"*.

Past grants

2019-2022: LabEx “Chemistry of Complex Systems”, Strasbourg (113000 €), project's title: *“Towards a systematically improvable density matrix functional embedding theory for strongly correlated electronic systems”*.

2014-2019: Young researcher **ANR** grant (JCJC), 127000 €.

2013-2016 : LABEX, “Chemistry of Complex Systems”, Université de Strasbourg, 96000 €.

Scientific production

51 publications in international peer-reviewed rank A journals (+3 papers in preparation); **52** oral communications in international conferences (including **44** invited lectures); **4** plenary lectures in French national meetings, **48** invited seminars; **1488 citations**; H-index **23** (Google Scholar on 19/10/2023).

A complete list of my publications is available on Google Scholar:

<https://scholar.google.fr/citations?user=6S8Or18AAAAJ&hl=fr>

Award

2017 Scientific young researcher Prize “Les espoirs de l’Université de Strasbourg” (10000€), University of Strasbourg.

Invited Professor positions

February 2017 University of Nagoya, Department of Physics, Nagoya, Japan.

January 2022 Tokyo Metropolitan University, Department of Chemistry, Tokyo, Japan.

Other activities

- **Appointed member** of the French national scientific research committee (CoNRS), “Chemical Physics” section (the so-called “section 13”), period: 2021-2025.
- **Head** (since February 2022) of the Laboratory of Quantum Chemistry in Strasbourg (LCQS), Institute of Chemistry, University of Strasbourg.
- **Elected member** of the “*Modeling and Simulation*” board, division of Physical Chemistry, French Chemical Society (SCF), periods: 2018-2021 and 2021-2024.
- **Board member** of the national research group on theoretical spectroscopy (GDR REST).
- **Board member** of the national research group on the many-body problem (GDR NBODY).
- **Founder and organizer** of the ISTPC summer school on correlation in electronic structure theory <<https://quantique.u-strasbg.fr/ISTPC/>>.
- **Scientific Committee member**, “*New horizons in density functional theory*” Faraday Discussion, 2 - 4 September 2020, Online, United Kingdom.

<https://www.rsc.org/events/detail/37136/new-horizons-in-density-functional-theory-faraday-discussion>

- **Chairman and organizer** of the ICQC satellite meeting on strong electron correlation, June 2018, Strasbourg, France. <https://quantique.u-strasbg.fr/icqc18-sat-strasbourg/index.php>.

Opponent/reviewer in PhD/Habilitation jurys

I have been member of **18** PhD jurys (8 times as reviewer) and **4** Habilitation jurys (3 times as reviewer).