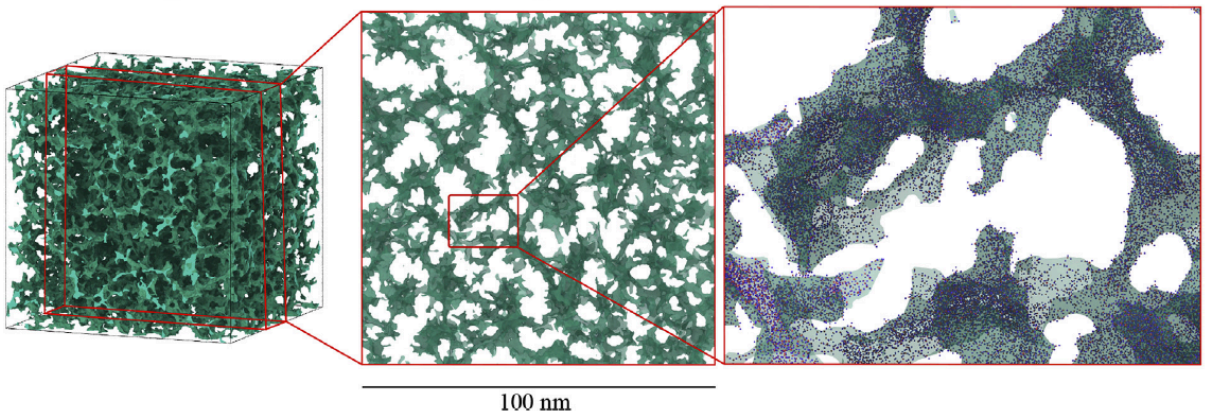
Water surface effects on the mechanical properties of silica aerogels: a molecular dynamics study

New optimized components with very high thermal resistance and minimal thickness are needed for the conservation of energy in the building industry. Based silica aerogel materials could match these strict standards, as they exhibit a very low thermal conductivity (< 20 mW/m.K). Their tortuous nano-porous structure with extremely high surface to volume ratio, see figure, and the ceramic nature of silica aerogels provides the required thermal properties but is also responsible for their poor mechanical properties.



Silica aerogel obtained by molecular dynamics simulation [1]. Right, zoom on the ligaments, brick of the silica aerogels structure

A recent molecular dynamics study of pure silica aerogels shows that their mechanical properties, like asymmetry in tension-compression tests, arise from preexisting surface stress [1]. The omnipresence of water in the environment of silica aerogels materials can affect this surface stress and therefore influences their mechanical properties. A development of ReaxFF-based molecular dynamics potential, validated with DFT simulations and experimental values, allows to simulate well water-silica interfaces [2].

The aim of this postdoctoral job is to study and simulate, with the ReaxFF-based molecular dynamics potential, the mechanical properties (tension-compression tests) of a silica ligaments, brick of the silica aerogels structure, see figure, in the presence of water on its surface.

The proposed job is funded by the AURA region as part of a collaborative project involving MATeB (MATEIS and EDF) and SIMaP laboratories, ENERSENS and the CSTB.

Candidate: Doctor in the field of mechanics of materials with knowledge in molecular dynamics.
Start: from now and before october 2018. Duration: 1 year
Localization: MATEIS Laboratory (INSA de Lyon - France)
PhD advisors: Julien Morthomas, Patrice Chantrenne and Geneviève Foray.
Salary: between 1800 and 2400€ net/month depending of the years of experience.
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[1] W. Goncalves, J. Morthomas, et al., Acta Mat. **145**, 165(2018)
[2] J.Yeon et al., *J. Phys. Chem. C* **120**, 305-317 (2016), J.M. Rimsza et al., *J. Phys. Chem. C* **120**, 24803-24816 (2016), M. Pitman et al., J Amer. Chem. Soc. **134** 3042-3053 (2012), J.C. Fogarty, et al., *J. Chem. Phys*. **132**, 174704 (2010),