Jessica Perrero

Curriculum Vitae

Academic career

2020 - 2024 **PhD, Chemistry**, *Universitat Autònoma de Barcelona & Università degli Studi di Torino*, Bellaterra, Spain & Torino, Italy, under the supervision of Prof. Albert Rimola Gibert and Prof. Piero Ugliengo, with a thesis project entitled "Phenomena at Interstellar Core and Mantle Grains: a Quantum Mechanical Approach". PhD thesis defended on November 20^{th}, 2024.

The aim of the project was to characterize chemical processes, such as adsorption and reactivity, taking place onto and into the dust grains present in the interstellar medium.

2018 - 2020 **MS, Chemistry**, *Università degli Studi di Torino*, Torino, awarded with a grade of *110/110 cum Laude with Honors* on October 20^{th}, 2020, under the supervision of Prof. Piero Ugliengo, with a thesis project entitled "Ab initio calculation of binding energies of sulphur containing astrochemical relevant species with crystalline interstellar ice models"

The objective of this project was to investigate the adsorption of 17 sulphur containing species, either observed or thought to be present in the interstellar medium, onto interstellar ices. The aim was to enhance the existing data on sulphur chemistry within the interstellar medium.

2015 - 2018 **BS, Chemistry and Chemical Technologies**, *Università degli Studi di Torino*, Torino, awarded with a grade of *110/110 cum Laude* on October 11^{th}, 2018, under the supervision of Prof. Piero Ugliengo, with a thesis project entitled "The sulphur depletion in the interstellar medium"

The thesis was a review of the existing literature on the topic available at the time.

Scientific profile

General subjects

During the doctorate I learned how to properly write research projects, how to deliver effective presentations to a vast audience (with expertise in different fields). Staying abroad gave me the opportunity to practice English with non-native speakers and to learn Spanish and a little of Catalan. I had the opportunity to work in a large team and learn how to organize the work. I also supervised the research of few students during their stays in the research group. I particularly appreciate writing and revising scientific articles as well as any other type of scientific text and report. I am known for being quick in completing tasks, but also for having a lot of patience and stubbornness when facing the most challenging tasks.

Computational Chemistry
During the Master and PhD theses, I gained a substantial expertise on solid modeling, using periodic quantum codes such as CRYSTAL and CP2K. Additionally, I delved into gas-phase processes utilizing well-established programs like Gaussian and Orca. The simulations conducted during this period encompassed a diverse range of studies, including adsorption processes, characterization of reaction paths (involving transition state searches and rate constant calculations), computation of IR/Raman spectra, and a limited exploration of molecular dynamics.

Prebiotic chemistry and Astrochemistry
During the Master thesis, I focused on exploring adsorption processes occurring on the surfaces of icy grains, employing models of both crystalline and amorphous water ice. The emphasis on sulphur chemistry persisted into my PhD research, where I delved into the interactions of sulfur-bearing species with silicates, specifically onto forsterite and olivine surfaces. More recently, my involvement expanded to include the examination of IR and Raman spectra of sulfur chains adsorbed onto water ice mantles. Another substantial area of investigation has been reactivity, with a particular focus on the formation of complex organic molecules (iCOMs) in the interstellar medium. This was explored on dirty ice models, composed of water and CO, as well as on small water clusters.

Experimental work
Recently, I collaborated with an experimental group from CY Cergy Paris Université, focusing on simulating the chemistry of the interstellar medium. During a one-month visit at the LERMA laboratory, I conducted experiments investigating the adsorption of ethanol and ethylamine onto both amorphous and crystalline water ice surfaces. The overarching objective is to establish concordance between computational and experimental data.

