Multi-scale Materials Under the Nanoscope 2016
Université Pierre et Marie Curie, Paris, 7–9 December 2016
Amphithéâtre Durand, bâtiment Esclangon

7th December

09:00 Welcome address – Pierre Levitz and Roland Pellenq

Introductory lectures
Chair: Roland Pellenq

09:15 Emanuela Del Gado (Georgetown University)
From statistical physics of complex materials to cement hydrates
09:45 Jean-Marie Tarascon (Chaire Chimie du Solide-Energie, Collège de France)
Materials advances for better Li(Na)-ion batteries: can theory help?
10:15 Paulo Monteiro (University of California at Berkeley)
Advances in high-resolution imaging of materials using x-ray synchrotron radiation

10:45 *Coffee Break*

Nano-micro poromechanics (Part I)
Chair: Paulo Monteiro

11:20 Sébastien Brisard (Laboratoire Navier, ENPC-CNRS-IFFSTAR)
Microstructure and macroscopic mechanical properties: polarization techniques to the rescue
11:50 Gyorgy Hantal and Gilles Pijaudier-Cabot (Laboratoire des Fluides Complexes et leurs Réservoirs, UPPA-CNRS-TOTAL)
Effects of surfaces on the mechanical properties of nanoscale materials
12:10 Pierre-Louis Valdenaire (Multi-Scale Materials Science for Energy and Environment, MIT)
Numerical Assessment of Kerogen's Flexibility at the Atomistic Scale

12:30 *Lunch (buffet) + Posters*

Multiscale materials for supercapacitors
Chair: Benjamin Rotenberg

14:00 Patrice Simon (Université Paul Sabatier Toulouse)
Ion adsorption and transport in porous carbons electrodes: application to Electrochemical Capacitor
14:30 Céline Merlet (Department of Chemistry, University of Cambridge)
NMR study of charge storage mechanisms and ion dynamics in supercapacitors
15:00 Dominique Petit (Laboratoire Charles Coulomb, Université de Montpellier-CNRS)
Multi-Scale Dynamics of free and confined ionic liquids
15:20 Trinidad Méndez Morales (Maison de la Simulation, CEA and PHENIX, UPMC-CNRS)
Computational study of graphene-based supercapacitors
15:40 Zhujie Li (Maison de la Simulation, CEA and PHENIX, UPMC-CNRS)
Marcus free energies for the Fe^{3+}/Fe^{2+} couple in ionic liquids

16:00 *Coffee Break*

Nano-micro poromechanics (Part II)
Chair: Sébastien Brisard

16:30 David Grégoire (Laboratoire des Fluides Complexes et leurs Réservoirs, UPPA-CNRS-TOTAL)
Characterisation of the confinement state of a fluid in a nanometric split pore by density functional theory in the context of adsorption-induced swelling in microporous media
16:50 Laurent Brochard (Laboratoire Navier, ENPC-CNRS-IFFSTAR)
A possible nano-scale origin of the surprising thermal expansion of clays
17:10 Matthieu Vandamme (Laboratoire Navier, ENPC-CNRS-IFFSTAR)
Experimental study of stresses induced in model cement-based materials by in-pore crystallization
17:30 Christian Hellmich (Institute for Mechanics of Materials and Structures, Vienna University of Technology)
Molecular-to-continuum poroelasticity upscaling of hydrating cement pastes, considering progressive C-S-H gel densification

8th December

Dynamics and thermodynamics of confined fluids (Part I)
Chair: Emanuela Del Gado

09:00 Katerina Ioannidou (MIT)
Mesoscale modelling of cement hydrates: application to freeze-thaw damage
09:30 Eric Ferrage (Institut de Chimie des Milieux et Matériaux de Poitiers)
A multiscale investigation of structure and dynamics of water confined in swelling clay porous media
10:00 Mohammad Javad Abdolhosseini Qomi, University of California - Irvine
Intermolecular forces between C-S-H Layers

