Wednesday, December 7, 2016

TIME	EVENT
09:00 - 09:15	Welcome address - Pierre Levitz and Roland Pellenq
09:15 - 10:45	Introductory lectures
09:15 - 09:45	› From statistical physics of complex materials to cement hydrates - *Emanuela Del Gado, Georgetown University*
09:45 - 10:15	› Materials advances for better Li(Na)-ion batteries: can theory help ? - *Jean-Marie Tarascon, Chimie du Solide-Energie, UMR 3680, Collège de France, Réseau sur le stockage électrochimique de l'énergie*
10:15 - 10:45	› Advances in high-resolution imaging of materials using x-ray synchrotron radiation - *Paulo Monteiro, University of California at Berkeley*
10:45 - 11:20	Coffee break
11:20 - 12:30	Nano-micro poromechanics (Part I)
11:20 - 11:50	› Microstructure and macroscopic mechanical properties: polarization techniques to the rescue - *Sébastien Brisard, Laboratoire Navier*
11:50 - 12:10	› Effects of surfaces on the mechanical properties of nanoscale materials - *Gyorgy Hantal, Laboratoire des Fluides Complexes et leurs Réservoirs - Gilles Pijaudier-Cabot, Laboratoire des Fluides Complexes et leurs Réservoirs*
12:10 - 12:30	› Numerical Assessment of Kerogen's Flexibility at the Atomistic Scale - *Pierre-Louis Valdenaire, Massachusetts Institute of Technology (MIT), Multi-Scale Materials Science for Energy and Environment*
12:30 - 14:00	Lunch (Buffet) + Posters
14:00 - 16:00	Multiscale materials for batteries and supercapacitors
14:00 - 14:30	› Ion adsorption and transport in porous carbons electrodes: application to Electrochemical Capacitors - *Patrice Simon, Université Paul Sabatier Toulouse III,, FR CNRS 5085*
14:30 - 15:00	› NMR study of charge storage mechanisms and ion dynamics in supercapacitors - *Céline Merlet, Department of Chemistry (Cambridge, UK)*
15:00 - 15:20	› Multi-Scale Dynamics of free and confined ionic liquids - *Dominique Petit, Laboratoire Charles Coulomb*
15:20 - 15:40	› COMPUTATIONAL STUDY OF GRAPHENE-BASED SUPERCAPACITORS - *Trinidad Méndez Morales, Maison de la Simulation - CEA*
15:40 - 16:00	› Marcus free energies for the Fe3+/Fe2+ couple in ionic liquids - *Zhujie LI, Maison de la Simulation*
16:00 - 16:30	Coffee break
16:30 - 17:50	Nano-micro poromechanics (Part II)
16:30 - 16:50	› 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 - *David Grégoire, Laboratoire des Fluides Complexes et leurs Réservoirs*

TIME	EVENT
16:50 - 17:10	› A possible nano-scale origin of the surprising thermal expansion of clays - *Laurent Brochard, Laboratoire Navier*
17:10 - 17:30	› Experimental study of stresses induced in model cement-based materials by in-pore crystallization - *Matthieu Vandamme, Universite Paris-Est, Laboratoire Navier (UMR 8205), CNRS, ENPC, IFSTTAR, F-77455*
17:30 - 17:50	› Molecular-to-continuum poroelasticity upscaling of hydrating cement pastes, considering progressive C-S-H gel densification - *Christian Hellmich, Institute for Mechanics of Materials and Structures, Vienna University of Technology, TU Wien - Vienna University of Technology*

Thursday, December 8, 2016

TIME	EVENT
09:00 - 10:30	Dynamics and thermodynamics of confined fluids (Part I)
09:00 - 09:30	› Mesoscale modelling of cement hydrates: application to freeze-thaw damage - *Katerina Ioannidou, Massachusets Institute of Technology*
09:30 - 10:00	› A multiscale investigation of structure and dynamics of water confined in swelling clay porous media - *Eric Ferrage, INSTITUT DE CHIMIE DES MILIEUX ET MATERIAUX DE POITIERS*
10:00 - 10:30	› Intermolecular forces between C-S-H Layers - *Mohammad Javad Abdolhosseini Qomi, University of California - Irvine*
10:30 - 11:00	Coffee break
11:00 - 12:40	Dynamics and thermodynamics of confined fluids (Part II)
11:00 - 11:20	› NICKEL-CARBON NANOPARTICLES: SIZE DEPENDENT PHASE DIAGRAMS AND INTERACTION WITH GRAPHENIC LAYERS - *Yann Magnin, Centre Interdisciplinaire de Nanoscience de Marseille, Aix-Marseille University and CNRS*
11:20 - 11:40	› Transport of Hydrocarbons Mixtures in Disordered Nanoporous Materials - *Obliger Amael, Massachusetts Institute of Technology (MIT), Multi-Scale Materials Science for Energy and Environment*
11:40 - 12:00	› Permeation of supercritical fluids through nanoporous constrictions : theory and simulations - *Fouad Oulebsir, LFC-R, Université de Pau et des Pays de l'Adour*
12:00 - 12:20	› Non-equilibrium simulations of flow in clay nanopores using a wall thermostat - *Pauline Simonnin, Université Pierre et Marie Curie - Paris 6, IFP Energies Nouvelles*
12:20 - 12:40	› Probing saturation, dynamics and wettability of oil and water in Shale Oils - *Jean-Pierre Korb, Sorbonne Université, UPMC Univ. Paris 06, Laboratoire Physicochimie des Electrolytes, Nanosystèmes Interfaciaux*
12:40 - 14:00	Lunch (Buffet) + Posters
14:00 - 15:40	New synthetic approaches to multiscale porous materials (Part I)
14:00 - 14:30	› Coupling soft chemistry and processing for designing hierarchical functional materials. - *Cédric Boissière, Laboratoire de Chimie de la Matière Condensée de Paris (site Collège de France)*
14:30 - 15:00	› Looking for nano in nano: heterostructures within nanomaterials - *David Portehault, Lab. Chimie de la Matière Condensée de Paris*

