



*2015 Workshop of the International Research Network GdRi - M2UN
a joint Micromeritics / MIT / CNRS event*

MIT, Media Lab, E14, August 26 – 28 2015

Organizers : Drs J. Kenvin (Micromeritics), R. Pellenq (CNRS-MIT)

Program

Wednesday Aug 26th

8h30 - 9h00: Registration

9h00 - 9h15: Welcome, J. Kenvin, R. Pellenq

Session 1, Chair: E. Del Gado
From the fundamentals of adsorption and confinement

09h15 – 10h00: P1. Using High Throughput Computation to Accelerate Development of Nanoporous Materials for Real World Applications, D. Sholl

10h00 – 10h45: P2. Corresponding States Theory of Adsorbed Films: Influence of Wetting and Wall-roughness, K. Gubbins

10h45 – 11h15: Coffee break

11h15 – 12h00: P3. Adaptability of Molecules and Ions to Nanoscale Environments, K. Kaneko

12h00 – 12h20: T1. Comprehensive Characterization of Porous Carbon Materials Using Adsorption of N₂, Ar and CO₂ analyzed by 2D-NLDFT Models, J. Jagiello

12h20 – 12h40: T2. A Differential Approach to Modeling Pore Throats and Cavities, J. Kenvin

12h40 – 02h00: Lunch



Session 2, Chair: F. Ulm
Dynamics of confined fluids

02h00 – 02h45: P4. Probing Confined Fluid Dynamics in Nanoporous Materials: from the Pore to the Pore Network, P. Levitz

02h45 – 03h30: P5. Shock Electrochemistry in Porous Media, M. Bazant

03h30 – 04h00: *Coffee break*

04h00 – 04h45: P6. Probing Confined Fluid Dynamics in Heterogeneous Porous Materials by Multi-scale NMR: from Laboratory to Industrial Applications, J.-P. Korb

04h45 – 05h05: T3. Transport of Alkane Mixtures Through Nanoporous Carbon Membranes, A. Obliger

05h05 – 05h25: T4. Non-Equilibrium Thermodynamics of Porous Electrodes in Li-ion Batteries, R. Smith

05h25 – 05h45: T5. The Use of Multi-scale Sequential Packing and Genetic Algorithms for Porosity Investigation, K. Sobolev

05h45 – 06h15: *Break*

06h15 – 07h00: Special seminar, Game Changing Energy Technologies from MIT, R. Armstrong

07h00 – 09h00: *Cocktail Reception / Poster Session*



Thursday Aug 27th

**Session 3, Chair: P. Levitz
Chemoporomechanics**

09h15 – 10h00: P7. On the Impact of Adsorption in Compliant Nanoporous Materials, A. Fuchs

10h00 – 10h20: T6. Failure of Porous Materials, Stress or Energy?, L. Brochard

10h20 – 10h40: T7. Effect of Water on Mechanical Properties of Clay-based Materials: Molecular Simulations of Clay Layers and Experiments on Self-standing Thin Clay Films, M. Vandamme

10h40 – 11h15: *Coffee break*

11h15 – 12h00: P8. Permeability and Relative Permeability of a Porous Material : a Stochastic Hierarchical Bundle Approach, Gilles Pijaudier-Cabot

12h00 – 12h20: T8. Multiscale Mechanics of Shale-Rock from X-ray Microscopy Scans, H. Laubie

12h20 – 12h40: T9. Mineral Surface Area and Organic Carbon Preservation in Organic-Rich Shale Rocks, J. Berthonneau

12h40 – 02h00: *Lunch*



Session 4, Chair: R. Pellenq

The real world: from natural to synthetic materials (Porous carbons, coral, shale-rocks, zeolites, geopolymers, cement ...)

02h00 – 02h45: P9. Nanometer Scale Texture and Pore Size Distribution (PSD) of Unconventional Hydrocarbon Reservoirs, D. K. McCarty

02h45 – 03h30: P10. Storage and Transport of Hydrocarbons in Organic-Rich Mudstones, R. Kleinberg

03h30 – 04h00: *Coffee break*

04h00 – 04h45: P11. Design of Hierarchically-Organized Zeolite Catalysts, J. Pérez-Ramírez

04h45 – 05h05: T10. Advances in the Physical Adsorption Characterization of Nanoporous Materials with Hierarchical Pore Structure, M. Thommes

05h05 – 05h25: T11. Multi-scale Texture and Porosity in Red Coral, J. Perrin

05h25 – 05h45: T12. Characterization of Geopolymers Porous Network, A. Poulesquen



Friday Aug 28th

Session 5: Chair J. Kenvin

The real world: from natural to synthetic materials (colloids, coral, shale-rocks, zeolites, geopolymers, cement ...), continued

09h15 – 10h00: P12. Internal Stresses, Non-Equilibrium Conditions and Yielding in Amorphous Solids: from Soft Gels to Cement Hydrates, E. Del Gado

10h00 – 10h45: P13. Porous Carbons for Energy Storage: Synthesis, Application and Operando Characterization, G. Yushin

10h45 – 11h15: *Coffee break*

11h15 – 12h00: P14. Industrial Gas Applications in Oil & Gas Recovery from Unconventional Reservoirs, J. Mc Andrew

12h00 – 12h20: T13. Meso-scale Modeling of C-S-H, K. Ioannidou

12h20 – 12h40: T14. The Texture of Geopolymers from Solid-State NMR, J.-B. d’Espinoise

12h40 – 02h00: *Lunch*

02h00 – 02h20: T15. Mechanisms of Nanomaterial Release from Photocatalytic Cements Identified by Multi-scale X-ray Based 2D and 3D Imaging Techniques, J. Rose

02h20 – 02h40: T16. Hydrothermal Processing of K-feldspar as a Source of Potash, D. Ciceri

02h40 – 03h00: T17. Porous Materials for Ion-electrospray Propulsion, I. Jivanescu

03h00 – 03h15: Final remarks, J. Kenvin, R. Pellenq