PhD THESIS: **In silico design of molecular systems for nano and opto-electronics applications**

Research Group: **Inorganic Theoretical Chemistry Group**
Institute of Chemical Sciences of Rennes (ISCR)
CNRS - University of Rennes 1 - FRANCE
https://iscr.univ-rennes1.fr/cti/

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Supervisors: **Karine Costuas** - Senior researcher CNRS - ISCR
Jérôme Cornil - Senior researcher FNRS - University of Mons - BELGIUM

Collaborations: Christophe Lescop - Researcher - ISCR - INSA engineering school, Rennes
Stéphane Rigaut - Professor- ISCR, University of Rennes 1

Research Group: The team of Theoretical Inorganic Chemistry of the ISCR is a research group gathering 14 researchers of the CNRS, the University of Rennes 1 and the Engineering School of Chemistry of Rennes (https://iscr.univ-rennes1.fr/cti/). Its research topics are dealing with the rationalization using quantum chemical tools of chemical structures and physical properties of i) complex architectures (i. e. large clusters, glasses), ii) solid-state materials for energy, and iii) multifunctional molecular systems for opto-electronics or spintronics. The present project is part of the latter research axis. The group works complementarily in collaboration with the team in Mons, specialized in multi-scale modeling of materials for opto-electronics.

Scientific Context: Important worldwide financial supports have been devoted those last two decades to the researches developing technologies in molecular electronics, opto-electronics or spintronics leading recently to promising applications. The main interest of these systems is to have a high efficiency at the nanometric scale (small amount of atoms / low energy in use) that is fully in line with environmental challenges that the world faces. Molecular materials have demonstrated their potential applications in a wide array of sectors like data storage and information technologies, medicine, food, energy (solar energy, lighting…). The development of these technologies is focusing important private and public research efforts toward i) the optimization of properties for industrial processes, ii) the search for new functionalities to enlarge the application domains.

Research Project: The present research project aims at contributing to these research efforts using computational chemistry as a molecular screening tool to access to high-level functionalities in the aim of conceiving molecular-based devices. A particular focus will be devoted to stability in-use of the resulting devices. The past results of the Theoretical Inorganic Chemistry Group performed in collaboration with experimentalists of the ISCR and with several foreign research teams clearly demonstrate that quantum chemical studies are crucial to the understanding and strongly help in the design of functional inorganic and organometallic molecular compounds. Moreover, simulation of the properties of molecular devices are fully accessible.*[1] The present research project will be devoted to two applications: low-cost lighting and (thermal) energy harvesting at the nanoscale. For the first objective, our effort will be driven toward copper containing molecules for the availability and the low cost of this metal. Indeed, by a careful choice of its ligand sphere, luminescent compounds can be obtained. The in silico design will consist in finding the structural arrangements that show intense emission by focusing on the energies of the excited states and on the relativistic effects. Indeed, metal containing compounds are known to facilitate phosphorescence or late fluorescence leading to emission properties usually much more interesting that those of most of pure organic materials. Our recent work with C. Lescop team at the ISCR in collaboration with the one of V. W.-W. Yam in Hong-Kong demonstrates interesting thermally activated delayed fluorescence phenomenon at room temperature for a polymetallic copper complex.*[2] Based on this result, important molecular design will be performed toward improvement of emission properties. Our colleagues will perform the synthesis of the best molecular candidates in order to adapt and optimize directly the molecular systems.

The same research approach will be applied to the in silico design of molecular systems for thermoelectric applications with the aim of harvesting and converting wasted energy (heat) in in-use nano-devices into electricity (to prevent over-heating damages also). This part of the project will be done in collaboration with the team of Mons University. The aim here is to evaluate the thermoelectric ability of the best molecular targeted systems inserted in a junction to convert a thermal gradient into electric current, or reversely to cool

down a device by applying an electric potential. This domain of research is emerging and a lot has yet to be discovered. This project follows a recent result of the consortium which includes the team of S. Rigaut at the ISCR and the team of X. Chen in Singapore Nanyang University that reports the first molecular junction showing photo-switchable electronic transport.

Applicants: The PhD student will work in an international environment of research in which his/her researches will be crucial to the global project. Applicants should be graduated in chemistry or physical chemistry. Skills in quantum chemistry and/or molecular modeling experiments will be appreciated.

To apply or obtain additional information send an email to Karine Costuas (kcostuas@univ-rennes1.fr)

* **1 -** F. Meng, Y.-M. Hervault, L. Norel, K. Costuas, C. Van Dyck, V. Geskin, J. Cornil, H. H. Hng, S. Rigaut, X. Chen*, Chem. Sci., **2012**, 3, 3113*

*** 2 -** M. El Sayed Moussa, S. Evariste, H.-L. Wong, L. Le Bras, C. Roiland, L. Le Polles, B. Le Guennic, K. Costuas, V. W.-W. Yam, C. Lescop*, Chem. Commun. **2016**, 52, 11370.*