

**PhD position: "Reactive transport in porous media: A multi-scale imaging and modelling approach"**

Univ. Bordeaux / CNRS / MUMMERING

**A 3-years PhD position** will be available at ICMCB, Institute of Condensed Matter Chemistry from Bordeaux, in the interdisciplinary field of 3D imaging, materials science and computation.

As PhD student, you will be part of MUMMERING (MUlti-scale, Multimodal and Multidimensional imaging for EngineeRING), an Innovative Training Network (ITN) accepted in 2017 (European call H2020-MSCA-ITN-2017). The position will be open the 1<sup>st</sup> of January 2018 to the earliest, and the contract will begin preferably before the 1<sup>st</sup> of May 2018.

**About MUMMERING:** ITN are Marie Skłodowska-Curie Actions aiming to support the career development and training of early-stage researchers through international and inter-sectorial mobility. MUMMERING is a European Training Network that will comprise 15 PhD students in 13 academic and 2 non-academic institutions from 9 different European countries. The scientific project is divided in 5 work-packages: WP1 "Data acquisition, electron and X-ray tomography. New modalities, atomic resolution, adaptive acquisition" (3 PhD). WP2 "Data management and HPC. Robust and automatized" (2 PhD). WP3 "3D reconstruction. Live reconstruction, missing data and direct inversion from Fourier space" (4 PhD). WP4 "Segmentation. Trained algorithms, segmentation without reconstruction" (4 PhD). WP5 "Modelling. 4D modelling and multi-scale" (2 PhD). ***This PhD position is part of WP5, and you can find information about all the MUMMERING PhD positions [here](#).***

**PhD project:** The objective is to develop a multi-scale imaging and modelling procedure for reactive transport in porous media. Indeed, in this kind of problems heterogeneous reactions are fundamental, meaning that the solid boundaries must be precisely described at the local scale, on the other hand the global spatial distribution of the solid must also be precisely characterized because it determines the average transport properties. Multi-scale imaging techniques can provide a "low" resolution (LR) image that can be used as input for computing the average transport properties, and a "high" resolution (HR) image that describes the solid boundaries in details. For numerical modelling we need the LR image of all the computation domain, and HR information of the zones where important reactions take place. Acquiring a HR image of the full computation domain is not realistic, and, if an average value is not sufficient for modelling (effective reactive surface), we need a way to incorporate in a multi-scale model both HR and LR information. The solution we propose to explore is based on a super-resolution approach: A limited region of the considered material is imaged at LR and HR. From this couple of images, a statistical model of the way they locally relate is built. This model allows to compute the most probable HR image associated to a LR one, and reciprocally. In the iterative multi-scale numerical modelling this model will be used to locally increase the resolution. After a first simulation at the LR scale (i.e. relevant for the transport at the global scale), the zones where grid refining is necessary are selected using an error estimate procedure. Super-resolution can then be used to complement LR image in these zones and generate finer grid to improve the quality of the results. As PhD student, you will mainly focus on the numerical aspects of the project, but you will also be actively associated to the super-resolution approach developments (Y. Berthoumieu from IMS, and JF Aujol from IMB) and to several topics covered in the network (multi-scale imaging, HPC, etc.)

**Requirements:** To apply you must meet Marie Curie Early Stage Researcher (ESR) eligibility criteria. In particular, you must not have resided in France for more than 12 months in the last 3 years immediately prior to commencing in the role, and, at the date of recruitment, you must be in the first four years (*full-time equivalent research experience*) of your research career.

Mobility within the MUMMERING network (trainings provided by MUMMERING and secondment to industry and academic partners) is mandatory. In the network you will participate in summer schools, workshops, and scientific meetings with top scientists and the 14 others PhD students of MUMMERING. During your secondment, you will work with multi-scale data acquisition at synchrotron facility and with High Performance Computation at top level laboratories.

A MSc degree is required with a strong background in numerical modelling, computer programming, transport properties of materials, and 3D image analysis. Skills in large data processing will be appreciated.

There is no condition of citizenship, but the applicant will have to be agreed by the French government, ICMCB being a classified laboratory.

**Academic supervision:** As PhD student, you will be supervised by Dominique BERNARD, CNRS senior scientist at ICMCB, by Yannick BERTHOUMIEU, Prof. at Bordeaux INP, and by Jean-François AUJOL, Prof. at Bordeaux University.

**Terms of employment:** The position is a three-years full time appointment under PhD student contract with the French National Centre for Scientific Research (CNRS) following the rules of the Marie Skłodowska-Curie Actions. Contract will start between January and May 2018.

**Application:** Candidates are requested to submit a single pdf file containing:

- A letter motivating the application
- A detailed CV
- Academic transcripts

to Dominique.Bernard@icmcb.cnrs.fr

Selection will be based on merit and potential, measured in terms of academic records and personal achievements. Creativity, proactivity and capacity for teamwork will also be taken into account.