MC17: Physical Properties in Confined Environments, Fundamentals & Applications

Organisers : Yann Magnin & Nicolas Chanut

Monday August 22 – 16:15-17:45

16:15 - 16:45 **INVITED MC17-1**	**Nanoporous materials for CO_2 capture: hurdles and opportunities** **P. L. Llewellyn**, C. Pereira and Y. Magnin *TotalEnergies S.E., Pau, France. philip.llewellyn@totalenergies.com*
16:45 - 17:05 **MC17-2**	**Enhancement of gas adsorption & separation via entropic effects: Statistical-mechanics modeling of nanoconfined H_2, CO_2, H_2O/CO and CO_2/N_2** **M. Polak** and L. Rubinovich *Ben-Gurion University of the Negev, Israël. mpolak@bgu.ac.il*
17:05 - 17:25 **MC17-3**	**A novel computational screening methodology for the design of effective solvents for CO_2 capture** **F. de Meyer**, A. Orlov and X. Rozanska *TotalEnergies S.E., Paris, France. frederick.de-meyer@totalenergies.com*
17:25 - 17:45 **MC17-4**	**Modelling Carbon Capture on Metal-Organic Frameworks with Quantum Computing** G. Greene-Diniz, D. Zsolt Manrique, **W. Sennane**, Y. Magnin, E. Shishenina, P. Cordier, P. L. Llewellyn, M. Krompiec, M. J. Rančić, and D. Muñoz Ramo *TotalEnergies S.E., Saclay, France. wassil.sennane@totalenergies.com*

Tuesday August 23 – 15h00-18h30

15:00 - 15:30 **INVITED** **MC17-5**	**Water and ionic separation by highly porous ultrathin carbon-nanomembranes: a molecular dynamic study** **G. Monet**, M-L. Bocquet and L. Bocquet *École Normale Supérieure, Sorbonne Paris, France. geoffrey.monet@phys.ens.fr*
15:30 - 15:50 **MC17-6**	**Nanofluidique pour l'étude du transport de particules virales à travers un système confiné** **L. Chazot-Franguiadakis** and F. Montel *École Normale Supérieure, Lyon, France. lea.chazot-franguiadakis@ens-lyon.fr*
15:50 - 16:10 **MC17-7**	**Molecular dynamics investigation of non-Fickian effects on desorption from source rocks' organic matter** K. Walczak and **A. Obliger** *Institut des Sciences Moléculaires, Bordeaux, France. amael.obliger@u-bordeaux.fr*
16:10 - 16:30 **MC17-8**	**Pore network simulator for large pore scale simulations** **M. Regaieg**, T. Farhana Faisal, C. Varloteaux and R. Rivenq *TotalEnergies S.E., Pau, France. mohamed.regaieg@totalenergies.com*
COFFEE BREAK, 16:30 – 17:00	
17:00 - 17:30 **INVITED** **MC17-9**	**Simulations atomistiques des processus électrochimiques lors de la charge et la décharge des supercondensateurs en carbone** R. Dupuis, P-L. Valdenaire, **R. J.-M. Pellenq** and K. Ioannidou *MIT and CNRS - George Washington University (USA), pellenq@mit.edu*
17:30 - 17:50 **MC17-10**	**Wetting/drying mechanisms associated with nanoconfined salt solutions: an optical reflectance study on vapour phase imbibition and adsorption** **S. Dutta**, H. Bellezza, P. Huber and O. Vincent *Institut Lumière Matière, CNRS, Lyon, France. sujeet.dutta@univ-lyon1.fr*

17:50 - 18:10 **MC17-11**	**Phonon drag-electric current generation at the liquid-graphene interface** A. Marcotte, **M. Lizee**, B. Coquinot, N. Kavokine, C. Barraud, A. Nigues, L. Bocquet and A. Siria *École Normale Supérieure, Sorbonne Paris, France. mathieu.lizee@phys.ens.fr*
18:10 - 18:30 **MC17-12**	**CONCLUDING REMARKS & DISCUSSION** **Y. Magnin & N. Chanut** yann.magnin@external.totalenergies.com, nchanut@mit.edu

Poster Tuesday August 23 – 18h30-21h00

MC17-13	**Compréhension des mécanismes de bouchage de milieu poreux par des émulsions de Pickering** A. Le Beulze, **N. Santos De Pera**, B. Levaché, M. Questel, P. Panizza, F. Lequeux, M. Levant and N. Passade-Boupat *ESPCI & TotalEnergies S.E., Paris, France. nathalie.santos-de-pera@totalenergies.com*
MC17-14	**Single orientation random hexagonal close-packed colloidal crystals from capillary action induced shear** N. H. P. Orr, T. Yanagishima, I. P. Dolbnya, A. V. Petukhov and R. P. A. Dullens *University of Oxford, Oxford, UK & Université Montpellier 2, Montpellier, France. nicholas-henry-pache.orr@umontpellier.fr*