Postdoc Position Offer

Job reference: boostcrop-pd1
Project title: Molecular dynamics and electronic structure simulations of photoexcited chromophores in the gas-phase and complex environments
Research area: theoretical and computational chemistry
Laboratory: Institut de Chimie Radicalaire, Aix Marseille Université, Marseille
Period: 1 year + up 2 years extension
Application deadline: March 30, 2019
Starting date: October 1, 2019
Salary range: 2 466 € - 3 156 € (monthly gross salary)
Funding: ERC FET Open Boostcrop
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).

Prof. Barbatti is part of the research consortium BoostCrop, which has been recently awarded a FET Open European grant. The aim of BoostCrop is to develop a novel approach to improve crop yields by protecting plants from cold stress. The approach is based on 'molecular heaters'; nature-inspired molecules that absorb light at wavelengths that are either harmful to the plant or not used in photosynthesis and converting this light energy to heat.

The goal of this postdoctoral research project is to develop models for nonadiabatic excited state dynamics of chromophores in isolation and in complex environments. Comparison of computer simulations with experimental data will establish structure-dynamics-function relationships, and thus a molecular rationale for photon-to-molecule heaters. Such knowledge will also enable tuning the absorption profiles to be compatible with leaf photosynthetic machinery.

The research work will focus on electronic structure calculations of chromophores in the gas-phase and in complex environments. These calculations will run in tandem with the experiments by our coworkers. The researcher will also help develop models for the nonadiabatic relaxation of the photon energy absorbed by the chromophore. These calculations will be carried out through a two-pronged strategy involving: i) static techniques for determining conical intersections, excited state critical points, and reaction pathways connecting them; and ii) nonadiabatic dynamics simulations. The nonadiabatic relaxation models will determine how the photon energy is converted into ground state vibrational energy (heat) and how possible chemical functionalization will aid retention of excess vibrational energy near the cellulose wall.

Job tasks

- To perform computational calculations and analysis of diverse chromophores proposed by the BoostCrop consortium.

- To prepare full reports on the advances of the research.
- To coordinate the work of a graduate student.
- 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 applications. 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 BoostCrop 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 BoostCrop 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 BoostCrop.
- To drive the research to properly meet BoostCrop 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 **boostcrop-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
	Evidence of IT literacy including Linux system	E
	Knowledge of programming in Perl or other script language	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.