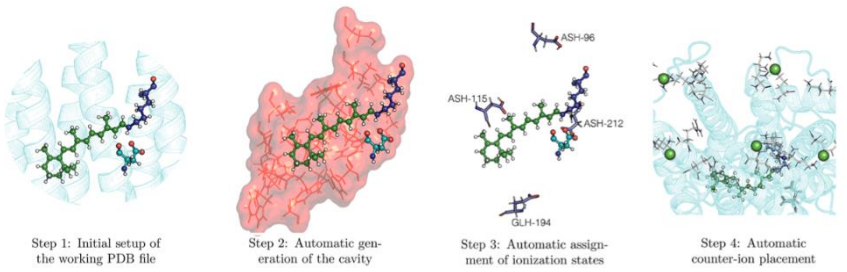
Research Software Engineer position, Marseille, France

A 1-year research software engineer position is immediately available in Aix-Marseille University, Institut de Chimie Radicalaire, Marseille, France. The engineer will make a major contribution to the delivery of a professional software especially developed for large scale simulations of photo-induced processes at work in rhodopsin proteins for biochemical and biological applications like optogenetics.

The Automatic Rhodopsin Modeling (ARM) protocol [Pedraza-Gonzalez, JCTC 15, 2019, DOI: 10.1021/acs.jctc.9b00061] is a computational chemistry-based workflow dedicated to the calculation of spectroscopic and photochemical properties of all kinds of rhodopsin photoactive proteins. It has been successfully applied to reproduce experimental trends in absorption and emission maximum wavelengths of natural and synthetic rhodopsins, with a controlled accuracy [Pedraza-Gonzalez, Top. Curr. Chem. 21, 2022, DOI: 10.1007/s41061-022-00374-w, Pedraza-Gonzalez, JCTC 19, 2023, DOI: 10.1021/acs.jctc.2c00928, Cardenas, JPCA 127, 2023, DOI: 10.1021/acs.jpca.3c05413].

ARM remarkable features have attracted the attention of many experimental research groups around the world, some of them willing to use it as a black box and/or suggesting including new features. In its current state, ARM is a collection of python scripts interfacing time-consuming steps, like molecular dynamics simulation or QM/MM calculations. The research software engineer will primarily work on a significant update of the ARM workflow, including the rewriting of its key components, adding more internal controls, improving its parallelization, enhancing the post-processing analysis, and improving the packaging of ARM and its dependencies.



Step 1: Initial setup of the working PDB file | Step 2: Automatic generation of the cavity | Step 3: Automatic assignment of ionization states | Step 4: Automatic counter-ion placement

Candidates must hold a PhD or an engineer degree in theoretical chemistry, theoretical physics or applied computer science. Previous experience in molecular modeling is desirable. Knowledge in modern scientific programming is required, especially in, but not limited, to Python or Fortran.

Marseille is the 2nd largest city in France. Located at the very South of the country, it gives immediate access to the Mediterranean Sea as well as the beautiful Provence countryside. The University campus can be easily reached from the city center. The salary depends on the experience (regular salary is comprised between 2000 and 2300€/month, after taxes) and may be negotiated, based on the candidate curriculum and achievements. Aix-Marseille University can cover 50% of the daily home-work public transport expenses and participate to the health insurance costs.

Applications will be considered as they are received. Applicants are encouraged to contact Prof Nicolas Ferré (nicolas.ferre@univ-amu.fr) and Dr Miquel Huix-Rotllant (miquel.huix-rotllant@cnrs.fr) for informal inquiries about the position, before submitting a formal application.

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