

# Edison Florez Ph.D., M.Sc.

Computational Physicist | Algorithm Developer  
Data Scientist | Business Analyst

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**Technical Skills:** Python • C++ • Fortran • Data Base (SQL/NoSQL) • Visualization • Linux • Bash • OpenMP • HPC • Git • Testing/TDD • CI/CD • Docker • L<sup>A</sup>T<sub>E</sub>X

**Key Skills:** Complex problem solving • Critical thinking • Creativity • Leadership • Teamwork • Project Management • Communication • Time management

**Profile:** As a data scientist with a profound background in quantum mechanics, biophysics, and mathematics, I bring over eight years of experience, having served as a researcher, algorithm developer, data scientist, business analyst and team leader. My passion lies in extracting fundamental insights from data, thinking critically, and understanding the rationale behind each task. With my ability to learn quickly and motivation to take on challenges, I have

excelled as a team player and individual contributor, taking calculated risks and showing initiative. My experience spans consulting for biotech startups and the financial industry, where I develop and validate scalable algorithms, and work collaboratively to deliver top-quality, data-driven solutions. In my spare time, I enjoy intellectual pursuits like drawing and writing about science fiction. I am a beer and cycling enthusiast, although not all simultaneously.

## Academic Background

- **Doctor of Philosophy** July 2023  
Computational Physics, Massey University, New Zealand
- **Master of Science** December 2014  
Computational Chemistry, University of Antioquia, Colombia
- **Bachelor of Science** July 2012  
Chemistry, University of Antioquia, Colombia

## Fellowships and Awards

- **Ph.D. in Physics:** Massey University Doctoral Scholarship
- **M.Sc. in Chemistry:** Honours and research work with meritorious award.

## Professional Experience

- **Computational Physics** Aug.2021 - Aug 2023  
HelicoBio [[helico.bio](https://helico.bio)], New Zealand  
COMPUTATIONAL PROTEIN DESIGNER: Leveraging in-depth knowledge of biophysics and protein design, I created and validated scalable algorithms to advance plant biology research.

As a **TEAM LEADER**, I collaborated with cross-functional groups to deliver high-quality, data-driven solutions. I contributed to all phases of the software development lifecycle, including the development, testing, and deployment of new functionalities using Python and C++. A notable achievement was leading the development of a protein design platform for running all-atom molecular dynamics simulations. I have direct experience using Molecular Dynamics packages like GROMACS and OpenMM, also Alphafold and other bioinformatics tools.

- **Freelancer Editor**

Enago [[enago.com](https://enago.com)], Remote

Since Apr.2023

MDPI [[mdpi.com](https://mdpi.com)], Remote

Apr.2018 - Dec.2018

**COPY & SUBSTANTIVE EDITING:** I perform Copy Editing, refining grammar and scientific terminology; and Substantive Editing, enhancing manuscript structure and content, clarifying ambiguous text, and verifying citation relevance. This helps authors aiming for high-impact journals and those requiring extensive language assistance.

- **Demonstrator**

Aug.2018 - Mar.2020

Massey University [[massey.ac.nz](https://massey.ac.nz)], New Zealand

**PHYSICS:** Instruct and advise students in workshops, with an emphasis on intricate topics such as advanced mechanics, thermodynamics, fluid dynamics, magnetic field theory, electromagnetism, and circuit analysis. My role is instrumental in enhancing students' understanding of these complex physical concepts and principles.

- **Data Scientist**

Aug.2016 - Mar.2018

EY-ibf [[ey.com](https://ey.com)], Colombia.

**SAP-IMPLEMENTATION AND BANK-ANALYZER:** Develop tailored solutions based on thorough business and technical analyses, primarily within SAP for Analytical Banking and Business Intelligence. I specialize in crafting complex models and implementing them, addressing economic problems through customized solutions. Additionally, I developed and implemented mathematical models related to financial inquiries, providing detail-oriented and pragmatic solutions.

- **Graduate Teaching Assistant**

Sept.2015 - Aug.2016

University of Antioquia [[udea.edu.co](https://udea.edu.co)], Colombia.

**QUANTUM & COMPUTATIONAL CHEMISTRY:** Guide advanced college students through the intricate domain of Quantum Chemistry. I ensure students achieve proficiency in the quantum language, comprehend relevant methods, and grasp key concepts. Furthermore, I facilitate their understanding of the interpretation and application of these principles in chemically interesting systems.

