Thesis Proposition

Post reference: subnano-gs1
Project title: Nonadiabatic relaxation of DNA fluorescent markers
Level: graduate student (doctorand)
Thesis supervisor: Prof Mario Barbatti
Research area: theoretical and computational chemistry
Laboratory: Institut de Chimie Radicalaire, Aix Marseille Université, Marseille
Application deadline: May 15, 2019
Starting date: October 1, 2019
Stipend: 1768 € (monthly gross value)
Duration: 36 months
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 thesis proposition is to test and apply the ML-based NA-MQC dynamics. These tests will be focused on simulations of 2-aminopurine (2AP)[2]—one of the main DNA fluorescent markers—in the gas phase, in diverse solvents, and connected to alkyl chains.

Job tasks

- To develop original, independent research on NA-MQC dynamics.
- To collaborate with other group members and external coworkers.
- To participate in conferences and training courses.
- To draft scientific papers.
- To perform other additional research and scholarly duties in line with University guidelines

Candidate profile

The ideal candidate will have a strong background in physical chemistry, molecular physics, or both. Knowledge of either computational chemistry, machine learning, or software programming is considered a plus. Good communication and team-work skills are also essential, as the doctorand should closely collaborate with the other group members and external coworkers.

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

Post profile

The doctorand 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.

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.
- To write and defend a Ph.D. thesis by the end of the third year.

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-gs1** in the subject of any message.

The application should include a cover letter and the CV, containing undergraduate and graduate grades, a list of publications, and contact information of one referee. Do NOT send a recommendation letter with the application. The referee 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	Master degree (or equivalent) in chemistry, physics, or related field	E
Experience	Evidence of independent research	D
	Experience in investigations using atomistic modeling and simulation techniques	D
	Experience with development and use of ML techniques	D
	Evidence of IT literacy including Linux system	D
	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	D
	Ability to work largely on their own initiative with minimum supervision	D
	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) Barbatti, M.; Lischka, H. Why Water Makes 2-Aminopurine Fluorescent? *Phys. Chem. Chem. Phys.* **2015,** *17*, 15452-15459.