

IT Engineer Position Offer

Job reference: subnano-ite

Project title: Computer science support for computational photochemistry

Laboratory: Institut de Chimie Radicalaire, Aix Marseille Université, Marseille

Period: Up to 5 years (August 31, 2024)

Application deadline: May 31, 2019

Starting date: October 1, 2019

Salary range: 3600 € - 4000 € (monthly gross salary)

Funding: ERC AdG SubNano

Contact: mario.barbatti@univ-amu.fr

Post description

The Light and Molecules research group (www.barbatti.org) is coordinated by Prof. Mario Barbatti at the Institut de Chimie Radicalaire of the Aix Marseille University, in Marseille, France. The group is specialized in excited state simulations of organic molecules using nonadiabatic mixed quantum-classical dynamics (NA-MQC). The group is also responsible for the development of the software Newton-X for NA-MQC (www.newtonx.org).

Recently, Prof. Barbatti has been awarded an ERC Advanced Grant to develop the SubNano project. The project aims at creating computational methods to extend nonadiabatic dynamics from the current picosecond scales into the sub-nanosecond regime.

The goal of the subproject concerning this IT engineer position is to support the implementation of the new methodology at the software and hardware levels.

Job tasks

- To optimize Newton-X with the best practices from computer science, eliminating current bottlenecks.
- To parallelize Newton-X.
- To propose programming protocols to be adopted by the community of developers.
- To help with the implementation of the new codes developed by other group members and external co-workers.
- To propose and implement standard data formats complying with the H2020 Open Research Data pilot. A hierarchical data format, likely HDF5, should be adopted for the interface.
- Interact with the staff of the university and national HPC clusters, specially concerning software installation.
- To provide technical support on Newton-X issues to group members and the community of Newton-X users.
- To manage the local computer resources, in terms of hardware (maintenance and security) and software (installation, maintenance, and security).

Candidate profile

The ideal candidate will have a strong background in computer sciences, including high-performance scientific programming in Linux system. Knowledge of Fortran is required and of Perl or Python,

desirable. Experience with computational chemistry is a plus. We are looking for a candidate with the potential for staying for the five years of the project. Good communication and team-work skills are also essential, as the engineer should closely work with the other group members and the community of developers and users of Newton-X.

There are no restrictions concerning nationality, provided a work permit is granted.

Post profile

The IT engineer is expected:

- To prepare technical reports for group members and external coworkers.
- To interact and work with other members of SubNano and external coworkers.
- To keep up-to-date with the latest developments in the field.
- To work independently, taking initiative in the planning and execution of tasks.
- To provide effective support to the SubNano team.
- To drive the work to properly meet SubNano milestones and deliverables.

Working place, environment, and employment policy

The work will be developed at the Aix Marseille Université, Institut de Chimie Radicalaire, Campus Saint Jérôme, Marseille, France.

The working language is English.

Our group is committed to promoting gender equality and cultural diversity, as well as to guarantee a friendly, professional, and free of prejudice work environment.

Applications and contact

Applications and further inquiries should be sent to Prof. Mario Barbatti (mario.barbatti@univ-amu.fr).

Please, refer to the job offer **subnano-ite** in the subject of any message.

The application should include a letter of motivation and the CV containing information of two potential referees. Do NOT send recommendation letters with the application. The referees may be contacted in a later stage of the selection process. Your authorization will be asked before they are contacted.

Person Specification

When preparing the letter of motivation, CV, and for an occasional interview, bear in mind that we will be evaluating the following attributes.

Attributes	Criteria	Essential / Desirable
Education and qualification	Bachelor's degree in computer sciences, or large working experience in the field.	E
Experience	Evidence of independent work.	D
	Experience with Linux and HPC systems.	E
	Experience with Fortran.	E
	Experience with Perl or Python.	D

Skills and abilities	Experience with software for scientific computing.	D
	Basic knowledge of computational chemistry.	D
	Good communication skills in English both verbal and written (B1 to B2 CEF language level)	E
	Ability to work largely on own initiative with minimum supervision	E
	Ability to work in a team	E
	Ability to plan and execute tasks of different nature	D
