Postdoc Position Offer

Job reference: subnano-pd5
Project title: Mixed quantum-classical dynamics: methods and applications
Research area: theoretical and computational chemistry
Laboratory: Institut de Chimie Radicalaire, Aix Marseille Université, Marseille
Period: 1 year + 2 years
Application deadline: until filled
Starting date: September 1, 2021
Salary: € 2780 (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 Marseille, France. The group is specialized in excited state simulations of organic molecules using nonadiabatic mixed quantum-classical dynamics (NA-MQC).[1] The group is also responsible for the development of the software Newton-X for NA-MQC (www.newtonx.org).

In 2019, Prof. Barbatti was awarded an ERC Advanced Grant to develop the SubNano project (www.subnano.org). SubNano aims at creating computational methods to extend nonadiabatic dynamics from the current picosecond scales into the sub-nanosecond regime, using Machine Learning and other acceleration algorithms.

The goal of the subproject concerning this postdoc position is to develop and apply the SubNano methodology to investigate excitonic processes. The researcher in this position should be able to 1) work on the development and implementation of new algorithms into the Newton-X program and 2) independently apply these methods to the study of photoexcited molecules.

Job tasks

- To develop and implement new methods into Newton-X.
- To simulate statical (reaction paths), statistical (reaction rates), and dynamical (surface hopping) simulations of excited states of molecules, using a variety of quantum chemistry methods.
- To collaborate with other group members and external coworkers.
- To participate in conferences and training courses.
- To write scientific papers and deal with the peer-reviewing process.
- To perform other additional research and scholarly duties in line with University guidelines.

Candidate profile

The ideal candidate will have a strong background in computational chemistry. Experience with Fortran, Perl, or Python is essential. We are looking for a candidate with the potential to stay for the three years of the project. Good communication and teamwork skills are also essential, as the postdoc should closely collaborate with the other group members and external coworkers.

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

Post profile

The postdoc is expected:

1. Communication, networking, and teamwork

- To give high-quality oral and poster presentations in English at meetings and conferences.
- To promote SubNano at meetings and conferences.
- To publish high-quality papers based on their research outcome.
- To prepare technical and progress reports for group members and external coworkers.
- To interact and work with other members of SubNano staff and external coworkers.
- To participate in the supervision of junior researchers.

2. Analysis and research

- To acquire the latest research knowledge.
- To develop independent, original research.
- To take the initiative in the planning of research.
- To provide practical support to other research projects in SubNano.
- To drive the research to meet SubNano milestones and deliverables adequately.

Working place, environment, and employment policy

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

The working language is English.

Training on project leading, project management, and technological innovation in the public and private sectors will be provided.

Our group is committed to promoting gender equality and cultural diversity and guarantee a friendly, professional, and inclusive 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-pd5** in the subject of any message.

The application should include a cover letter and a CV containing the complete publication list and contact information of two referees. Do NOT send recommendation letters with the application. The referees may be asked for a recommendation letter in a later stage of the selection process.

Person Specification

When preparing the cover letter and CV, bear in mind that we will be evaluating the following skills and attributes.

Attributes	Criteria	Essential / Desirable
Education and qualification	PhD in theoretical, computational chemistry, or theoretical molecular physics	E
Experience	Evidence of independent, original research	D
	Experience in investigations using atomistic modeling and simulation techniques	E
	Experience with mathematical derivations	E
	Experience with excited-state simulations	D
	Evidence of IT literacy including Linux system	E
	Knowledge of programming in Fortran, Perl, or Python	E
Skills and abilities	Good communication skills in English, both verbal and written (minimum B2 CEF language level)	E
	Ability to draft research papers for publication in appropriate academic journals.	E
	Ability to work largely on own initiative with minimum supervision	E
	Ability to give presentations at academic conferences and meetings	D
	Ability to work in a team	D

References

(1) Crespo-Otero, R.; Barbatti, M. Recent Advances and Perspectives on Nonadiabatic Mixed Quantum-Classical Dynamics. *Chem. Rev.* **2018,** *118*, 7026-7068.