

Post-doctoral fellowship

MD investigations of non-covalent interactions ruling out crystallophores association to proteins

Supervisor: Elise Dumont (elise.dumont@ens-lyon.fr)

Location: Chemistry Department ([LCh](#)) of ENS Lyon (France)

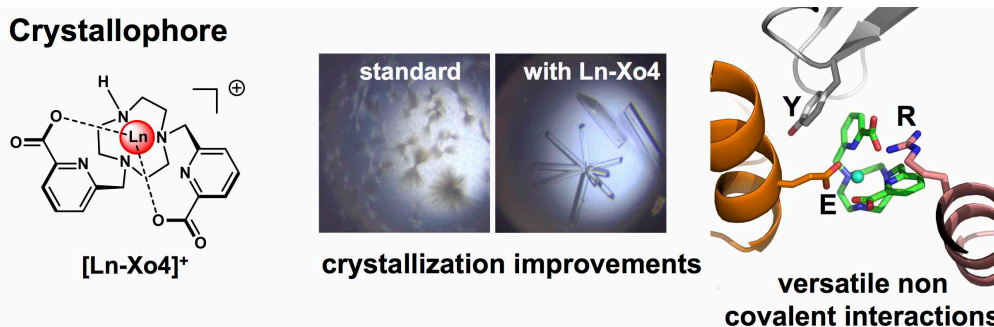
Starting date: 1st September 2018

Syllabus:

Obtaining protein crystals to solve their structures is amongst the most daunting tasks in Structural Biology. Chemists have recently designed “molecular glues” to assist the nucleation process and obtain high-quality, well-resolved crystals, such as lanthanides complexes or calixarenes.

The 1,5-year project is focused on a new generation of complex lanthanides, so-called crystallophores, synthesized in the host laboratory, which have been recently patterned and show promising behavior^[1,2]. The aim will be to use molecular dynamics approaches (both classical and QM/MM) to derive rules-of-thumb to rationalize the binding of this system on peptides and proteins. We will also scrutinize the protein-protein interface, which appears to be significantly mediated by the crystallophore^[3].

The candidate will benefit from state-of-the-art computational facilities of the PSMN cluster and of a rich scientific environment (LCh, Centre Blaise Pascal at ENS de Lyon, IBS Grenoble).



Skills:

The candidate must have a strong background in molecular dynamics, and experience with biological systems would be a definitive plus. He/she will be interacting on a very regular basis with inorganic chemists and bio-crystallographers.

References:

[1] E. Dumont, G. Pompidor, A. d'Aléo, J. Vicat, L. Toupet, R. Kahn, E. Girard, O. Maury N. Giraud *Phys. Chem. Chem. Phys.*, 2013, 15:18235-18242

[2] S. Engilberge, F. Riobé, S. Di Pietro, L. Lassale, N. Coquelle, C.-A. Arnaud, D. Pitrat, J.-C. Mulatier, D. Madern, C. Breyton, O. Maury, E. Girard *Chem. Sci.*, 2017, 8:5909-5917

[3] S. Engilberge, F. Riobé, T. Wagner, S. Di Pietro, C. Breyton, B. Franzetti, S. Shima, E. Girard, E. Dumont, O. Maury *Chem. Eur. J.* 2018, in press