TIME	EVENT
15:00 - 15:20	› Radiolytic hydrogren emissions: from hydrates to cement pastes - *Adeline Dannoux-Papin, CEA - Jérémy Haas, CEA*
15:20 - 15:40	› DEGRADATION OF ORGANIC MATTER UNDER GEOLOGICAL CONDITIONS: A ROUTE TOWARDS THERMODYNAMIC SOLID/FLUID EQUILIBRIUM USING REPLICA EXCHANGE MOLECULAR DYNAMICS SIMULATIONS - *Léa Atmani, CINAM and UMI-CNRS-MIT*
15:40 - 16:20	Coffee break
16:20 - 18:10	New synthetic approaches to multiscale porous materials (Part II)
16:20 - 16:50	› Irradiation-Induced Damage in Concrete: The Enthalpy Landscape Viewpoint - *Mathieu Bauchy, Physics of AmoRphous and Inorganic Solids Laboratory*
16:50 - 17:10	› Modeling soft-particle materials: shear behavior and effect of porosity - *Saeid Nezamabadi, Laboratoire de Mécanique et Génie Civil (LMGC), Université de Montpellier, CNRS, Montpellier, France*
17:10 - 17:30	› Atomic-scale modeling of the Alkali-Silica Reaction - *Alice Dufresne, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology (MIT), 77 Massachusetts Avenue, Cambridge, 02139, MA, USA, Multi-Scale Materials Science for Energy and Environment 2, the joint MIT-CNRS laboratory, MIT, 77 Massachusetts Avenue, Cambridge, 02139, MA, USA*
17:30 - 17:50	› Effect of hydration temperature on the pore structure of cement paste - *SARA BAHAFID, Ecole des Ponts ParisTech/ Laboratoire Navier/ CERMES*
17:50 - 18:10	› Hydrophobization of Silica Nanoparticles in Water: Resulting Porous Nanostructure and Response to Drying Stress - *Jean-Baptiste d'Espinose de Lacaillerie, Sciences et Ingénierie de la Matière Molle*
19:30 - 22:00	Conference Dinner

Friday, December 9, 2016

TIME	EVENT
09:00 - 10:30	Multiscale materials of our cultural heritage: challenges and perspectives
09:00 - 09:30	› A few challenges posed by multiscale ancient materials - *Loïc Bertrand, Institut photonique d'analyse non-destructive européen des matériaux anciens, Synchrotron SOLEIL*
09:30 - 10:00	› Multiscale approaches to characterize historical oil paintings - *Laurence de Viguerie, Laboratoire d'Archéologie Moléculaire et Structurale*
10:00 - 10:30	› Neutron imaging investigation of fossil woods: non-destructive characterization of microstructure and detection of in-situ changes. - *Laurent Michot, Phenix CNRS Sorbonne Université UPMC*
10:30 - 11:00	Coffee break
11:00 - 12:40	New developments in imaging multiscale porous materials
11:00 - 11:30	› In situ multi-scale tomographic imaging of topological changes in phase-separated glasses - *Emmanuelle Gouillart, Unité mixte CNRS/Saint-Gobain Surface du Verre et Interfaces*

TIME	EVENT
11:30 - 12:00	› Experimental characterization of the organic pore network of source rocks at the nano-scale - *Jeremie Berthonneau, Massachusets Institute of Technology*
12:00 - 12:20	› Morphological characterization of ceramic membranes from 3D X-ray computed tomography - *Jonathan Perrin, CINAM, Université Aix-Marseille*
12:20 - 12:40	› STRUCTURE AND PROPERTY ALTERATIONS IN GRAPHITE UNDER HIGH ELECTRON DOSE: A COMBINED TEM/MD INVESTIGATION - *Jean-Marc Leyssale, Laboratoire des Composites ThermoStructuraux*
12:40 - 12:45	Closing words - Pierre Levitz and Roland Pellenq