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, "Cyclo70: A new challenging pericyclic benchmarking set for kinetics and thermochemistry evaluation," 2025. DOI: 10.26434/chemrxiv-2025-vqx4m-v2.

[2] M. Ferrer, B. Deng, J. E. **Alfonso-Ramos**, and T. Stuyver, "Screening diels-alder reaction space to identify candidate reactions for self-healing polymer applications," 2025. DOI: 10.26434/chemrxiv-2025-kv6n0.

Published

[3] J. E. **Alfonso-Ramos**, C. Adamo, E. Bremond, and T. Stuyver, "Improving the reliability of, and confidence in, DFT functional benchmarking through active learning," *J. Chem. Theory Comput.*, 2025.

[4] M. Piejko, J. E. **Alfonso-Ramos**, J. Moran, and T. Stuyver, "Abiotic ribonucleoside formation in aqueous microdroplets: Mechanistic exploration, acidity, and electric field effects," *ChemistryEurope*, 2025.

[5] 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.

[6] 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.
[7] 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.
[8] 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.
[9] 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.
[10] 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.

Book Chapter

[11] T. Stuyver and J. **Alfonso-Ramos**, "Construction of training datasets for chemical reactivity prediction through computational means," in *Artificial Intelligence in Catalysis*. John Wiley & Sons, Ltd, 2025, ch. 4, pp. 83–104.

Teaching Experience

at Chimie ParisTech - PSL Université

2023 - 2025 Practical classes of *Introduction to C language* to 1^{st}-year, Engineer Cycle (64 h, 16 students)

at University of Havana

2021 - 2023 Practical classes of *Spectroscopy* to 4^{th}-year, BSc Chemistry, School of Chemistry

2021 - 2022 Practical classes of *Informatics in Chemistry* to 1^{st}-year, BSc Chemistry, School of Chemistry

2021 - 2022 Practical classes of *General Chemistry* to 1^{st}-year, BSc Biochemistry, School of Biology

2019 - 2022 Workshops of *Fundamentals of Structure and Bonding* to 1^{st}-year, BSc Chemistry, School of Chemistry

2018 - 2019 Practical classes of *General Chemistry* to 1^{st}-year, BSc Microbiology, School of Biology

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

Awards, Fellowships, & Grants

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

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 screeing, 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

Volunteer

2023 **55^{th} International Chemistry Olympiad**, Team Guided *Switzerland*