


Marie Skłodowska-Curie Actions
Second call for COFUND PhD fellowships

Employer	University Paris-Saclay
Doctoral School	EDOM (Waves and Matter)
Selection Domain	EDOM (Waves and Matter)

Supervision

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PHD THESIS PROJECT
QUASAR - QUAntum chemical and experimental Spectroscopy of Astrochemical Reactive isomers
Summary / Abstract

The project aims to uncover reactive isomers of astrophysical relevance by combining high-resolution laboratory spectroscopy with advanced quantum chemical calculations. This work incorporates high-level quantum chemical models to guide experimental detection and spectral assignment of reactive molecular species. The PhD fellow will conduct both the quantum calculations and laboratory spectroscopic characterization of selected isomeric families expected to be abundant in space but lacking experimental data. These new spectra will then support astronomical collaborators in targeted searches within existing radio to submillimeter wave surveys. By merging experimental and theoretical molecular science, the project will deliver essential spectroscopic data to improve astrochemical models, while offering the fellow comprehensive training in quantum chemistry and gas-phase molecular spectroscopy.

Principal 3i dimension: international. **Additional 3i dimension:** interdisciplinary

Keywords

- **Laboratory Astrophysics**
- **Reactive Species**
- Molecular Physics
- High Resolution Spectroscopy
- Quantum Chemical Calculations
- Atomic, molecular and plasma physics



QUASAR - QUAntum chemical and experimental Spectroscopy of Astrochemical Reactive isomers

Key Objectives

The main objective of this PhD fellowship is to identify and characterize reactive isomers of astrochemical relevance by combining high-resolution gas-phase spectroscopy and high-level quantum chemical calculations. The student will work at ISMO for two years, performing experimental rotational spectroscopy of selected reactive isomers using state-of-the-art microwave and terahertz instruments. Guided by calculations performed during a one-year stay at the University of Bologna, the fellow will predict structural and spectroscopic parameters to support experimental identification and spectral assignment. Additional short visits to collaborating laboratories will provide complementary training in astrochemical modeling and data interpretation. The ultimate goal is to build a reliable spectroscopic database for newly characterized isomers, enabling their astronomical search and improving the chemical networks used to model interstellar environments.

Project

Context and state-of-the-art of Scientific Research project

The interstellar medium (ISM) is a molecularly rich environment where more than 350 species have been identified, largely thanks to modern radio and millimeter wave observatories. Yet this inventory is still incomplete: many energetically accessible isomers of known molecules—especially reactive ones—remain undetected. These elusive molecules likely play crucial roles in astrochemical networks, but their observation is hindered by the absence of precise laboratory spectra, which are essential for reliable astronomical identification.

Only a few research teams worldwide pursue such short-lived isomers, due to experimental and theoretical challenges. These species typically require specialized production techniques (e.g. flash pyrolysis, plasma discharge) and highly sensitive rotational spectrometers. At the same time, accurate predictions of their spectroscopic properties demand high-level quantum chemical methods—well beyond standard DFT—and are indispensable for interpreting laboratory spectra.

The QUASAR project is designed to tackle this dual experimental and theoretical challenge by combining high-level quantum chemical calculations with high-resolution laboratory rotational spectroscopy, all within a focused doctoral training program. This integrated approach will enable the characterization of reactive isomers that are currently absent from astronomical and spectroscopic databases. By extending laboratory astrophysics into this unexplored molecular territory, the project will generate essential reference data to support future interstellar detections and refine astrochemical models.

A major strength of the project lies in the complementary expertise of the two host institutions. At ISMO (Université Paris-Saclay), the PhD fellow will be trained in rotational spectroscopy using millimeter (mm) and submillimeter (submm) instruments optimized for reactive molecules, both at room temperature and under cold gas-phase conditions. A one-year stay at the University of Bologna will provide training in high-level quantum chemical calculations, particularly coupled-cluster methods (e.g. CCSD(T)/F12) using the CFOUR suite. During this stay, the fellow will also be introduced to reactive species production by flash pyrolysis and gain experience with an under-development microwave spectrometer, completing a multidisciplinary profile.

