



1 PhD position open in the framework of the ERC-QUANTUMGRAIN project

One PhD fellowship is available in the Dept. of Chemistry of Universitat Autònoma de Barcelona to work on the project Quantum Chemistry on Interstellar Grains (QUANTUMGRAIN, <https://cordis.europa.eu/project/id/865657>), awarded by the European Research Council (ERC Consolidator Grant, grant agreement number 865657) and led by Dr. Albert Rimola. The project is related to the grain surface chemistry occurring in the Universe. You can know more about the QUANTUMGRAIN project in <https://www.quantumgrain.eu/>.

Scope: Simulations of Molecule Formation on Interstellar Grain Surfaces

The objective of the PhD position is to simulate, by means of computational chemistry and molecular modelling methods, processes occurring on the surfaces of interstellar grains (silicates, ices, carbonaceous materials), in particular those that lead to the formation of molecules identified in the interstellar medium and that are essential for the increase in the molecular complexity in space. The tasks to develop are: i) to construct realistic structural models for surfaces of interstellar grains, ii) to characterize the elementary physico-chemical steps involved in the synthetic routes occurring on the grain surface models with static (i.e., PES characterization) and molecular dynamics (AIMD and metadynamics) simulations, complemented by kinetic calculations, and iii) to determine the actual role of the surfaces in the studied reactions.

What we offer

- Training on surface modelling and *ab initio* simulations of surface chemistry phenomena (i.e., adsorption, diffusion, reactivity) with static and dynamics computations.
- Access to a well-developed research infrastructure, including supercomputing facilities.
- Interactions with senior and young researchers (astronomers, experimentalists and modellers) of other European institutions (and worldwide), who actively participate in other projects of excellence in the field of Astrochemistry.
- A research climate inviting lively, open and critical discussion within and across different fields of research.
- A working environment with teamwork, close working relations, network activities among young scientists and social activities
- A workplace characterized by professionalism, equality and a healthy work-life balance



Applicant's profile

Applicants must hold a Master degree specialized in Computational Chemistry, or is going to defend their MSc dissertation between July-September 2021. Previous experience in Astrochemistry will be valued. Knowledge of relevant program languages will be appreciated. Very good track record (publications, presentations, etc.) is desired. Teamwork ability is essential.

Starting Date and Period

Starting date: September-November 2021.

Duration of the employment: 4 years.

Contact Information

Further information may be obtained by e-mailing to the QUANTUMGRAIN official electronic address: pr.quantumgrain@uab.cat. Please use as e-mail subject: "predoctoral position".

Application

Applications should be submitted between 1st - 16th, June 2021.

The application must be submitted via Universitat Autònoma de Barcelona's recruitment system, which can be accessed under the job advertisement on the UPAC's website (<https://convocatoriesupac.uab.cat>). Register, sign in, and apply for the **2021DILEUA52** call. All interested candidates are encouraged to apply. Applications from women are especially welcome.

Place of Work and Area of Employment

The QUANTUMGRAIN project is being developed in the Dept. Chemistry (<https://www.uab.cat/departament/quimica/>) of Universitat Autònoma de Barcelona (UAB, <https://www.uab.cat/>), one of the major public universities of Spain. UAB is placed in a university campus outside from the downtown and framed by the beautiful surrounding landscape of wooded areas.