## Publications

1. **Flórez, Edison;** Zapata-Escobar, Andy; Ferraro, Franklin; Ibarguen-Becerra, César; Chamorro, Yuly; and Maldonado, Alejandro F. "Coordination of Mercury (II) in Water Promoted over Hydrolysis in Solvated Clusters  $[\text{Hg}(\text{H}_2\text{O})_{1-6}]_{(aq)}^{2+}$ : Insights from Relativistic Effects and Free Energy Analysis." [Accepted by The Journal of Physical Chemistry A](#)

2. **Flórez, Edison**; Reuvers, Tom; Schwarz, WH Eugen and Peter Schwerdtfeger. "The Stability of the Noble Gas Fluorides from Nonrelativistic and Relativistic Density Functional and Coupled Cluster Studies." [Submitted](#)
3. **Flórez, Edison**; Odile R. Smits; Jan-Michael Mewes; Paul Jerabek; and Peter Schwerdtfeger. "From the gas phase to the solid state: The chemical bonding in the superheavy element flerovium." *The Journal of Chemical Physics* 157, no. 6 (2022): 064304. DOI: [10.1063/5.0097642](https://doi.org/10.1063/5.0097642)
4. Chamorro, Yuly; **Flórez, Edison**; Alejandro F. Maldonado; Gustavo A. Aucar; and Albeiro Restrepo. "Microsolvation of heavy halides." *International Journal of Quantum Chemistry* 121, no. 7 (2021): e26571. DOI: [10.1002/qua.26571](https://doi.org/10.1002/qua.26571)
5. **Flórez, Edison**; Helgaker, Trygve; Klopper, Wim; Teale, Andrew; Stopkowitz, Stella; and Pahl, Elke. "Melting Under Extreme Conditions: Ab Initio Monte Carlo Simulations." In *APS March Meeting Abstracts*, vol. 2019, pp. C17-001. 2019. [ui.adsabs.harvard.edu/abs/2019APS..MARC17001F](https://ui.adsabs.harvard.edu/abs/2019APS..MARC17001F)
6. **Flórez, Edison**; Alejandro F. Maldonado; Gustavo A. Aucar; Jorge David; and Albeiro Restrepo. "Microsolvation of methylmercury: structures, energies, bonding and NMR constants ( $^{199}\text{Hg}$ ,  $^{13}\text{C}$  and  $^{17}\text{O}$ )." *Physical Chemistry Chemical Physics* 18, no. 3 (2016): 1537-1550. DOI: [10.1039/c5cp04826e](https://doi.org/10.1039/c5cp04826e)

## Open-Source Contributions

- **Parallel Tempering Monte Carlo (PTMC)**: This project introduces an advanced Fortran (2003) code that uses the Parallel Tempering Monte Carlo (PTMC) method for an accurate and efficient analysis of phase transitions in atomic and molecular clusters. Code available on [github.com/e-florez/PTMC](https://github.com/e-florez/PTMC)
- **Atomic and Molecular Cluster Energy Surface Sampler (AMCESS)**: An open-source Python package that automates the exploration of the Potential Energy Surface (PES) for atomic and molecular clusters. AMCESS uses advanced optimization techniques to generate candidate structures for critical points on the PES, enhancing research accuracy and efficiency. Code available on [github.com/e-florez/amcess](https://github.com/e-florez/amcess)

## Supervisions

- Co-supervisor M.Sc. thesis, computational chemistry Apr.2018 - Feb.2020  
**Microsolvation of Heavy Halides  $[\text{X}(\text{H}_2\text{O})_{1-6}]^-$  ( $\text{X} = \text{Br}, \text{I}, \text{At}$ )**  
University of Antioquia [[udea.edu.co](https://udea.edu.co)], Colombia.
- Co-supervisor B.Sc. thesis, computational chemistry Nov.2015 - Dec.2017  
**Relativistic and Electron Correlation Effects on the Calculation of Nuclear Magnetic Resonance Parameters on MX Diatomic Molecules ( $\text{M}=\text{Cu}, \text{Ag}, \text{Au}$  and  $\text{X}=\text{F}, \text{Cl}, \text{Br}, \text{I}$ )**  
University of Antioquia [[udea.edu.co](https://udea.edu.co)], Colombia.

References available upon request

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Yours sincerely,

**Edison Florez**

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Auckland, New Zealand.