This rare dual training in high-resolution experimental spectroscopy and high-level theoretical chemistry is ambitious but perfectly aligned with the excellence-driven vision of the Horizon Europe COFUND program LIGHT in Paris. It positions the fellow at the interface of physical chemistry, molecular physics, and astrochemistry, enabling them to make unprecedented contributions to the detection and understanding of elusive interstellar molecules.

Description

---Impact---

The QUASAR PhD project addresses a critical bottleneck in molecular astrophysics: the absence of laboratory spectroscopic data for many reactive isomers of known interstellar molecules. These species are predicted to play essential roles in the chemical pathways that drive the formation of complex and prebiotic molecules, but their detection is currently limited by the lack of precise rotational spectra. By producing high-accuracy laboratory measurements supported by quantum chemical predictions, this project will enable targeted astronomical searches and refinement of astrochemical models. The outcomes of this work will directly support the interpretation of data from observatories such as ALMA, NOEMA, and JWST. In parallel, the project will train a researcher with rare expertise at the interface between molecular spectroscopy, quantum chemistry, and astrochemistry, aligned with the excellence-based mission of the LIGHT in Paris programme.

---Relevance for the Sciences of Light---

Light is both the central probe and the connecting thread of this project. In the laboratory, electromagnetic radiation in the microwave, mm and submm ranges reveals the rotational spectra of molecules, providing a molecular fingerprint through light-matter interactions. In space, the same transitions are observed as emission or absorption lines, allowing molecules to be detected across interstellar environments. QUASAR therefore exemplifies the sciences of light by linking molecular spectroscopy and quantum chemistry to astrochemical observations, connecting laboratory photons to astronomical signals. This continuum from fundamental molecular physics to astrophysical application is fully aligned with the dual scientific and training goals of the LIGHT programme.

---Methodology---

The project targets three isomeric molecular families of increasing complexity: $[\text{CH}_2\text{O}]$, $[\text{C}_2\text{H}_3\text{N}]$, and $[\text{C}_3\text{H}_8\text{O}_2]$. It will unfold in three complementary and collaborative phases:

1/ Theoretical Prediction (Months 4–15, Bologna):

The fellow will compute accurate rotational constants, equilibrium geometries, and centrifugal distortion parameters using coupled-cluster methods (e.g. CCSD(T)/F12) implemented in CFOUR. Computations will include vibrational corrections and isotopic variants to achieve sub-MHz accuracy. Training at Bologna will also include flash pyrolysis and high-resolution microwave spectroscopy techniques.

2/ Laboratory Spectroscopy & Spectral Assignment (Months 1–3 and 16–36, ISMO):

Experiments at ISMO will be performed using mm and submm spectrometers covering the 75–1500 GHz domain. Reactive species will be produced at room temperature or under supersonic expansion, using pyrolysis or plasma discharge sources. Experimental spectra will be iteratively assigned with support from theoretical predictions. The forthcoming pyrolysis setup and two complementary spectrometers are key to these measurements.

3/ Data Integration and Dissemination (Months 24–36):

Assigned spectra, line lists, and molecular constants will be deposited in public databases (e.g. CDMS, JPL) and disseminated through at least three peer-reviewed publications in journals such as *Journal of Chemical Physics*, *PCCP*, or *Astrophysical Journal*. Presentation of results at international conferences will accompany publication.

The project will benefit from the financial support of an ANR grant (SMILE, Searching for Metastable Isomers in the Laboratory and in space) with similar scientific goals and providing useful collaboration with astronomers and astrochemical modellers.

Throughout the project, coordination between ISMO and Bologna will ensure a seamless link between theory and experiment, with potential short technical visits to external laboratories where necessary.

