MaCSE Group
Institut des Sciences Chimiques de Rennes
Université de Rennes 1 - CNRS UMR 6226
+33(0)2 23 23 63 62
https://iscr.univ-rennes1.fr/macse/

PhD position (2023-2026) in Molecular Materials

Chalcogen bonding in organic conductors

Exploitation of multifunctionalities on the nano scale is a critical challenge in modern chemistry to satisfy the rapidly growing demands in electronics. In particular, materials that combine both electrical conductivity and magnetism could find applications in magnetic sensors, memories, magnetoelectronics and spintronics. Molecular materials offer a formidable playground to introduce multiple functionalities with almost endless possibilities to fine-tune the desired chemical and physical properties owing to the tremendous synthetic modularity. To introduce both electrical conductivity and magnetism in such materials, one attractive strategy relies on introducing paramagnetic metal complexes within organic conductors to generate interactions between π electrons of organic conductive stacks and metallic d spins.[1]

In this project, we want to take advantage of an intermolecular interaction called chalcogen bonding (ChB),[2] to induce strong spin-charge couplings. To this end, **new electron rich organic molecules different from the commonly used tetrathiafulvalene derivatives** will be designed and explored. This includes synthesis of electron-rich chalcogenated molecules where the spin density, in their cation radical state, is not only located on the chalcogen atoms but in a position readily available for direct interactions with a magnetic counterion. The project will not only broaden the utility of chalcogen-containing electron rich molecules other than tetrathiafulvalene as electronic functional materials but also provide new insight into chalcogen-bonding mediated spin-charge interactions. The project will also include active dissemination of the obtained results in scientific articles and through participation in national meetings and interactional conferences.

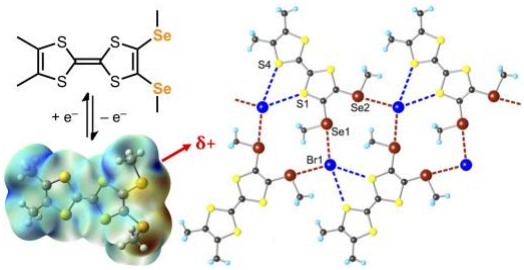

Figure. Activation of chalcogen bonding interactions in a radical salt of tetrathiafulvalene as an example[2d]

Specifically, the PhD student will be highly engaged in the preparation (**synthetic organic chemistry, manipulations under inert atmosphere**) of precursor π-donor molecules and magnetic building blocks. New organic conductor materials will be crystallized by **electrocrystallization** method (**crystal growth techniques**) and their structure and the formation of chalcogen bonding will be analyzed systematically by single crystal X-ray diffraction (**analysis of structural organizations**). The electric and magnetic measurements on the obtained crystals will be performed through local collaborations, where the interplay between conductivity and magnetism will be evaluated. The student will participate regular group meetings to present the progress, be also involved in writing reports on the advancement of project and of scientific publications. The project will be co-supervised by Dr. Ie-Rang Jeon and Dr. Marc Fourmigué at the Institut des Sciences Chimiques de Rennes in France.

Qualifications:
The successful candidate should have good knowledge and experience on **organic synthesis** and interest in pursuing multidisciplinary research (synthetic chemistry, crystallography, solid-state properties, etc.). Experience with crystallography and synthesis of air-sensitive compounds are considered strong advantages. Most importantly, the candidate should be highly motivated and possess organizational skills as well as the

ability to work both independently and as a part of a team. The candidate should be confident both in written and spoken English.

Other information:
The student should obtain their PhD degree within 3 years of the financial support. The university of Rennes offers French courses for foreign students and hosts an international Erasmus Mundus program.

Applications, sent to ie-rang.jeon@univ-rennes1.fr, should include a CV, a cover letter, at least one referent person, and a short summary of your master work.

Contacts: Dr. Ie-Rang Jeon, CR CNRS, (ie-rang.jeon@univ-rennes1.fr)
Dr. Marc Fourmigué, DR CNRS, (marc.fourmigue@univ-rennes1.fr)

[1] (a) G. Kawaguchi, M. Maesato, T. Komatsu, H. Kitagawa, T. Imakubo, A. Kiswandhi, D. Graf, J. S. Brooks, *Angew. Chem. Int. Ed.* **2015**, 54, 10169. (b) M. Maesato, T. Kawashima, Y. Furushima, G. Saito, H. Kitagawa, T. Shirahata, M. Kibune, T. Imakubo, *J. Am. Chem. Soc.* **2012**, *134*, 17452. (c) S. Uji, H. Shinagawa, T. Terashima, T. Yakabe, Y. Terai, M. Tokumoto, A. Kobayashi, H. Tanaka, H. Kobayashi, *Nature* **2001**, *410*, 908.

[2] ChB-related papers from the group: (a) M. Beau, S. Lee, S. Kim, W.-S. Han, O. Jeannin, M. Fourmigué, E. Aubert, E. Espinosa, I.-R. Jeon, *Angew. Chem. Int. Ed.* **2021**, *60*, 366. (b) A. Dhaka, O. Jeannin, I.-R. Jeon, M. Fourmigué, E. Aubert, E. Espinosa, *Angew. Chem. Int. Ed.* **2020**, *59*, 2383. (c) A. Dhaka, I.-R. Jeon, O. Jeannin, E. Aubert, E. Espinosa, M. Fourmigué, *Angew. Chem. Int. Ed.* **2022**, e202116650. (d) M. Beau, O. Jeannin, M. Fourmigué, P. Auban-Senzier, F. Barrière, I.-R. Jeon. *CrystEngComm*, **2022**, *24*, 7535.