HPC projects for computational resources

2023 Computational modeling of interstellar olivine surfaces and their interaction and reactivity with HCN (QHS-2023-2-0011 & QHS-2023-3-0032): awarded with 1 500 000 + 1 500 000 CPU-hours on Picasso (UMA). PI: Albert Rimola. Co-PI: Jessica Perrero

Quantum mechanical simulations of the physico-chemical features of the silicate/water interface in interstellar nanograins (QHS-2023-2-0032): awarded with 1 600 000 CPU-hours on MareNostrum4 (BSC). PI: Albert Rimola. Co-PI: Jessica Perrero

2022 Modeling and theoretical characterization of interstellar porous ice models and their reactivity with the carbon dimer (CC) molecule (QHS-2022-3-0007 & QHS-2023-2-0011): awarded with 1 000 000 + 1 000 000 CPU-hours on MareNostrum4 (BSC). PI: Albert Rimola. Co-PI: Jessica Perrero

2021 Dynamical effects on the formation of interstellar complex organic molecules. Energy dissipation versus chemical desorption (QHS-2020-3-0018 & QHS-2021-2-0014): awarded with 950 000 + 800 000 CPU-hours on La Palma (IAC). PI: Albert Rimola. Co-PI: Jessica Perrero

Projects

2020 - present days: QUANTUMGRAIN - Quantum Chemistry on Interstellar Grains: PI: Albert Rimola. Enrolled as a PhD student.

Computer skills

Operative systems	Windows, Linux
Programming skills	Bash, Python, HTML
Office productivity softwares	Office (Word, Powerpoint, Excel), Latex
Image manipulation and videomaking	Inkscape, POVRAY, ChemSketch, Flashback Express

Chemistry softwares

Simulation codes	CRYSTAL, CP2K, Gaussian, Orca
Visualization codes	MOLDRAW, VMD, Gaussview, ArgusLab

Languages

Italian	Mother language
English	B2
Spanish	B2

Publications

Summary: Total number of publications on peer-reviewed journals: 10

2024

J. Perrero, and L. Beitia-Antero, A. Fuente, P. Ugliengo, and A. Rimola, Binding energies and vibrational spectral features of S_n species on amorphous water-ice mantles: a quantum mechanical study *Astrophys. J.*, **2024**, *971*, 36. DOI: 10.3847/1538-4357/ad5548.

J. Perrero, J. Vitorino, E. Congiu, P. Ugliengo, A. Rimola, and F. Dulieu, Binding energies of ethanol and ethylamine on interstellar water ices: synergy between theory and experiments *PCCP*, **2024**, *26*, 18205.

J. Perrero, and A. Rimola, Synthesis of urea on the surface of interstellar water ice clusters. A quantum chemical study, *Icarus*, **2024**, *410*, 115848. DOI: 10.1016/j.icarus.2023.115848.

D. Campisi, **J. Perrero**, and N. Balucani, Computational Astrochemistry Journey towards the molecular universe, *accepted for publication*, **2024**. DOI: 10.48550/arXiv.2407.15204.

2023 **J. Perrero**, L. Beitia-Antero, A. Fuente, P. Ugliengo, and A. Rimola, Theoretical Modeling of the Adsorption of Neutral and Charged Sulfur Bearing Species onto Olivine Nanoclusters *MNRAS*, **2023**, *527*, 10697. DOI: 10.1093/mnras/stad3896.

J. Perrero, P. Ugliengo, C. Ceccarelli, and A. Rimola, Quantum mechanical modelling of the grain-surface formation of acetaldehyde on H_2O:CO dirty ice surfaces, *MNRAS*, **2023**, *525*, 2654. DOI: 10.1093/mnras/stad2459.

2022 **J. Perrero**, J. Enrique-Romero , S. Ferrero , C. Ceccarelli , L. Podio, C. Codella, A. Rimola, and P. Ugliengo, Binding Energies of Interstellar Relevant S-bearing Species on Water Ice Mantles: A Quantum Mechanical Investigation *Astrophys. J.*, **2022**, *938*, 158. DOI: 10.3847/1538-4357/ac9278.

J. Perrero, J. Enrique-Romero, B. Martínez-Bachs, C. Ceccarelli, N. Balucani, P. Ugliengo, and A. Rimola, Non-energetic Formation of Ethanol via CCH Reaction with Interstellar H_2O Ices. A Computational Chemistry Study, *ACS Earth Space Chem.*, **2022**, *6*, 496. DOI: 10.1021/acsearthspacechem.1c00369.

2021 **J. Perrero**, A. Rimola, M. Corno, and P. Ugliengo, Ab initio Calculation of Binding Energies of Interstellar Sulphur-Containing Species on Crystalline Water Ice Models, *Computational Science and Its Applications – ICCSA 2021*, **2021**, *12953*, 608. DOI: 10.1007/978-3-030-86976-2_41.