---Expected Results---

- Spectroscopic characterization and publication of at least three reactive isomers across the aforementioned molecular families
- Public release of the data : All spectroscopic data and molecular line lists generated during the project will be released in open-access databases such as CDMS and JPL, ensuring full interoperability with ongoing astronomical surveys and aligning with FAIR data principles promoted across the European Research Area.
- Improvement of astrochemical models through incorporation of new species (via collaborations)
- Three or more peer-reviewed publications and international presentations
- Training of a researcher with dual experimental and theoretical expertise, prepared for leadership in laboratory astrophysics

---Timeline---

- Months 1–3 (ISMO): Host institution onboarding, introductory spectroscopy training
- Months 4–15 (Bologna): Theoretical training and complementary experimental experience
- Months 16–36 (ISMO): Full experimental campaign, data analysis, dissemination, thesis writing and defense

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Facilities and quality of research environment available for the researcher

The PhD fellow will be hosted at the Institut des Sciences Moléculaires d'Orsay (ISMO, Université Paris-Saclay) under the supervision of Marie-Aline Martin-Drumel and will join the SYSTEMAE group, which brings together a cluster of laboratory astrophysics specialists notably Olivier Pirali (high-resolution spectroscopy of reactive species from the mm-wave to the far-infrared), Béranger Gans (VUV spectroscopy of reactive molecules), Ugo Jacovella (spectroscopy of large carbon molecules of astrophysical interest), and Laurent Coudert (theoretician specialized in tailored models for non-rigid species with large amplitude motions). This rich team environment ensures immediate access to diverse expertise in instrument operation, data analysis, and modelling of challenging molecular systems. ISMO offers state-of-the-art instrumentation for gas-phase molecular spectroscopy, including source-frequency-modulation based mm/sub-mm wave spectrometers, a broadband chirped-pulse mm wave spectrometer, room-temperature and supersonic expansion set-ups, and discharge sources. The fellow will benefit from an environment calibrated for reactive isomers, both at room temperature and under cold expansion conditions, and will contribute to the development of pyrolysis sources at ISMO.

In parallel, the international partner at the University of Bologna (Italy) will host the fellow during a one-year secondment supervised by Cristina Puzzarini, joined by Luca Bizzocchi and Mattia Melosso, both experts in experimental pure rotational spectroscopy. The Bologna group's facility includes source-frequency-modulated mm/sub-mm wave spectrometers and a flash-vacuum pyrolysis cell for generation of reactive intermediates. They combine experimental and computational capabilities to link quantum-chemical prediction of spectroscopic constants with laboratory measurement—a synergy directly aligned with the QUASAR project.

These two institutions have a long-standing collaboration (more than 7 co-authored publications since 2020) that provides a seamless theoretical–experimental workflow and ensures strong institutional support, excellent research infrastructure, and a stimulating international environment. The fellow will therefore benefit from highly complementary facilities and expertise, broad professional networks, and a research culture tuned to frontier problems of molecular astrophysics.

3i Dimensions - international; interdisciplinary

Description and expected outcomes

The QUASAR PhD project fully meets the interdisciplinary and international requirements of the MSCA COFUND program. Its core scientific objective—detecting and characterizing reactive interstellar isomers—relies on the integration of two distinct yet complementary approaches: high-resolution rotational spectroscopy (experiment) and high-level quantum chemical calculations (theory). While both fall under molecular physics and physical chemistry, they represent different scientific cultures with their own methods and training paths. The interdisciplinarity in QUASAR thus stems from uniting experiment and theory to solve a frontier problem in astrochemistry.

The international dimension is ensured through a mandatory 12-month secondment at the University of Bologna (Italy), under Prof. Cristina Puzzarini. The fellow will be trained in advanced quantum chemical methods (e.g. CCSD(T)/F12 via CFOUR) and exposed to experimental techniques including flash-vacuum pyrolysis and microwave spectroscopy. The Bologna host is affiliated with a Chemistry doctoral school, while the home institution, ISMO (Université Paris-Saclay), belongs to a Physics doctoral school (EDOM), reinforcing the project's interdisciplinary scope across institutional boundaries.

