# PhD position, at Laboratoire de Réactivité et Chimie des Solides (LRCS), Amiens (France)

# TOPIC: « Search, by simulation and modelling, of optimal low-gap materials for use as organic electrodes in batteries »

**Keywords**

Organic electrodes for batteries, DFT calculations & electronic structure analysis, Materials design, Structure-property relationships

**Summary of thesis project**

The research work on this project will involve various simulation and modelling methodologies to lead to optimised engineering of new categories of organic electrodes for batteries. More specifically, these investigations will be oriented towards the resolution of their current main drawback – *i.e.* their lack of favourable properties at the level of electronic conduction. Following various advanced strategies, an extensive search for redox-active and low-gap organic materials will be undertaken.

**General context**

The PhD candidate will work on the computational design/theoretical prediction and characterization of new materials for the development of eco-friendly organic batteries. She/He will provide guidelines as well as complementary characterization of innovant electrodes. The objectives will be to define suitable protocols as well as efficient selection strategies towards the engineering of performant materials and a support to the development of new prototypes in view of tackling current challenges of the field. The research work will consist in applying various theoretical approaches mainly based on Density Functional Theory calculations and chemical bonding analysis complemented by accurate exploration of electrochemical,

structural, and spectroscopic properties. Within an inspiring environment, through international interdisciplinary collaborations, and in close link with high-profile key-partners, this three-years PhD position will give the opportunity to contribute to strategic innovation routes towards the advent of advanced organic batteries. All these investigations will be conducted with cutting-edge resources and access to leading supercomputers. The starting date is October 1st 2024.

**General environment**

The PhD candidate will join the Laboratory of Reactivity and Chemistry of Solids, LRCS (https://www.lrcs.u-picardie.fr/), a French leading institution in the field of batteries and the Institut de Chimie de Picardie (https://www.u-picardie.fr/icp/index.php) at the University of Picardie Jules Verne. The PhD training and research will thus be carried in the vibrant environment of the city of Amiens, France.

**Profile and skills required**

The candidates must hold (or be about to receive) a Master's degree in Chemistry, Physical Chemistry, Materials Science or a similar relevant degree with an academic level equivalent to the master's degree in Engineering. Outstanding and highly motivated students from Chemistry and Physical Chemistry Departments with either organic synthesis, materials science/condensed matter chemistry or computational modelling experience are strongly encouraged to apply for this post. The successful candidates will have an excellent academic track record and shall be creative and highly motivated. Another mandatory requirement for the position is a personal interest in computational/theoretical research. Good knowledge of solid-state chemistry or organic synthesis and/or quantum chemistry/electronic structure theory would also be highly desirable. Hands-on experience with High Performance Computing is a plus. The candidate should be highly motivated by scientific challenges, be meticulous and perseverant. He/she will have to interact with several collaborators. He/she will have to communicate at conferences, etc. Therefore, the candidate should have excellent English skills.

## Applications

In addition to the https://adum.fr/ procedure, interested applicants are encouraged to send their application documents (letter of application, CV, academic transcript of B.Sc. and M.Sc. education/diploma, description of research experience and motivation, names of at least two academic references) as one pdf document per e-mail to Christine Frayret (email: christine.frayret@u-picardie.fr). The selection procedure starts now and candidates are encouraged to apply immediately. Applications will be considered till June 7th 2024 on the https://adum.fr/ web site.