

# Javier Emilio Alfonso Ramos

PHD STUDENT · COMPUTATIONAL CHEMIST

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“Be brave enough to be bad at something new.”

## Summary

PhD student at Chimie ParisTech - PSL Université. My research is focused on combining machine learning methods and density functional theory calculations to accelerate the exploration and analysis of chemical reactivity. Previous experience in the use of computational methods to investigate the chemical reactivity of diverse molecular systems. Interested in learning new technologies and tools if the need arises.

## Education

### Chimie ParisTech - PSL Université

Paris, France

#### PHD CHEMISTRY

2023 - present

- Advisor: Prof. Thijs Stuyver

### University of Havana

Havana, Cuba

#### BSC CHEMISTRY

2017 - 2022

- Thesis: “Origins of regioselectivity in 1,3-dipolar cycloaddition of acylnitrile ylides”
- Advisor: Dr. Gerardo M. Ojeda Carralero

## Skills & Softwares

Languages	Spanish, English
Programming	Python, Bash, elementary C
Quantum chemistry package	Gaussian, xTB, CREST, ORCA, MOPAC, MultiWFN
Machine learning package	Keras, TensorFlow, PyTorch, scikit-learn
Molecular visualization	GaussView, CYLView, VMD, ChemCraft, Avogadro

## Publications

### PREPRINTS

- [1] J. E. **Alfonso-Ramos**, C. Adamo, E. Bremond, and T. Stuyver, “Improving the reliability of, and confidence in, dft functional benchmarking through active learning,” ChemRxiv, 2024.
- [2] M. Piejko, J. E. **Alfonso-Ramos**, J. Moran, and T. Stuyver, “Abiotic ribonucleoside formation in aqueous microdroplets: Mechanistic exploration, acidity, and electric field effects,” ChemRxiv, 2024.

### PUBLISHED

- [3] L. A. Montero-Cabrera, A. L. Montero-Alejo, A. Aspuru-Guzik, J. M. García de la Vega, M. Piris, L. A. Díaz-Fernández, Y. Pérez-Badell, A. Guerra-Barroso, J. E. **Alfonso-Ramos**, J. Rodríguez, M. E. Fuentes, and C. M. de Armas, “Alternative CNDOL Fockians for fast and accurate description of molecular exciton properties,” *J. Chem. Phys.*, 2024.
- [4] J. E. **Alfonso-Ramos**, R. M. Neeser, and T. Stuyver, “Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: Application to hydrogen atom transfer reactions,” *Digit. Discov.*, 2024.
- [5] N. Casetti, J. E. **Alfonso-Ramos**, C. W. Coley, and T. Stuyver, “Combining Molecular Quantum Mechanical Modeling and Machine Learning for Accelerated Reaction Screening and Discovery,” *Chem. A Eur. J.*, 2023.

- [6] J. E. **Alfonso-Ramos**, R. Van Lommel, D. Hernández-Castillo, F. De Proft, R. González-Alemán, E. V. Van der Eycken, and G. M. Ojeda-Carralero, "Origins of the Reactivity in 1,3-Dipolar Cycloadditions of Acyl Isocyanide Ylides," *Eur. J. Org. Chem.*, 2023.
- [7] S. Pillitteri, P. Ranjan, G. M. Ojeda-Carralero, L. Y. Vázquez Amaya, J. E. **Alfonso-Ramos**, E. V. Van der Eycken, and U. K. Sharma, "Merging dual photoredox/cobalt catalysis and boronic acid (derivatives) activation for the Minisci reaction," *Org. Chem. Front.*, 2022.
- [8] J. Coro-Bermello, E. R. López-Rodríguez, J. E. **Alfonso-Ramos**, D. Alonso, G. M. Ojeda-Carralero, G. A. Prado, and E. Moreno-Castillo, "Identification of novel thiadiazin derivatives as potentially selective inhibitors towards trypanothione reductase from *Trypanosoma cruzi* by molecular docking using the numerical index poses ratio Pr and the binding mode analysis," *SN Appl. Sci.*, 2021.

## Teaching Experience

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### AT CHIMIE PARISTECH - PSL UNIVERSITÉ

**2023 - 2025** Practical classes of *Introduction to C language* to 1<sup>st</sup>-year, Engineer Cycle (64 h, 16 students)

### AT UNIVERSITY OF HAVANA

**2021 - 2023** Practical classes of *Spectroscopy* to 4<sup>th</sup>-year, BSc Chemistry, School of Chemistry

**2021 - 2022** Practical classes of *Informatics in Chemistry* to 1<sup>st</sup>-year, BSc Chemistry, School of Chemistry

**2021 - 2022** Practical classes of *General Chemistry* to 1<sup>st</sup>-year, BSc Biochemistry, School of Biology

**2019 - 2022** Workshops of *Fundamentals of Structure and Bonding* to 1<sup>st</sup>-year, BSc Chemistry, School of Chemistry

**2018 - 2019** Practical classes of *General Chemistry* to 1<sup>st</sup>-year, BSc Microbiology, School of Biology

**2018 - 2022** Independent tutor of *General Chemistry* and *Organic Chemistry* to undergraduate student

## Awards, Fellowships, & Grants

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2023 **National Award for Most Outstanding Student**, Cuban Chemical Society

2022 **Best Teaching Assistant Student**, School of Chemistry, University of Havana

**Best Student in Research**, School of Chemistry, University of Havana

**Scientific Merit**, University of Havana

**Mention**, IX National University Chemistry Olympiad

2015 **Gold Medal**, National Chemistry Olympiad

2014 **Gold Medal**, National Chemistry Olympiad

2013 **Silver Medal**, National Chemistry Olympiad

## Conference Presentations

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### POSTERS

#### V LatinXChem

ONLINE TWITTER EVENT. POSTER #COMP033

2024

- "Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: Application to hydrogen atom transfer reactions", **Javier E. Alfonso Ramos**; Rebecca M. Neeser; Thijs Stuyver

#### III LatinXChem

ONLINE TWITTER EVENT. POSTER #COMP068

2022

- "Drug repositioning for SARS-COV-2: Search for 3CL protease inhibitors using pharmacophore-based virtual screening, molecular docking and molecular dynamics", Rafael Perurena; **Javier E. Alfonso Ramos**; Karel A. Barberena Morales; Osmany Guirola Cruz

## II LatinXChem

ONLINE TWITTER EVENT. POSTER #COMP099

2021

- "Origins of regioselectivity in 1,3-dipolar cycloaddition of acylnitrile ylides", **Javier E. Alfonso Ramos**; Roy Gonzalez Aleman; Gerardo M. Ojeda Carralero; David Hernandez Castillo

## Extracurricular Activity

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### VOLUNTEER

2023 55<sup>th</sup> International Chemistry Olympiad, Team Guided

*Switzerland*