From clay minerals to cement and charcoal and to the urban environment: bridging time and length scales in the modeling of complex porous materials

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We investigated the formation and mechanical, transport, aging… properties of multi-scale materials such as clays, cement, geopolymer, charcoals...

Concerning length-scales, I will introduce the concept of Potential of Mean Force, PMF,as a way to implement upscaling modeling from the nano-scale to micron-scale. As regards to time scales, I will introduce meta-dynamics concepts as a way to implement upscaling modelling from the time scale of the elementary chemical reaction to geological time scales.

A PMF is a free energy function representing in an effective way the interactions between objects (cement hydrates, clay platelets, etc.) at thermodynamics conditions. The PMF is therefore the key piece of information allowing to coarse-grained Physical Chemistry information in a meso-scale model formulation. The use of PMF offers a huge computational advantage as it allows a straight up-scaling to the meso-scale while keeping essential interactions information that are the hallmark of Physical Chemistry processes. Such a coarse-grained modeling integrates atomistic response into inter-particle potentials that fully propagate molecular scale information all the way to the meso-scale.

Concerning time scales, I will introduce the reactive replica exchange molecular dynamics (RExMD) to investigate the geological conversion of two important classes of gas-forming constituents of terrestrial organic matter (lignin and cellulose) into charcoal. This conversion takes place over a time window of hundreds of millions of years and has so far remained a no man's land to theoreticians. Using reactive molecular dynamics and the RExMD framework, I will show that one can now simulate the full transformation of cellulose and lignin into charcoal and its associated fluid phase under prevailing geological conditions.

In the last part of this talk, I will present the concepts of Urban Physics in which cities are seen as porous systems for the prediction of urban climatic events (heat islands, storms, hurricanes, floods…) from the scale of neighborhoods to that of urban systems. Urban Physics is based on descriptors such as the two-point spatial correlation function, g(r), the average number of first...n-neighboring buildings, a local order parameter quantifying the organization of the buildings constituting the immediate neighborhood… directly imported from the analysis of the texture of matter at the molecular scale in a physics by analogy approach.