**Unveiling the chemical bond under confinement....**

**A-B@Cn**

Emilie-Laure Zins, Vanessa Labet, Bruno Madebene, MONARIS UMR SU-CNRS 8233

Quantum characterisation of chemical bonding enables chemical processes to be rationalised, understood and predicted. Although it has been widely explored over the last century, chemical bonding under stress has been little studied so far. However, real chemical systems mostly operate in complex environments and are subject to a variety of constraints (electrical, mechanical, …).

The primary objective of this project is to provide insight into the behaviour of molecular systems under spatial confinement. We will start by characterising the response of main types of chemical bonds to spatial confinement and then study the effects of this response on the reactivity of small molecules. To this end, we will use well-established dedicated tools (QTAIM, ELF, MESP, conceptual DFT) that we will have to adapt to the case of encapsulated systems. In order to be able to decompose the effects of spatial confinement, we will consider different types of cages. First, we will implement "physical" cages whose size will be varied in order to control the "pressure" exerted on the structure. It will allow us to evaluate the magnitude of the quantum effect of the cage. Then we will consider molecular cages, first inert (e.g. fullerene) then reactive (e.g. fullerene doped with nitrogen).

This ambitious project brings together the complementary skills of the E=MCT researchers of the MONARIS laboratory. Furthermore, a one-year post-doctoral researcher specialized in quantum physics and with strong programming skills will be recruited for this project.

***Key words***: Topological characterization of the Chemical bond, Confinement in a molecular cage, Quantum chemistry, Reactivity under constraint