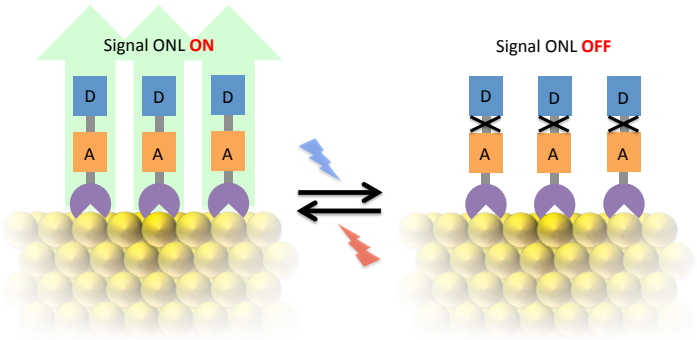
PhD Thesis

Simulation of Multi-States Nanometric Switches for Nonlinear Optical Applications

A PhD position is open in joint supervision between the University of Bordeaux (Frédéric Castet, Institut des Sciences Moléculaires) and the University of Namur (Benoît Champagne (Laboratoire de Chimie Théorique). The PhD will be conducted in the framework of the project *Integrated Photonic Architectures* within the excellence cluster LAPHIA (*LAsers and PHotonics In Aquitaine*, http://laphia.labex.u-bordeaux.fr), aiming at designing new organic-inorganic hybrid architectures of interest for photonic applications.

The objective of the PhD will focus on the simulation of nonlinear optical (NLO) properties of monolayers of organic photochromic compounds grafted onto metal or metal oxides surfaces, by using complementary quantum chemical methods. The morphology and electronic properties of large-size hybrid interfaces will be determined by means of order-N density functional theory (DFT) calculations, as implemented within the CONQUEST package. The NLO properties will be investigated by performing high level *ab initio* calculations on small-size aggregates extracted from the O(N) DFT calculations. These latter will serve as reference for evaluating the performances of computationally cheaper methods such as Tight-Binding DFT semiempirical approaches.



A 3-years PhD Grant will be provided for one half by the University of Bordeaux (funded by the Aquitaine Région) and for the other half by the University of Namur. The thesis will be carried out in both universities.

Candidates should have a solid background in physical and theoretical chemistry, with working knowledge on computational and numerical methods. They must be able to work in collaboration within international multidisciplinary teams including experimentalists, and demonstrate high-level communication skills in both written and spoken English.

Interested candidates are encouraged to contact Frédéric Castet (f.castet@ism.u-bordeaux1.fr) and Benoît Champagne (benoit.champagne@unamur.be). Necessary documents for the application are: a CV including the grades of previous education (in particular during the MSc) and the name of one reference (or one letter of recommendation), as well as a letter of motivation.

RÉGION AQUITAINE

université de BORDEAUX

UNIVERSITÉ DE NAMUR