Short research visits to other French or international partners may occur throughout the project, supporting methodological transfer and broadening the fellow's network across laboratory astrophysics, computational chemistry, and observational astronomy.

Expected outcomes include: (i) a researcher trained in both theoretical and experimental molecular science; (ii) transfer of experimental know-how (e.g. flash pyrolysis) from Bologna to ISMO; and (iii) publicly available spectroscopic datasets and publications, reinforcing European excellence in laboratory astrophysics. The project aligns directly with the goals of LIGHT in Paris by promoting excellence, mobility, and cross-disciplinary training in the sciences of light.

Approximate timeline of internships / external stays corresponding to the 3i dimension

- Year 1 (October 2026 – September 2027)**

Months 1–3 (ISMO): Host institution onboarding, introductory spectroscopy training

Months 4–12 (Bologna): Theoretical training and complementary experimental experience

- Year 2 (October 2027 – September 2028)**

Months 12–15 (Bologna): Theoretical training and complementary experimental experience (continued)

Months 16–24 (ISMO): Full experimental campaign, data analysis, dissemination

- Year 3 (October 2028 – September 2029)**

Months 16–36 (ISMO): Full experimental campaign, data analysis, dissemination (continued) thesis writing and defense

The fellow will complete a primary international secondment at the University of Bologna (Italy) during Months 4–15 of the PhD (12 months total). This stay provides essential training in high-level quantum chemical calculations (e.g. CCSD(T)/F12) using the CFOUR suite under the supervision of Prof. Cristina Puzzarini, as well as hands-on experience in molecular synthesis via flash pyrolysis and introductory microwave spectroscopy. This secondment ensures full compliance with the international and interdisciplinary (3i) requirements of the LIGHTinPARIS program.

Additional short scientific visits (1–2 weeks each) may take place during the fellowship to collaborate with other project partners, including groups in France and abroad, depending on experimental or theoretical needs.

The secondment will be supported by the standard mobility allowance (150 €/month) from LIGHTinPARIS, while travel and relocation costs for the Bologna stay will be covered by ISMO through the ANR SMILE grant, which shares scientific objectives with this PhD project. Living expenses in Bologna will be covered by the fellow's standard salary.

Profile of PhD fellow

PhD studies and research work require curiosity, creativity, rigour, teamwork, and organisational skills. A minimum B2 level of English is mandatory. The below criteria are specific to the thesis project.

pre-requisite	Academic background covers molecular physics or physical chemistry
pre-requisite	Academic background covers quantum chemistry and spectroscopy
pre-requisite	Experience in spectroscopic measurements in the laboratory
advantageous	Experience working experimental high-resolution spectroscopy (high spectral resolution)
advantageous	Experience with quantum-chemical calculations

Ethics issues in the project as per Horizon Europe Ethics Self-assessment

Section 1. Human embryonic stem cells (hESCs) and human embryos (hEs)			No
Section 2. Humans	No	Section 3. Human cells and tissues	No
Section 4. Personal data	No	Section 5. Animals	No
Section 6. Third Countries	No	Section 7. Environment, health and safety	Yes
Section 8. Artificial Intelligence	Yes	Section 9. Other ethics issues	No
Section 10. Crosscutting issue: potential misuse of results			No

7. Environment, health and safety

All French labs are required to have health and safety procedures in place, which takes into account the use of high-energy light sources such as lasers of class 3 and above, and the use of hazardous / toxic chemical and biological products. The institution and the laboratory comply with the highest safety requirements, and all PhD fellows have mandatory health and safety training, with additional training if required.

8. Artificial intelligence

The use of machine learning and artificial intelligence is used to fit data and analyse results. This is typically used to improve fits and complex models with multiple parameters. The data in question is related to physical experiments and is not human data.

Artificial Intelligence is not developed during this project and is thus not impacted by the AI Act.