

Postdoctoral position on “AI-based assistant for molecular QUantum chemistry”

1 year (with opportunity of extension), starts on fall 2018 in LERIA - MOLTECH Anjou CNRS (Angers, France).

Objectives of the project

This project addresses scientific and societal challenges around data science and artificial intelligence applied to molecular computational chemistry. For the chemists, the ambition of this project is to radically change the approach, developing artificial intelligence and optimization methods in order to explore efficiently the highly combinatorial molecular space. The recent abundance of data is an incredible opportunity, but also an additional challenge and therefore an added value to this project: we will develop original and highly scalable methods.

Job description

The postdoctoral researcher will start the machine learning development based on already available DFT calculations databases. Firstly, the goal of the predictive models is to generate for a new uncalculated molecule, precise approximations for different important results, saving hundreds hours of computation and making a broader exploration of the molecular space feasible. In addition to predictive models, generation of new molecules with constraints on one or more characteristics (such as electronic energies, the number of synthesis steps, etc.) will be investigated. We expect to study the integration of neural networks (objective functions) with neighborhood algorithms (molecular space exploration), but also emerging techniques like Generative Adversarial Networks (GAN).

Desired skills and experience

Since the information system is quite mature and being created, the work will directly be focused on the machine learning part. The candidate should therefore have experience in machine learning or data sciences. Additional computational chemistry experience will be appreciated. Fluency in Python language and solid knowledge of machine learning algorithms is furthermore mandatory.

About us and Contacts

Our project is a multidisciplinary collaboration between two researchers in two separate laboratories of the University of Angers. The LERIA for computer science tasks related to artificial intelligence and MOLTECH-Anjou for computational chemistry backed up by experimental facilities.

Application (CV + cover letter) has to be sent by email to Benoit Da Mota (benoit.damota@univ-angers.fr) and Thomas Cauchy (thomas.cauchy@univ-angers.fr). Don't hesitate to request for more information.