Antoine Aerts

Email : antoine.aerts@ulb.be
+32 476 70 23 79
Professional address: CP 160/09 Av. Roosevelt 50, 1050 Bruxelles, Belgique

Education

- **Université libre de Bruxelles** — Brussels, Belgium
  PhD of Science (Chemistry). — *Oct 2017- Aug 2022*
- **Université libre de Bruxelles** — Brussels, Belgium
  Master of Science in Chemistry; Research Focus Program. A (ECTS grading scale) — *2015 - 2017*

Languages

French: Mothertongue. **English**: Very good command. **Dutch**: Basic communication skills.

Programming Skills

- **Languages**: Python, Fortran, Bash
- **Technologies and Frameworks**: Tensorflow, Keras, LaTeX, jobs scheduling (TORQUE, SLURM)

Experience

- **Université libre de Bruxelles** — Brussels, Belgium
  Post-doc *at SQUARES (Department of Chemistry);* ***Lecturer*** *- Science and SBS-EM* — *Oct 2022 - Sept 2025*
  - **Teaching:**
    - 2022 - ... Structures et symétries moléculaires (CHIMF304, bachelor)
    - 2022 - ... Approches computationnelles des états de la matière (CHIMF443, master)
    - 2022 - ... Chimie physique moléculaire : structure, spectroscopie et dynamique (CHIMF401, master)
    - 2024 - 2025 Chemistry (CHIMS171, bachelor)
- **Université libre de Bruxelles** — Brussels, Belgium
  Teaching assistant *- first year general chemistry course - Faculty of Science* — *Oct 2017 - Sept 2022*
  - Design, setup and improvement of online ressources using Moodle : quizzes (recurrent tests and finals (COVID)) and laboratory learning material.
  - Recurrent (in person and online) seminars for supervised numerical problems solving.
  - Recurrent (in person) laboratory co-supervision (groups of 48 students): basic analytic laboratory equipment and methods.
  - Supervision of end-of-the-year bibliographic research.
  - Design and marking of student reports and finals.
- **University of Alberta** — Edmonton, Canada
  Research assistant - Computational and Theoretical Chemistry Group (A. Brown) — *Sep 2016 - Dec 2016*
  - High accuracy computation of Electric Field Gradients around aluminum nucleus in small molecules.
  - Co-supervision of an undergraduate project in computational chemistry.
- **Consultant - Junior Data Architect** — La Hulpe, Belgium
  Society for Worldwide Interbank Financial Telecommunication (SWIFT) — *2013 - 2017*
  - Consultant for the SWIFTRef team. Reference : Karel Spiritus, karel.spiritus@swift.com

Awards and fellowships

- **Gustave Boël Sofina Fellowship 2020** (20 800 eur) Awarded by the Roi Baudoin foundation (7 recipients in 2020 amongst all universities and all disciplines in Belgium). **12 months** research project at the university of Alberta in 2021: "Laser quantum control of model chemical processes and accurate electronic structure of polyatomic molecules."
- **Bourse d'Excellence WBI 2020** (6360 eur) Travel and research grant, summer 2020, declined (COVID 19).
- **Bourse de voyage de la communauté Française 2020** (∼4000 eur) Declined.
- **CCCI ULB 2019** (4000 eur) Travel and research grant, summer 2019 (**5 months**) at the University of Alberta, Canada.
- **Solvay Award 2017** (250 eur) Best master thesis of the chemistry department of the Université libre de Bruxelles, invited talk at the annual conference of the Royal Chemistry Society of Belgium.
- **Prigogine Award 2017** (400 eur) Best GPA amongst chemistry master students in 2016-2017 academic year. Awarded by the Instituts Internationaux de Physique et de Chimie.

Peer-reviewed Publications

- Mahsa N. Ashani, Qinan Huang, A. Mackenzie Flowers, Alex Brown, Antoine Aerts, Alberto Otero-de-la-Roza, and Gino A. DiLabio. **Accurate Potential Energy Surfaces Using Atom-Centered Potentials and Minimal High-Level Data.** *J. Phys. Chem. A*, 127(38):8015, 2023.
- Antoine Aerts, Spencer W. Jolly, Pascal Kockaert, Simon-Pierre Gorza, Jean Vander Auwera, and Nathalie Vaeck. **Modulated super-Gaussian laser pulse to populate a dark rovibrational state of acetylene.** *J. Chem. Phys.*, 159(8):084303, 2023.
- Antoine Aerts, Alex Brown, and Fabien Gatti. **Intramolecular Vibrational Redistribution in Formic Acid and its Deuterated Forms.** *J. Chem. Phys.*, 157(1):014306, 2022.
- Antoine Aerts, Moritz R. Schäfer, and Alex Brown. **Adaptive Fitting of Potential Energy Surfaces of Small to Medium-Sized Molecules in Sum-of-Product Form: Application to Vibrational Spectroscopy.** *J. Chem. Phys.*, 156(16):164106, 2022.
- Antoine Aerts, Pascal Kockaert, Simon-Pierre Gorza, Alex Brown, Jean Vander Auwera, and Nathalie Vaeck. **Laser control of a dark vibrational state of acetylene in the gas phase - Fourier transform pulse shaping constraints and effects of decoherence.** *J. Chem. Phys.*, 156(8):084302, 2022.
- Antoine Aerts, Jean Vander Auwera, and Nathalie Vaeck. **Lindblad parameters from high resolution spectroscopy to describe collision-induced rovibrational decoherence in the gas phase – Application to acetylene.** *J. Chem. Phys.*, 154(14):144308, 2021.
- Antoine Aerts, Philippe Carbonnière, Falk Richter, and Alex Brown. **Vibrational states of deuterated *trans*- and *cis*-formic acid: DCOOH, HCOOD, and DCOOD.** *J. Chem. Phys.*, 152(2):024305, 2020.
- Antoine Aerts and Alex Brown. **A revised nuclear quadrupole moment for aluminum: Theoretical nuclear quadrupole coupling constants of aluminum compounds.** *J. Chem. Phys.*, 150(22):224302, 2019.

