Postdoc Position Offer

Job reference: subnano-pd1
Project title: Nonadiabatic mixed quantum-classical dynamics with machine learning
Research area: theoretical and computational chemistry
Laboratory: Institut de Chimie Radicalaire, Aix Marseille Université, Marseille
Period: 1 year + up 2 years extension
Application deadline: until filled
Starting date: October 1, 2019
Salary range: 2 466 € - 3 156 € (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).[1] 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 SubNano methodology is anchored on the conjoint use of Machine Learning (ML) and Hessian calculations to speed up and control the accuracy of the simulations.

The goal of the subproject concerning this postdoc position is to develop and implement ML-based NA-MQC dynamics. It should extend our initial implementation,[2] to allow the ML-prediction of nonadiabatic couplings and Hessians. It should also implement an adaptive ML algorithm to allow automatic retraining during the dynamics propagation. The project will be co-coordinated by Prof. Nicolas Ferré.

Job tasks

- To develop ML algorithms for NA-MQC dynamics.
- To implement these methods into Newton-X.
- To prepare full documentation and tutorials.
- To coordinate the work of a graduate student, who will be testing the 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 development. Experience with machine learning is a plus. Knowledge of Fortran and Perl is desirable. We are looking

for a candidate with the potential for staying for the three years of the project. Good communication and team-work 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 effective support to other research projects in SubNano.
- To drive the research 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.

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, 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-pd1** in the subject of any message.

The application should include a cover letter and the CV, containing the full 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, CV, and for an occasional interview, bear in mind that we will be evaluating the following 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 modelling and simulation techniques	E
	Experience with mathematical derivations	E
	Experience with development and use of ML techniques	D
	Evidence of IT literacy including Linux system	E
	Knowledge of programming in Perl, Fortran or both	D
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.

(2) Dral, P. O.; Barbatti, M.; Thiel, W. Nonadiabatic Excited-State Dynamics with Machine Learning. *J. Phys. Chem. Lett.* **2018,** *9*, 5660-5663.