2020 C. Codella, L. Podio, A. Garufi, **J. Perrero**, P. Ugliengo, D. Fedele, C. Favre, E. Bianchi, C. Ceccarelli, S. Mercimek, F. Bacciotti, K. L. J. Rygl, and L. Testi, ALMA chemical survey of disk-outflow sources in Taurus (ALMA-DOT) IV. Thioformaldehyde (H_2CS) in protoplanetary disks: spatial distributions and binding energies *Astron. Astrophys.*, **2020**, *A120*, 644. DOI: 10.1051/0004-6361/202039309.

Congresses

Summary Number of total congresses: 17

Number of invited communications: 2

Number of oral communications: 10

Number of poster presentations: 5

2024 EPSC2024, Berlin - Germany, September 8^{th}-13^{th}, oral communication.

XXVIII National Congress of Società Chimica Italiana, Milan - Italy, August 26^{th}-30^{th}, oral communication.

9th EuChemS, Dublin - Ireland, July 7^{th}-11^{th}, oral communication.

SUL4LIFE kick-off meeting, Madrid - Spain, January 22^{nd}-25^{th}, oral communication.

2023 Nanostructured Interfaces and Surfaces (NIS) colloquium: Heterogeneous catalysis based on naturally occurring materials: from prebiotic chemistry to applications, Torino - Italy, November 28^{th}, oral communication (invited).

2° Congresso nazionale di Astrochimica (Proto-)Planetaria, Trieste - Italy, September 11^{th}-14^{th}, oral communication.

XLIX Congress of the Physical Chemistry Division of the Società Chimica Italiana: a fresh glimpse into the microscopic world, Torino - Italy, September 4^{th}-7^{th}, oral communication.

XXXVIII Reunión Bienal de la Real Sociedad Española de Química, Zaragoza - Spain, June 25^{th}-29^{th}, poster presentation.

ACO Conference: chemical processes in Solar-type star forming regions, Tolouse - France, June 5^{th}-9^{th}, oral communication.

XRQTC (Xarxa de Referència en Química Teòrica i Computacional) - 1a Reunió de Química Teòrica i Computacional, Barcelona - Spain, January 30^{th}-31^{th}, flash communication + poster presentation.

2022 8^{th} ORCA User Meeting - Environmental effects: From solids to solutions to biology, Virtual meeting, December 6^{th}-7^{th}, poster presentation.

XVIII Simposio de Jóvenes Investigadores Químicos de la RSEQ, Sevilla - Spain, November 21^{th}-24^{th}, oral communication.

Workshop "New insights into Sulphur chemistry", Madrid - Spain, June 22^{nd}-24^{th}, oral communication (invited).

Astrochemistry meets Surface Science, Aarhus - Denmark, April 5^{th}-8^{th}, oral communication.

2021 Workshop on Interstellar Matter, Virtual meeting, November 17^{th}-19^{th}, poster presentation.

ACO Conference: chemical processes in Solar-type star forming regions, Torino - Italy, September 13^{th}-17^{th}, poster presentation.

The 2021 International Conference on Computational Science and its Applications (ICCSA 2021), Virtual meeting, September 13^{th}-16^{th}, oral communication.

Awards

Jun 2023 Best poster prize, XXXVIII Reunión Bienal de la Real Sociedad Española de Química, Zaragoza - Spain, June 25^{th}-29^{th}.

Sep 2022 Best poster prize, Paris International School on Advanced Computational Materials Science, Paris - France, August 29^{th}-September 2^{th}.

Other experiences

August 2024 Peer-review activity for a scientific journal

July 2024 Participation in the Astrochem Coffee (coffee.astrochem.net/) podcast.

Sep 2019 - Oct 2019 One-month internship at Laboratorio Chimico della Camera di Commercio di Torino to perform the analysis of potentially toxic components for humans in plastic and paper food packaging.

Oct 2018 - Jun 2019 Tutor for students with specific learning disabilities at Università degli Studi di Torino

Sep 2014 - Apr 2016 Volunteer activity: creation of an archive and management of the library of my birthplace, San Francesco al Campo, with bi-weekly opening.