Academic Conferences

- **HDQD, Hamburg, Germany 2024** (*Poster*) Aerts, A., and Vaeck, N. Defy the Curse of Dimensionality in Potential Energy Surfaces with Sparse Grids and Local Polynomial Interpolation.
- **ViRAPID Workshop, Vienna, Austria 2024** (*Poster*) Aerts, A., and Vaeck, N. Non-covalent interactions on interstellar water ice using xTB and AIQM1.
- **SMLQC2023, Uppsala, Sweden 2023**
- **IMAMPC2023, Innsbruck, Austria 2023** (*Poster*) Aerts, A., and Vaeck, N. Exploring the nature of the vibrational motion: Applications to laser quantum control.
- **METAMORPHOSE, Brussels, Belgium 2023** (*Talk*) Aerts, A., and Vaeck, N. The nature of molecular vibrations: theoretical investigation and use in laser quantum control.
- **HDQD, Groningen, Netherlands 2022** (*Talk*) Aerts, A., and Brown, A. "Black-box" methods for fitting potential energy surfaces for quantum dynamics.
- **HDQD, Groningen, Netherlands 2022** (*Poster*) Aerts, A., Schäfer R. M., and Brown, A. Adaptive Fitting of Potential Energy Surfaces of Small to Medium-Sized Molecules in Sum-of-Product Form: Application to Vibrational Spectroscopy.
- **International Symposium on Molecular Spectroscopy (ISMS), University of Illinois-Urbana Champaign, USA. 2022** (*Talk*) Aerts, A., Jolly, S., Kockaert, P., Gorza, S.-P., Vander Auwera, J., and Vaeck, N. Pulse induced dark state of acetylene.
- **Virtual Symposium on Theoretical and Computational Chemistry in Canada, Online Canada. 2021**
- **Solvay Workshop on "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics", Brussels, Belgium. 2019** (*Poster*) Aerts, A., and Brown, A. A revised nuclear quadrupole moment for aluminum: Theoretical nuclear quadrupole coupling constants of aluminum compounds.
- **Gordon Research Conference (and Seminar) on Quantum Control of Light and Matter, Newport (RI), USA. 2019** (*Poster*) Aerts, A., Brown, A., and Vaeck, N. Laser Control of a Markovian System : Populating a dark state.
- **HDQD, Lille, France. 2018** (*Poster*) Aerts, A., Brown, A., and Vaeck, N. Laser Control of a Markovian System : Experimental Constraints.
- **METAMORPHOSE, Louvain-la-Neuve, Belgium. 2018** (*Talk*) Aerts, A., Santos, L., and Vaeck, N. Quantum Control of a Markovian System.
- **Société Royale de Chimie One-day conference, Louvain-la-Neuve, Belgium. 2017** (*Talk*) Quantum Control of a Markovian System.
- **Quantum Chemistry in Belgium, Brussels, Belgium 2017** (*Poster*) Aerts, A., Santos, L., and Vaeck, N. Laser Control of a Markovian System.

Graduate students supervision

- **Moritz R. Schäfer (MSc Thesis)** Potential Energy Surface fitting - from the Heidelberg University (2021)
- **Dieter Maes (MSc Internship)** Potentiel Energy Curves and vibrational states of CO^{+2} - from KU Leuven (2023)
- **Anouar El Abbadi (MSc Thesis)** Potential Energy Surface fitting using POTFIT and Adaptive - ULB (2023)
- **Imad Agrida (MSc Internship)** Force fields for Iodine containing molecules in molecular dynamics - ULB (2023)
- **Richa Salaheddine (MSc Internship)** Atoms on Amorphous Water Ice - ULB (2023)
- **A. Mackenzie Flowers (MSc Thesis)** Vibrational spectra of molecules in interstellar media: highly accurate structures and PESs - from UofA, Edmonton (2023)
- **Xavier Huet (MSc Thesis)** Rovibronic Spectra of Carbon Monoxide Dication CO^{+2} - ULB (2024)
- **Gaetan Olbrechts (MSc Internship)** Atoms on amorphous ice: from physi- to chemisorption - from VUB (2024)

Service to the scientific community

- **Reviewer** for the *Journal of Chemical Physics*.
- **Contribution to ULB administration**
    - Representative of the scientific staff at the Department of Chemistry Council: 2018-2024, 2025-...
    - Member of the Teaching Committee: 2018-2024, 2025-...
    - Member of the Nomination Committee: 2018-2022
    - Member of the Department of Chemistry Board: 2018-2022, 2025-...