Master 2 Research fellow at LRCS, Amiens, France
"Charge-transfer complexes for energy storage"

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Scientific Project:

Charge-transfer complexes (CTC) are a specific class of materials obtained by combination of an electron-donating molecule (named generally D or p-type in battery field) and an electron-accepting molecule (noted A or n-type in battery field).[1] While the donor part tends to be semiconductors, the CT complex can have entirely different properties. Indeed, associated D-A systems can be an ambipolar semiconductors, can present metallic behaviour, or even display superconductor properties. Charge transfer complexes have been studied since the 1970's for their conduction properties which can reach values equivalent to metallic compounds.[2] The most famous CT complex is TTF-TCNQ presenting a tuneable electronic conductivity depending of the stack architecture.[3] These remarkable performances make them excellent materials for conception of optoelectronic devices, for organic photovoltaic applications and even in catalysis.

In the field of electrochemical energy storage, charge transfer compounds have recently started to appear with a first study on TTF-TCNQ.[4] In parallel, another study was published on a TCNQ-based complex associated with a phenazine (PNZ) or a dioxin (DD).[5] Although these two pioneering studies highlight the interest of using this type of compound as electrode materials or as a conductive coating, it is important to note that there are an infinite number of combinations, and therefore potentially much more interesting performances to be found.

The aim of this master thesis is to investigate electrochemical activity (in battery configuration) and electrical/ionic conductivity properties of a series of CTC in order to probe their possible application as positive electrode materials or as conductive additives. A specific attention will be paid to the evolution of the crystalline structure of the materials upon cycling and its impact on the molecular packing and associated electrical conductivity.

Techniques used: *Electrochemistry (GCPL, CV, EIS, GITT), X-rays diffraction techniques (PXRD, in-situ, operando), Spectroscopic characterization (FTIR, NMR), Ball-milling, TGA-DSC, SEM.*

Recent publications related to the topic:

[1] Geiser, U. ; Schlueter, J. A. *Chem. Rev.* **2004**, *104* (11), 5203–5241.

[2] Wudl, F. *Acc. Chem. Res.* **1984**, 17, 227–232.

[3] Kirtley, J. R.; Mannhart, J. *Nat. Mater.* **2008**, *7* (7), 520–521.

[4] Guan, Y. S. *et al. Chem. Commun.* **2019**, *55* (50), 7179–7182.

[5] Lee, S. *et al. Energy Storage Mater.* **2019**, *20*, 462–469.

List of documents to provide:

CV + Motivation Letter ° list of references

Marks and ranking during master degree