

# **Nanoscale analysis of the surface and interfaces between sediment and cementitious matrices**

**Ali Zaoui**

*Civil Engineering and geo-Environment Laboratory LGCgE-Lille Nord de France,  
Polytech'Lille. Université de Lille 1 Sciences Technologies. Cité Scientifique. Avenue Paul  
Langevin. 59655 Villeneuve D'Ascq Cedex, France*

*Email : [aзаoui@polytech-lille.fr](mailto:aзаoui@polytech-lille.fr)*

## **Abstract**

In this talk I will give, first, an overview on modeling and simulation at nanoscale level. I will explain the main background of the corresponding methods such as Molecular dynamics, Monte Carlo and first-principles. I will then introduce some examples based on recent studies on concrete, clays and minerals. The main focus of the talk will be on nanoscale modeling of the bulk and surface states of the nanogranular calcium silicates hydrates (C-S-H) gel. Regarding the mechanical properties as well as porosity, we identify two main phases: a ductile one, when porosity increases from 12.4 % to 27 % and a brittle phase for a porosity lower than 12.4% or higher than 27%. These studies show that 20 % of gel porosity makes C-S-H in a better structural stability, with a higher stiffness. I will show the (001) surface of C-S-H gel at the nanoscale level and explain how more water on the surface will stabilize thermodynamically the nanostructure. I will also show that the (001) surface of Low Density C-S-H tends to be more stable than the surface of High Density phase since the obtained surface energy decreases with increasing gel porosity. Finally, I will explain how and why calcite can consolidate C-S-H with 30% of gel porosity.