Thesis offer at Institut des Sciences Chimiques de Rennes

MaCSE team, starting date september 2023

Titre: Synthesis of conducting molecular materials for energy storage

Location : Equipe Matière Condensée et Systèmes Électroactifs (MaCSE) de l'Institut des Sciences Chimiques de Rennes (ISCR), UMR 6226 CNRS, Campus de Beaulieu bat 10A, 35042 Rennes cedex (France)

Supervisor : Pr Dominique Lorcy

Keywords : Molecular chemistry, Conducting Molecular Materials, Batteries, Energy.

Molecular conductors, be they built out of fully organic or coordination compounds, raise a lot of interest for their applications in organic electronics and in energy storage devices (batteries).[1,2] There are also many advantages to use organic compounds since organic synthesis requires less energy (compared with ceramic way) and organic materials can be easily recycled. Recently, the charge transfer complex TTF-TCNQ, resulting from the association of the tetrathiafulvalene (TTF) as electron donor with the tetracyanoquinodimethane (TCNQ) as electron acceptor, was reported very promising for application in electrochemical energy storage as conductive-additive free electrode but also inversely as conductive additive with storage properties.[1] These results obtained with TTF-TCNQ pave the way for new studies on conductive molecular materials for energy storage.

Indeed, different types of conducting molecular materials exist: charge transfer complexes, ion radical salts and single component molecular conductors. Such class of compounds displays remarkable electronic and ionic conduction properties and in the same time is based on electroactive molecules (n-type or p-type) able to store reversibly electrons, depending on their chemical composition and structural arrangement. The host laboratory has extensive experience in the synthesis of precursors of these materials and the development of conductive materials.[3]

This PhD project aims at developing novel families of organic molecules (tetrathiafulvalenes, bisrhodanine and analogues) and coordination complexes (dithiolene complexes), able not only to provide radical species upon oxidation or reduction but also to favor specific intermolecular interactions between molecules themselves or their counter-ions in the solid state, towards highly conducting molecular materials. In a second step, it aims at investigate the applicability of these classes of conductive organic materials, either as electrode material or as conductive additives for electrochemical energy storage applications. The evaluation of the interest of these materials for energy storage will be conducted in collaboration

with our colleagues from the University of Amiens at LRCS (Laboratory of Reactivity and Chemistry of Solids UMR CNRS 7314). This multidisciplinary subject involves an important work of design and synthesis (organic, coordination chemistry) of new organic compounds and complex dithiolene electroactive, their characterizations in solution (NMR, optical spectroscopy, electrochemistry) and in the solid state (X-ray diffraction).

Funding : ANR COMETS for 36 months (≈ 2135 € gross monthly)

Candidate profile : The future PhD student should have a solid background in molecular chemistry (organic synthesis, coordination and organometallic chemistry, work in an inert atmosphere), with skills in electrochemistry. A motivation for materials science and solid state properties is an asset (crystal growth, crystallography, electronic properties). Good communication skills are necessary to exchange with the partners associated with this multidisciplinary project.

Interested student can contact :

Dominique Lorcy Tél. :02 23 23 62 73, email : Dominique.lorcy@univ-rennes1.fr

Applications must be made before May 15, 2023. All applications must include the following elements : detailed CV, letter of motivation ; names and emails of two contacts for recommendations.

1 Y. Fujihara, H. Kobayashi, S. Takaishi, T. Tomai, M. Yamashita, I. Honma, *ACS Appl Mater Interfaces*, **2020**, *12*, 25748.

2 P. Poizot, J. Gaubicher, S. Renault, L. Dubois, Y. Liang, Y. Yao, *Chem. Rev.* **2020**, 120, 6490–6557.

3 Y. Le Gal, T. Roisnel, P. Auban, N. Bellec, J. Iniguez, E. Canadell, D. Lorcy, *J. Am. Chem. Soc*. **2018**, *140*, 6998.