INSTITUT DE CHIMIE

ANNÉE ACADÉMIQUE 2015-2016

COLLÈGE DE FRANCE 1530

Conférence

**Roland PELLENQ**
Directeur de Recherche CNRS, MIT

Mercredi 1er juin 2016 à 11h
Salle 2

Roland Pellenq is a computational materials scientist with a strong interest in the physics and mechanics of micro- and nanoporous materials and confined fluids. He graduated in 1994 with a PhD in Chemical Physics from Imperial College, London; and is currently Director of Research at CNRS, the French government research agency and a MIT Senior Research Scientist. Dr. Pellenq's research is dedicated to the development of bottom-up simulation approaches (starting at an atomistic level of description) for a large variety of critical problems in energy and environment, ranging from hydrogen and CH4 storage, CO2 sequestration/fracking, shale gas to the stability of nuclear fuels and fundamentals of cement and concrete research. R. Pellenq is the author or co-author of 160+ papers published in major peer reviewed scientific journals. He was one of the co-founders and lead scientist of the Concrete Sustainability Hub, CSH@MIT, opened in 2009, an interdisciplinary research center dedicated to the reduction of the environmental footprint of the cement and concrete industry. He is also principal investigator of the MIT X-Shale project focusing on gas-shale research. He was hired as a MIT Senior Research Scientist in November 2011 and is the head of the CNRS-MIT joint laboratory "Multi-Scale Material Science for Energy and Environment" open in June 2012 and located on the MIT campus.

## THE BOTTOM-UP MODELLING APPROACH TO CEMENT PASTE

Strength and other mechanical properties of cement paste and concrete rely upon the formation of calcium-silicate-hydrates (C-S-H) during cement hydration. Despite the potential for technological transformation, controlling the structure and properties of C-S-H phase is still a challenge, due to the complexity of this hydration product and of the mechanisms that drive its precipitation from ionic solution upon dissolution of cement grains in water. Departing from traditional models that are mostly focused on length-scales above the micrometer, molecular models have recently addressed the nanometer-scale structure and properties of C-S-H. However, small angle neutron scattering, electron-microscopy imaging, and mechanical nano-indentation experiments, all suggest that an even more important role is played by the mesoscale organization of the C-S-H structure that extends over hundreds of nanometers. New quantitative models are needed to address this unexplored meso-scale, elucidate the experimental observations, and complete the understanding of the multi-scale structure of cement paste. Here we present a novel description of the C-S-H meso-structure that offers an opportunity to translate results from the fundamental scales to the macro-scale of engineering properties. We use simulations that combine information of the nano-scale building units of C-S-H and on their effective interactions, obtained from atomistic simulations and experiments, into a statistical physics framework for aggregating nanoparticles. We compute small angle scattering intensities, pore size distributions and nano-indentation modulus and hardness, providing a new quantitative understanding of the relevant features observed experimentally. Our results suggest that specific heterogeneities developed during the early stages of hydration persist in the structure of C-S-H, impacting the rheological and mechanical performance of the hardened cement paste.