Theoretical design and rationalization of Metal-Azadipy multimodal probes

12-month Postdoctoral position founding
(Starting early 2023)

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The objective of the MAP project is to develop a new class of optimized fluorophores for optical imaging and Fluorescence Guided Surgery (FGS), based on azaBODIPYs (Figure 1). AzaBODIPYs, which are structurally closed to BODIPY have the advantages to be stable, to absorb and emit in the near-Infrared (NIR) region and may exhibit properties suitable for photo-acoustic imaging (PAI). More precisely, we are going to replace the boron atom of the azaBODIPYs by selected metals (azaMDIPY), in order to confer to the resulting systems unique photophysical properties. The metal can also be changed by a radiometal, in order to develop bimodal probes combining NIR Optical Imaging (OI) or photo-acoustic Imaging (PAI) with Positron Emission Tomography (PET) or Single Photon Emission Computed Tomography (SPECT).

In this context, quantum chemical calculations will provide helpful guidelines in the rationalization of the observed photophysical properties (absorption, emission) of all aza-DIPY & azaMDIPY dyes that will be developed. It will allow us to identify the main structural features controlling the optical properties and then drive the experimental development of a next generation of dyes and complexes. The theoretical work will consist in the determination and application of the most accurate quantum chemical protocol, mainly based on time-dependent Density Functional Theory (TD-DFT), for the proper description of the electronic structure of both ground and excited states, with a careful focus on the involved electronic transitions. Vibronic calculations will potentially be conducted to refine the computed spectra and evaluate the emission quantum yields.

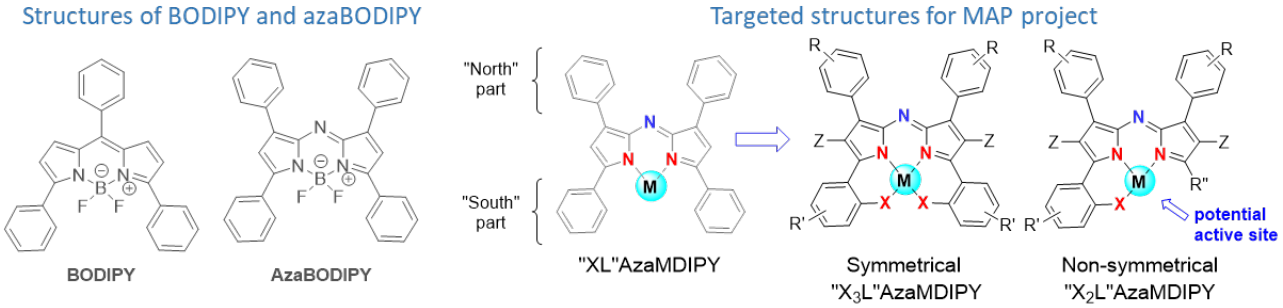

Figure 1. Structures of BODIPY and azaBODIPY (left); targeted structures of the project (right)

The Inorganic Theoretical Chemistry team:

The hired postdoctoral fellow will work in the Inorganic Theoretical Chemistry (ITC) team, in the Institute of Chemical Sciences of Rennes. The ITC team gathers a large number of theoreticians (14 permanent researchers, ca. 20 students), working with a wide range of quantum chemistry tools, from high precision *ab initio* wave-function theory to fast semi-empirical methods. The studied systems in ITC team are molecular, nano-structured or periodic, and most of the times of high experimental interest. This leads to fruitful joint experience/theory collaborations with other ISCR groups, and numerous others at the national and international level. We are also deeply involved in methodological efforts in the theoretical chemistry community to permit reaching practical applications of very recent and state-of the art quantum tools.

The ITC team provides a stimulating scientific environment, with regular team meetings, seminars and a constant communication with the other members of the group.

Profile of the candidate:

This 12-month postdoctoral funding is part of the **MAP** (**M**etal-**A**zadipy multimodal **P**robes: find your way in vivo) **ANR Project** coordinated by E. Bodio (ICMUB, Dijon). This project aims at developing a new class of near-infrared fluorophores for in vivo optical imaging, especially for fluorescence-guided surgery.

This project thus requires a motivated candidate with a solid background in **quantum chemistry** and **physical chemistry**. The work will be conducted with regular discussions and meetings with the experimentalists of the project. Scientific curiosity and general knowledge in chemistry are then also expected.

Application:

The PhD project will start in early 2023. Applications are already opened.
Candidates can submit their application on the CNRS platform:
https://emploi.cnrs.fr/Offres/CDD/UMR6226-BORLEG-004/Default.aspx