L'université de Bourgogne recrute

Ancrée depuis 300 ans sur son territoire, l'université de Bourgogne est un établissement historique, composé de 2800 personnels. Elle accueille 35 000 étudiants répartis sur 6 campus : Dijon, Auxerre, Chalon sur Saône, le Creusot, Macon, Nevers.

Université pluridisciplinaire, doté de 400 formations et de 32 laboratoires de recherche, allant de l'archéologie à l'Intelligence Artificielle, l'uB œuvre pour former les citoyens, et professionnels d'aujourd'hui et de demain, et à relever les défis sociétaux.

L'université de Bourgogne est membre fondateur de l'alliance européenne Forthem qui fait d'elle un campus européen avec possibilité de collaboration de travail avec des universités partenaires.

Travailler à l'uB c'est mettre ses compétences au service d'une mission de service public essentielle : contribuer à transmettre le savoir, créer des connaissances et développer la recherche.

Post-doctoral position in Artificial Intelligence for Materials Design

<u>Institution</u>: Université de Bourgogne

<u>Name of the project</u>: Artificial Intelligence Guided Materials Design

<u>Project Description</u>:
The work will be carried out within the framework of the AIMS (Artificial Intelligence for Material Science) alliance, which includes the materials science department of the University of Buffalo and the ImViA and CIAD laboratories of the University of Burgundy. The post-doc will work on the artificial intelligence part of the project in collaboration with the materials science department of the University of Buffalo.

Hydrogen can be produced from water electrolysis via hydrogen evolution reaction (HER), enabling sustainable energy supply and carbon footprint reduction. Earth-abundant two-dimensional (2D) layered transition metal dichalcogenides (TMDs) have demonstrated enormous potential as HER catalysts. Hydrogen can be produced from water electrolysis via hydrogen evolution reaction (HER), enabling sustainable energy supply and carbon footprint reduction. Earth-abundant two-dimensional (2D) layered transition metal dichalcogenides (TMDs) have demonstrated enormous potential as HER catalysts.

The overarching goal of this project is to integrate the AI approaches with experimental efforts to rationally design and develop next-generation electrocatalysts based on 2D TMDs at an accelerated pace for clean hydrogen production.

The project will consist in exploiting artificial intelligence techniques for informed and controlled 2D TMD synthesis. The manually selected synthesis parameters and in-situ morphology data collected in Buffalo encode rich mechanistic insights related to thermodynamic/kinetic control and surface diffusion of reactants. The post-doc will work on automatic microscopic image analysis collected in Buffalo and develop the ontological model representing the know-how of the 2D TMD materials synthesis process to extract critical knowledge related to nucleation, growth, and long-range transport. The extracted knowledge will assist in the systematic mapping of the parameter space and determining the optimal parameter combinations for the desired synthesis when combined with the design of experiment technique. This extracted knowledge will populate the ontology model to check their consistency. ML technics-assisted automatic microscopic image analysis will reveal the relationship and the ontological model will assist in growth condition prediction.

The second objective will consist in constructing a numerical twin to quantify the cross-correlation throughout the synthesis, characterization, and application stages to accelerate the overall development of high-performance TMD-based HER catalysts in an iterative, closed-loop fashion.

As part of the collaboration with the University of Buffalo, one or two trips to Buffalo will be required during the contract period.

Applicant profile
- Ph.D. in Artificial Intelligence (Ontology, Machine Learning, Deep Learning)
- Good programming knowledge and experience in programming environments
- Knowledge in image processing might be also appreciated
- Good communication skills in written and oral English
- High motivation for research work
- Eager to disseminate research results through publications and presentations at international conferences

Application:
Applicants are invited to submit their application to Stéphanie BRICQ stephanie.bricq@u-bourgogne.fr
Application must contain the following documents:
- Cover letter describing your training, experiences, knowledge and most significant contributions, and how you can contribute to this project.
- CV
- PhD diploma
- At least one reference letter
- Any other relevant information (webpage, github, publications, …).

Application deadline: 18 June 2023

Start of contract: between September and December 2023
Contract length: 12 months
Localization: ImViA laboratory, Dijon