





Modélisation et Simulation Multi Echelle

Postdoctoral Position

Molecular Dynamics applied to bone matrix nanoporosity

Cortical bone is intrinsically a multiscale living material. When studying mass transport phenomena within this type of tissue, it is then necessary to adopt a multiscale strategy. While the organ's scale characterized by the vasculature network (millimetre scale) and the lacunocanalicular scale (micrometer scale) are widely studied combining continuum mechanics with numerical simulation and imaging methods, the nanometric scale of the pore of the collagen-apatite matrix are less studied. In particular, the possibility of observing a mass transport between the mineral platelets of the collagen-apatite matrix is still an open question in bone biomechanics. To better understand some key phenomena such as the bone mineralization process or the paracrinal cell-to-cell communication, it is of high relevance to characterize the phenomena occurring at the scale of the hydroxyapatite platelets (nanometre scale). At this scale, the concepts of continuum mechanics fail and other methods such as molecular dynamics are required.

The main objective of this postdoctoral position is to participate in one of the transverse activities of the Laboratory MSME regrouping people from the four teams (Biomechanics, Chemistry, Mass transfers and Mechanics). The post-doc position is open to any candidate that presents skills in molecular dynamics involving water, ions and mineral platelets (hydroxyapatite). The candidate will have to develop molecular modeling and simulation to describe the water-hydroxyapatite interactions with typical ions that can be found in the bone context (typically calcium and sodium ions). Thus, the water structure and the effective diffusion coefficient could be provided as inputs in multiscale mass transport models developed in the laboratory.

The candidate should have a PhD with prior research experience in molecular modeling and simulation. Familiarity with scientific programming, molecular simulations and Linux system is also required.

For more information about the laboratory, please visit http://msme.univ-mlv.fr/

Application procedure: The application shall 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: salah.naili@univ-paris-est.fr and thibault.lemaire@univ-paris-est.fr. The search will continue until the position is filled.

Contact: Salah Naili (salah.naili@univ-paris-est.fr) and Thibault Lemaire (thibault.lemaire@univ-paris-est.fr)

Salary, **duration and localisation**: Net salary: about 2100€/month (gross salary: 2600€/month). The postdoctoral position is for 12 months and can start as soon as possible. The laboratory has two locations at Marne-la-Vallée and Créteil (Métro Créteil-Université).