



Post-doctoral fellowship – Call for application (Computational Chemistry)

Department of molecular chemistry (University Grenoble Alpes/ CNRS)

Prof. Anne Milet

<https://dcm.univ-grenoble-alpes.fr/>

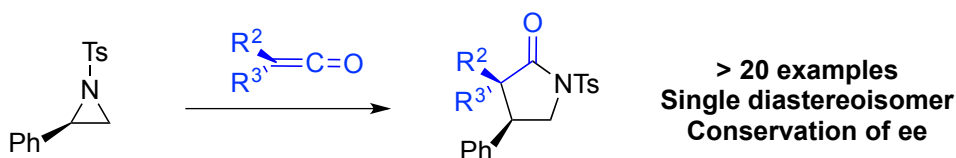
<https://dcm.univ-grenoble-alpes.fr/membre/anne-milet>

A Post-doctoral fellowship has opened up at the Department of Molecular Chemistry (DCM) at Grenoble, France. In an alpine setting and a remarkable scientific environment, the University of Grenoble Alpes welcomes more than 7000 PhD and post-doctoral students each year.

- Immediate opening
- Net salary: from 1900 to 2600 €/month (depending on experience).
- ANR funding.
- Duration: one year

Objectives:

The group of Prof. Jean-François Poisson (DCM, Grenoble) has recently found that aziridines can react with ketenes, affording lactams in excellent yields. With unsymmetrical ketenes, a single diastereoisomer is observed. **The objective of this part of the ANR Ketflo project is to determine the mechanism of this promising reaction and explain the selectivity observed using theoretical tools.**



In view of the reagents used and the reaction paths proposed, simulations that explicitly include solvent effects are necessary. We will therefore propose to use QM/MM methods coupled with metadynamics to determine the mechanisms involved. These methods are part of the know-how of our theoretical chemistry group. The candidate will interact regularly with the experimental team.

Applicant profile:

The successful candidate will have expertise in QM/MM calculations and knowledge of the cp2k software will be appreciated. An open mind and broader chemical culture will also be a key asset for interacting with the experimental team.

Further information and application:

Contact Prof. Anne Milet by email (Anne.Milet@univ-grenoble-alpes.fr) ASAP. Please attach a letter of motivation, CV, list of publications and recommendation letter(s) (pdf format).