POSTDOCTORAL POSITION

https://euraxess.ec.europa.eu/jobs/130175

Job Information
Organization: Université de Liège (ULiège, Belgium)
Department: Center for Integrated Technology and Organic Synthesis - CiTOS
Research Field(s): Computational chemistry, Machine Learning, Organic chemistry, Chemical Engineering

Type of Contract: Temporary (24 months, renewable)
Job Status: Full-time
Offer Starting Date: 1 Oct 2023
Application Deadline: 1 Sep 2023 - 12:00 (Europe/Brussels)

Offer Description
Overall context
This research proposal falls under the umbrella of a Wel-T advanced grant led by Prof. Jean-Christophe Monbaliu and strengthens current research efforts at the Center for Integrated Technology and Organic Synthesis (CiTOS).

The work will be carried out at the Center for Integrated Technology and Organic Synthesis (CiTOS, University of Liège, Belgium) in a competitive research environment and within a multidisciplinary team including synthetic chemists and chemical engineers. The candidate will have access to the most recent flow reactor technologies from Corning AFR and an internal analytical platform (LC, LC-MS, GC, GC-MS, benchtop NMR, IR, UV, etc.). Our large network of industrial collaborators stimulates research toward concrete industrial and/or societal challenges, making this a unique opportunity for candidates aspiring to continue either towards careers in academia or industry.

Research project
The goal of this project is to decrease the reliance on trial-and-error approaches to chemistry by using quantum mechanics computations to obtain a priori knowledge of a chemical reaction. This project brings together computational modeling to generate initial data, and machine learning to home in on an effective prediction model for reactivity. This model will be used to predict optimal reaction conditions, which will then be tested using a microfluidic flow reactor. Experiments will be conducted on an in-house automated platform equipped with inline monitoring. This approach will be applied to novel synthetic routes, for which there is no existing data, to showcase how novel, more efficient synthetic routes can be developed with a minimal number of experiments through the combination of these disciplines. The target compounds are active pharmaceutical ingredients.

Applicant's Profile
The candidate should have a PhD degree in Chemistry or Chemical Engineering and an interest in developing skills in organic synthesis, as well as in flow technology, automation. Candidates should have experience in machine learning, and ideally a background in Computational Chemistry (DFT). S/he should be comfortable with organic chemistry. Knowledge and/or experience in flow chemistry, process engineering, process analytical technology, electronics and/or automation will be considered as assets, though not required for the position. The successful applicant will be in

charge of 2 PhD students.
Eligible candidates must not have spent more than 24 months (for study or research/professional reasons) in Belgium for the past 3 years, regardless of citizenship, and must have obtained their PhD degree within less than 10 years at the time of the application.

Application

Interested candidates please send electronic applications including (a) a cover letter, (b) a curriculum vitae, (c) a short statement on your motivation and career objectives, and (d) the names and contact details of 3 professional references. The motivation letter should emphasize any previous research experience that aligns with this project. The application files should be addressed to Prof. Jean-Christophe M. Monbaliu (admincitos@uliege.be) (ref. Wel-T_ADV_Postdoc_2023). Candidates will be selected based on scientific excellence and achievements in research. Review of applications will begin on September 1, 2023 and will continue until the position is filled. Selected candidates will be interviewed.

Additional information

Prof. Jean-Christophe Monbaliu, Center for Integrated Technology and Organic Synthesis (CiTOS)
Email (for application files): admincitos@uliege.be
CiTOS: http://www.citos.uliege.be/
ULiège: https://www.uliege.be/
Wel Research Institute: https://welri.org/cms/c_16995060/en/welri-mission