10:30 *Coffee Break*

Dynamics and thermodynamics of confined fluids (Part II)
Chair: Eric Ferrage

11:00 Yann Magnin (Centre Interdisciplinaire de Nanoscience de Marseille, Aix-Marseille University and CNRS)
Nickel-carbon nanoparticles: size dependent phase diagrams and interaction with graphenic layers
11:20 Obliger Amael (Multi-Scale Materials Science for Energy and Environment, MIT)
Transport of Hydrocarbons Mixtures in Disordered Nanoporous Materials
11:40 Fouad Oulebsir (Laboratoire des Fluides Complexes et leurs Réservoirs, UPPA-CNRS-TOTAL)
Permeation of supercritical fluids through nanoporous constrictions : theory and simulations
12:00 Pauline Simonnin (PHENIX, UPMC-CNRS and IFP Énergies Nouvelles)
Non-equilibrium simulations of flow in clay nanopores using a wall thermostat
12:20 Jean-Pierre Korb (PHENIX, UPMC-CNRS)
Probing saturation, dynamics and wettability of oil and water in Shale Oils

12:40 *Lunch (buffet) + Posters*

New synthetic approaches to multiscale porous materials (Part I)
Chair: Mathieu Bauchy

14:00 David Portehault (Laboratoire Chimie de la Matière Condensée de Paris, UPMC)
Looking for nano in nano: heterostructures within nanomaterials
14:30 Cédric Boissière (Laboratoire Chimie de la Matière Condensée de Paris, UPMC)
Coupling soft chemistry and processing for designing hierarchical functional materials
15:00 Adeline Dannoux-Papin et Jérémy Haas (CEA)
Radiolytic hydrogren emissions: from hydrates to cement pastes
15:20 Léa Atmani (CINAM and UMI-CNRS-MIT)
Degradation of organic matter under geological conditions: a route towards thermodynamic solid/fluid equilibrium using replica exchange molecular dynamics simulations

15:40 *Coffee break*

New synthetic approaches to multiscale porous materials (Part II)
Chair: Mohammad Javad Abdolhosseini Qomi

16:20 Mathieu Bauchy (Physics of AmoRphous and Inorganic Solids Laboratory, UCLA)
Irradiation-Induced Damage in Concrete: The Enthalpy Landscape Viewpoint
16:50 Saeid Nezamabadi (Laboratoire de Mécanique et Génie Civil (LMGC), Université de Montpellier)
Modeling soft-particle materials: shear behavior and effect of porosity
17:10 Alice Dufresne (MIT)
Atomic-scale modeling of the Alkali-Silica Reaction

17:30 Sara Bahafid (Laboratoire Navier, ENPC-CNRS-IFFSTAR)
Effect of hydration temperature on the pore structure of cement paste
17:50 Jean-Baptiste d'Espinose de Lacaillerie (Sciences et Ingénierie de la Matire Molle, ESPCI)
Hydrophobization of Silica Nanoparticles in Water: Resulting Porous Nanostructure and Response to Drying Stress

19:30 *Conference dinner (La Baleine, jardin des plantes)*

9th December

Multiscale materials of our cultural heritage: challenges and perspectives
Chair: Pierre Levitz

09:00 Loïc Bertrand (Institut photonique d'analyse non-destructive europen des matériaux anciens, Synchrotron SOLEIL)
A few challenges posed by multiscale ancient materials
09:30 Laurence de Viguerie (Laboratoire d'Archéologie Moléculaire et Structurale, UPMC-CNRS)
Multiscale approaches to characterize historical oil paintings
10:00 Laurent Michot (PHENIX, UPMC-CNRS)
Neutron imaging investigation of fossil woods: non-destructive characterization of microstructure and detection of in-situ changes

10:30 *Coffee break*

New developments in imaging multiscale porous materials
Chair: Loïc Bertrand

11:00 Emmanuelle Gouillart (Unité mixte CNRS/Saint-Gobain Surface du Verre et Interfaces)
In situ multi-scale tomographic imaging of topological changes in phase-separated glasses
11:30 Jeremie Berthonneau (MIT)
Experimental characterization of the organic pore network of source rocks at the nano-scale
12:00 Jonathan Perrin (CINAM, Université Aix-Marseille)
Morphological characterization of ceramic membranes from 3D X-ray computed tomography
12:20 Jean-Marc Leyssale (Laboratoire des Composites ThermoStructuraux)
Structure and property alterations in graphite under high electron dose: a combined TEM/MD investigation

12:40 Closing words – Pierre Levitz and Roland Pellenq