

## LabEx MMCD

### Multi-Scale Modelling & Experimentation of Materials for Sustainable Construction

#### Post-doctoral position

#### Hybrid aerogels for sustainable construction: a new modelling approach to characterize effective properties

##### Summary

This post-doctoral project is a part of the structured project entitled "porous and biosourced materials" in the framework of the Laboratory of Excellence (LabEx) MMCD "Multi-scale Modeling & Experimentation for Sustainable Construction" of the "Université Gustave Eiffel". The aim of this project is to strengthen the actions undertaken for new processes for the preparation and characterisation of hybrid aerogels for sustainable construction, the properties of which are well understood. It draws on the complementary expertise of two LabEx laboratories: the "Institut de Chimie et des Matériaux Paris-Est" (ICMPE, UMR 7182 CNRS) and the laboratory "Modélisation et Simulation Multi Echelle" (MSME, UMR 8208 CNRS).

Two new classes of very promising materials, particularly in terms of thermal insulation and low environmental impact - vacuum insulation panels and silica-based aerogels - are now meeting with growing interest in the building sector. The highly porous structure of aerogels – gels in which a liquid has been replaced by a gas – means that up to 99.99% of the air can be confined, giving thermal conductivity values at atmospheric pressure that are lower than those of still air. They are therefore described as thermal super-insulators that block heat loss. The use of this type of ultralight nanostructured solid means that the thickness of the insulating material can be reduced by up to three times, while maintaining the same thermal conductivity. However, in addition to their high cost, pure silica aerogels, which are of great interest in the field of super-insulation, suffer from poor resistance to mechanical stress and thermal shock, which is holding back their large-scale industrialization and commercial success. More recently, transparent aerogels have been developed to replace window glass.

One of its objectives is to study the multi-physical behavior of aerogels in development and to better understand the microstructural effects on their effective properties. The obtained results are important to guide the elaboration task of these materials, which also actively is developed by the chemists within the project framework. We will focus on determination of the effective mechanical and thermal properties. The theoretical characterizations, together with experimental characterization, would provide more precise specifications for the elaboration.

The geometric configuration of these hybrid aerogels can be represented at the macroscopic scale by using the work of Kelvin and Weaire-Phelan, which consists of paving space by repeating cells made up of polyhedra with more or less regular hole faces. The division of space into polyhedra with a minimum total surface area is a fundamental issue in science, particularly mathematics. In 1887, Lord Kelvin conjectured that the optimal partition of space is obtained with a space-filling polyhedron with 14 faces, called a tetrakaiedecedron. Kelvin's conjecture held up for a century until, in 1994, Weaire and Phelan proposed a new structure, made up of eight polyhedra, obtained from numerical simulations. One of the scientific challenges in this work is to find the class of geometric configurations for homogenization on the macroscopic scale that best represents the aerogels developed by the ICMPE.

To achieve the desired result, it is proposed to use a 3-scale homogenization model developed by the MSME lab with these new geometric configurations and to use machine learning methods (in particular via artificial neural networks) to provide predictions. The artificial neural networks will be trained on a large dataset using the database obtained from the 3-length scale homogenization model. The model developed will need to be capable of efficiently estimating effective properties from a dataset defined by a large number of geometric (e.g. size and spatial distribution of chitosan chains and graphene sheets, porosity, characteristic aerogel length, etc) and physical parameters at all three scales. The model developed should be capable of efficiently estimating effective properties from a dataset defined by a large number of geometric (e.g. size and spatial distribution of chitosan chains and graphene sheets, porosity, characteristic length of aerogel, etc.) and physical parameters at all three scales. To achieve the desired result, a hybrid approach combining artificial neural networks and the 3-scale model is proposed. The use of neural networks will make it possible to quickly predict the actual behavior of the aerogel after a learning phase. The construction of suitable neural networks requires a detailed choice of model hyperparameters such as the activation function, the number of intermediate layers and the number of neurons in each layer, optimization algorithms, etc. In order to speed up the generation of data for the simulation, we also aim to introduce a model reduction strategy using the orthogonal eigenvalue decomposition method.

The successful candidate will develop new multiscale analysis for modeling the physical behavior of elaborated hybrid aerogels. To obtain the effective properties, this model uses a homogenization method based on explicit relationships of multilayer laminated structures at the smallest scale (nanometric) and then on asymptotic developments at the other scales (hundreds of nanometers and hundreds of micrometers).

The numerical solution will be obtained by using the finite element method and/or the Fast Fourier Transform method. The candidate will implement the numerical methods and provide some useable tools which allow other PhD students to do their own numerical tests.

### **Keywords**

Mean-field homogenization, asymptotic homogenization, numerical methods, machine learning

### **Required competences**

The candidate should have a PhD in solid mechanics with strong backgrounds in numerical methods for solving partial differential equations. A taste of modelling and programming is also appreciated. Knowledge of multiscale and homogenization methods using double-scaled asymptotic development methods will be a plus. The candidate is supposed to work on a transverse project with strong collaborations between specialists in mechanics and chemists. He/she should be able to participate to their discussions with certain open-mindedness.

### **Application procedure**

The application should be written in English or French. Please send your cover letter and CV (including publication list, prior research experience and contact information of two references) as a single pdf file to:

MSME :                Salah Naili ; naili@u-pec.fr  
                             Vu-Hieu Nguyen ; vu-hieu.nguyen@u-pec.fr

### **Salary, duration and location**

Net salary about 2300€/month. The postdoctoral position is for 12 months and can start in October or November 2023.

The laboratory is located at the "Campus Centre" (Métro Créteil-Université, about 10 km from Paris center).

### **Date of starting diffusion**

July 2023