PhD Project starting 1st October 2020

Laboratory: MOLTECH-Anjou (SOMaF group), University of ANGERS
(http://moltech-anjou.univ-angers.fr/)

Title of the PhD subject: Organometallic coupling methodologies from nitroarenes for active materials in organic photovoltaics

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Grant: PhD grant from University of Angers

Presentation of project:

The objective of this PhD aims to develop original organometallic couplings methodologies involving nitroarenes, to prepare new molecular materials or polymers, donor or acceptor. These materials will be integrated in organic electronics devices, in particular for applications in organic solar cells.

Most of the methods known today for synthesizing these molecules are using palladium-catalyzed organometallic couplings from halogenated derivatives. In our group, we have very recently successfully carried out the Suzuki-Miyaura reaction\(^1\) using a nitroarene as electrophile substrate, in particular on nitrated perylenedimide (PDI).\(^2\) These reactions turn out to be more interesting in terms of synthetic accessibility of the starting materials, selectivity, scalability and industrial applications than those using halogenated analogs.

In this PhD work, we will extend the study of the reactivity of this nitro function introduced on the bay-region of the PDI core, engaging it in various organometallic coupling methodologies, conducting mechanistic studies, and to probing the influence of the nature of the metal catalyst (Pd or the less onerous Ni). This study will then be extended to various nitroarenes, in particular other opto- or electroactive polyaromatic dyes in order to evaluate the potential of this coupling methodology, and open new possibilities in organic electronics.

This organic synthetic challenge will be completed by the study of the electrochemical and optical properties of these new molecular systems, and by their use as donors or acceptors in organic solar cells. This complementarity will thus enable the PhD candidate to acquire multidisciplinary training in the field of functional organic materials applied in organic electronics.

Profile of the candidate: The candidate must be an organic chemist and have a good university background. Knowledge in the field of organic materials, electrochemical and spectroscopic techniques (UV-Visible, fluorescence), and practical methods of organometallic couplings will be appreciated.

Application: The PhD project will start 1st October 2020. Candidates must send CV and cover letter showing motivation, including clear description of previous Master internship(s) to the following addresses:
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