Multiscale modeling of geopolymers

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Research Field: Geopolymers, Numerical Simulation, Microstructure, Mechanics

Context: Geopolymers are amorphous multi-scale aluminosilicate binders synthesized at room temperature by alkaline activation of aluminosilicate raw materials (metakaolin, fly ash…). These materials are intrinsically porous materials with a wide pore size distribution and a variable pore shape. The interest in geopolymers stems from their high compressive strength, high chemical and thermal resistance, complying with the main durability criteria that are beneficial for a number of industrial applications. For example, dense and lightweight geopolymers are used in civil engineering, chemical and nuclear industries, typically for conditioning certain toxic metals and radioactive elements or treating liquid nuclear waste. To achieve optimum mechanical properties for industrial applications, the dissolution and the polycondensation reactions are the key processes to understand in order to control the multiscale pore network of geopolymers.

The aim of this project is the multiscale modeling of the geopolymerization process using the numerical toolbox of soft matter and granular physics to elucidate the relation between chemical composition and pore network formation. The first step is to establish a realistic and consistent atomistic model of geopolymers. Atomistic modeling is important for understanding the chemical reactions of polycondensation. Modelling all atoms with reactive potential is computationally expensive and limited to the subnano scale. Therefore, the next step is to use the atomistic findings to identify a meaningful coarse-graining unit and effective interactions between these units in order to simulate the structure and mechanics at larger scales.

Websites of the laboratories: (<MSE>2 @ MIT**) & (**PMMD @ LMGC @ UMontpellier**) & (**CEA Marcoule**)**

Remarks: The PhD thesis is funded by CEA in France. The successful candidate will be located at Université de Montpellier with the possibility to spend a year as visiting PhD student at MIT in <MSE>^{2} the MIT-CNRS-AMU joint laboratory. Background in statistical physics and/or computational physics and/or soft matter physics and/or physical chemistry are preferred. This project is interdisciplinary between physics, chemistry and civil engineering.

How to apply? Send a cover letter, a CV and copies of transcripts (including lectures followed and grades/rankings when available) to hekate@mit.edu