

Post-doctoral position on excited-state molecular dynamics of organic crystals

Duration: 2025–2027 (24 months, starting November 2025)

Location: Aix-Marseille Université, Institut de Chimie Radicalaire (Marseille, France)

A postdoctoral position is available in the theoretical chemistry group of the Institut de Chimie Radicalaire (ICR) in Marseille, under the supervision of Prof. Mario Barbatti (www.barbatti.org). The ICR team develops advanced computational approaches to simulate chemical processes induced by light, with a particular focus on excited-state dynamics and photochemistry.

The project aims to establish new strategies for simulating photoinduced processes in organic crystals. These systems pose specific challenges due to their periodic structure and electronic complexity. The postdoctoral researcher will contribute to method development and computational modeling efforts to make the excited-state simulation of these materials tractable and predictive.

This position is funded by the **PEPR LUMA** program, within the **ChirExCo** project, which explores chirality in organic crystals for next-generation energy transport and conversion. The work will lay the methodological foundations for future applications within this multi-partner national initiative.

Qualifications:

Applicants must hold a PhD in theoretical or computational chemistry, or a closely related discipline. Prior experience in electronic structure theory and molecular dynamics is expected. Familiarity with periodic-boundary condition simulations and/or excited-state calculations is advantageous. Proficiency in scientific programming and the ability to work in a high-performance computing environment are essential. The successful candidate will be motivated, collaborative, and eager to contribute to a multidisciplinary research effort.

Application:

Interested candidates should send a CV, a motivation letter, and contact information for at least two referees to Prof. Mario Barbatti (mario.barbatti@univ-amu.fr).

The position starts on **November 1st, 2025**. Please note that administrative processing may take up to two months. Salary will be based on experience and includes full social security and health coverage.