

Papers presented at honorary sessions at AIChE meeting

Monday, November 14, 2016: 12:30 PM - 3:00 PM

Cyril Magnin II (Parc 55 San Francisco)

Description: This plenary comprises invited papers.

Sponsor: Adsorption and Ion Exchange

Chair: Matthias Thommes **Email:** matthias.thommes@quantachrome.com

Co-Chair: Stefano Brandani **Email:** s.brandani@ed.ac.uk

- 12:30 PM** (174a) Intermolecular Structure of Binary Mixture in Confined Spaces
Taku Iiyama, Masatsugu Yoshimoto, Ryusuke Futamura, Toshiya Otomo and Sumio Ozeki
- 12:50 PM** (174b) Dynamic Mean Field Theory with Hydrodynamic Interactions: Theoretical Development and Applications in the Study of Fluid Transport in Porous Adsorbents
Eustathios Kikkinides and Peter A. Monson
- 1:10 PM** (174c) Adsorption Stress in Nanopores
Alexander V. Neimark
- 1:30 PM** (174d) Computer Simulations of Chemical Reactions and Proton Transport in Porous Materials and Functionalized Surfaces
Karl Johnson, Jingyun Ye and Abhishek Bagusetty
- 1:50 PM** (174e) Understanding Gate Adsorption of CO₂ on Elastic Layer-Structured Metal-Organic Framework-11
Hideki Tanaka, Shotaro Hiraide, Narutomo Ishikawa, Atsushi Kondo and Minoru Miyahara
- 2:10 PM** (174f) Confinement-Induced High Pressure Phases in Nanopores: Can the Pressure be in the Megabar Range?
Keith E Gubbins
- 2:30 PM** (174g) On the Role of Surface Chemistry in Carbon Adsorption
L.R. Radovic
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Monday, November 14, 2016: 3:15 PM - 5:45 PM

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Description: The purpose of this session is to showcase the most important advances in the fundamentals of adsorption and ion exchange.

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Chair: Stefano Brandani **Email:** s.brandani@ed.ac.uk

Co-Chair: Matthias Thommes **Email:** matthias.thommes@quantachrome.com

- 3:15 PM** [\(227a\) A Refined Model for Adsorption of Simple Gases on Graphite](#)
Duong D. Do, Yonghong Zeng, Luisa Prasetyo, Shiliang Tan, Chunyun Fan and David Nicholson
- 3:40 PM** [\(227b\) Adsorption and Transport Properties of Alkanes in Kerogen-Containing Shale-Rocks](#)
Roland J.-M. Pellenq, Amaël Obliger and Franz-Josef Ulm
- 4:05 PM** [\(227c\) Mapping the Adsorption and Phase Behavior of Fluids in Micro-Mesoporous Adsorbents with Hierarchical Pore Structure: *Towards an Advanced Pore Structural Characterization*](#)
Matthias Thommes and Katie Cychoz
- 4:30 PM** [\(227d\) Speedy Standing Wave Design and Splitting Strategies for the Separation of Mixtures with Three or More Components Using Simulated Moving Beds](#)
George S. Weeden Jr., Nicholas Soepriatna and Nien-Hwa Linda Wang
- 4:55 PM** [\(227e\) Adsorptive Recovery of Biobutanol in Vapor Phase](#)
Stijn Van der Perre, Miguel Palomino, Susana Valencia, Fernando Rey, Ranjeet Singh, Paul A. Webley, Gino Baron and Joeri Denayer
- 5:20 PM** [\(227f\) Molecular Insight into Water Effects in a Stable Metal-Organic Framework: An *in-situ* Experimental and Molecular Modeling Analysis](#)
Nicholas C. Burtch, Cody R. Morelock, Yang Jiao, Jurn Heinen, Julian T. Hungerford, Andrey A. Yakovenko, Wenqian Xu, David Dubbeldam and Krista S. Walton
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