INFLUENCE OF CRYSTAL ENVIRONMENT ON MOLECULAR PROPERTIES

Supervisor: Pr. Enrique Espinosa (HdR) 03 83 68 49 53 *enrique.espinosa@crm2.uhp-nancy.fr*
Co-Supervisor: Dr. Emmanuel Aubert 03 83 68 48 81 *emmanuel.aubert@crm2.uhp-nancy.fr*
Laboratoire de Cristallographie, Résonance Magnétique et Modélisation (CRM2)
Institut Jean Barriol, Université de Lorraine - Nancy - FRANCE (www.crm2.uhp-nancy.fr)

The project is focused on the modeling of molecular properties upon the influence of the crystal environment, of either a single molecule or a group of them, presenting directional intermolecular interactions such as halogen and hydrogen bonding. The project aims to get insight on the crystal effect on the intermolecular interactions and how this can be used to tune desired molecular properties in the crystal phase. As an example, the cohesion energy is a crystal property of noticeable importance in pharmacology, where the efficient dissolution of an active compound of a drug must be controlled. To model this process, both the crystal energy and the competition between crystalline intermolecular interactions and those taking place in a biological medium (mainly hydrogen bonds) must be accurately described. In order to characterize the molecular interactions, the electron density and the electrostatic potential topologies will be analyzed. Main methods to be employed will be single crystal (and powder) X-ray and neutron diffraction, along with theoretical calculations in both periodic and gas phase systems. In addition, spectroscopic and calorimetric characterization techniques will be also employed. Target materials will be co-crystals and/or polymorphs of small molecules with biological activities.

Motivated candidates with good academic scores should contact us as soon as possible, sending a detailed *CV*, two recommendation and one motivation letters. The position will be opened by September 2013. A solid background in crystallography and diffraction methods is required. Knowledge on quantum chemistry will be appreciated.

Financing: '*Contrat Doctoral*': 3 years contract - Master diploma required - income = 1684€ (gross amount) or 2024€ if teaching & other tasks are also performed (indicative amounts)

Selected references of our previous works on the subject

1) *The nature of halogen···halogen interactions: A model derived from experimental charge-density analysis.* Angew. Chem. Int. Ed., **2009**, *48*, 3838-3841.
2) *Universal Features of the Electron Density Distribution in Hydrogen-Bonding Regions: A Comprehensive Study Involving H···X (X=H, C, N, O, F, S, Cl, π) Interactions*
Chem. Eur. J. **2010**, *16*, 2442 – 2452.
3) *Periodic projector augmented wave density functional calculations on the Hexachlorobenzene crystal and comparison with the experimental multipolar charge density model.*
J. Phys. Chem A, **2011**, *115*, 14484-14494.
4) *Charge Density Analysis and Topological Properties of Hal3-Synthons and Their Comparison with Competing Hydrogen Bonds*.
Cryst. Growth Des., **2012**, *12*, 5373-5386.