

May 19-24, 2013 • Hyatt Regency on the Inner Harbor • Baltimore, Maryland, USA

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FOA11

11th International Conference on
the Fundamentals of Adsorption

FINAL PROGRAM



International Adsorption Society



- 4:20 PM (L-137) **Synthesis and Application of Nanocomposites of Reduced Graphene Oxide and Periodic Mesoporous Silica with Vertically Aligned Mesochannels.** Zheng-Ming Wang, Shigeru Kurosawa, Katsunori Kosuge, Shiori Kubo, Noriko Yoshizawa, Geoffrey A. Ozin, AIST
- 4:40 PM (L-138) **The Structure Directing Effect of Cross-Linked Methacrylate Polymers used for the Synthesis of Nanoporous Solids.** Charalambos Papatryphonos, Charis Theocharis, University of Cyprus
- 5:00 PM (L-139) **Facile Synthesis of All-silica DD3R Crystals with Uniform Shape and Size and their Application to Adsorption-based Separations.** Anna Peng, Chunhui Xu, Yijun Zhong, Weidong Zhu, Zhejiang Normal University
- 5:20 PM (L-140) **Adsorption of Horseradish Peroxidase onto Functionalized Titanate Nanotubes.** João Victor Nicolini, Douglas Caffaro, Neuman S. de Resende, Helen C. Ferraz, Federal University of Rio de Janeiro
- 5:40-6:00 PM (L-141) **A Procedure for Building Models of Equilibria on Surfaces of Hybrid Silica-organic Materials.** Anton Panteleimonov^{1,2}, Yuriy Kholin², Yoshitaka Gushikem¹, ¹State University of Campinas; ²V.N. Karazin Kharkiv National University



- 6:00-7:30 PM **POSTER SESSION / SOCIAL**
Posters in the P-1000 series will be presented
Authors of posters in the P-1000 series should stand at their posters and be available to discuss the research during Poster Session-I from 6:00 PM to 7:30 PM.

Tuesday, May 21, 2013

- 7:30 AM **Light Breakfast in Constellation Ballroom A/B** (included in the registration fee)
- 10:10 AM - 6:00 PM **EXHIBITION OPEN in the Constellation Ballroom Foyer**



- 8:30 AM (L-201) **Physical Adsorption Characterization of Nanoporous Materials: Progress and Challenges.** Matthias Thommes, Quantachrome Corporation



- 9:10 AM (L-202) **Rapid Characterization of Porous Materials by Thermal Response Measurements.** Matthias Leistner¹, Wulf Grählert¹, Stefan Kaskel², ¹Fraunhofer IWS; ²Technische Universität Dresden
- 9:30 AM (L-203) **On the Description of Hysteresis Loops of IUPAC Classification with a Simple Pore Model - The Interplay of Pore Size and Capacity.** Duong Do, Phuong Nguyen, Chunyan Fan, David Nicholson, University of Queensland

- P-1048 **In-situ Powder Diffraction during the Gas Adsorption on Metal-organic Frameworks.** Andreas Heerwig¹, Volodymyr Bon¹, Irena Senkovska¹, Nicole Klein¹, Dirk Wallacher², Ivo Zizak², Esther Dudzik², Ralf Feyerherm², Stefan Kaskel¹, ¹Dresden University of Technology; ²Helmholtz-Zentrum Berlin
- P-1049 **New Hydrolytically Stable Zr and Hf based Metal-organic Frameworks.** Volodymyr Bon¹, Volodymyr Senkovskyy¹, Irena Senkovska², Stefan Kaskel¹, ¹Dresden University of Technology; ²Leibnitz-Institut für Polymerforschung Dresden e. V.
- P-1050 **Ad- and Desorption in a Trienzymatic Production Process for Laminaribiose.** Thomas Waluga¹, Marwan Zein², Jördening Hans-Joachim², Scholl Stephan¹, ¹TU Braunschweig Institute for Chemical and Thermal Process Engineering; ²TU Braunschweig Institute for Technical Chemistry
- P-1051 **Comparative Study of Protein Adsorption onto Silica Nanoparticles.** Jens Meissner, Bhuvnesh Bharti, Gerhard Findenegg, Technical University Berlin
- P-1052 **Synthesis, Characterization and n-Hexane Adsorption on MIL/Graphite Oxide Composites.** Qibin Xia, Xuejiao Sun, Jinpeng Miao, Hongxia Xi, Zhong Li, South China University of Technology
- P-1053 **Adsorption Isotherms and Kinetic Curves of H₂/ CO/ CO₂/H₂O on MIL-100(Fe) and their Breakthrough Curves in Fixed Bed.** Sha Wang, Xin Zhou, Chen Ma, Qibin Xia, Zhong Li, South China University of Technology
- P-1054 **Adsorption Isotherms and Surface Activation Energies of Desorption of Toluene on the Metal-Organic Framework HKUST-1 and MIL-101.** Feng Xu, Zhong Li, South China University of Technology
- P-1055 **Understanding and Prediction of Breathing Transition in MIL-53(Al): A Thermodynamics and Statistical Mechanics Study.** Yu Liu, Xueqian Chen, Jun Hu, Honglai Liu, Ying Hu, East China University of Science and Technology
- P-1056 **Computer Simulation of Gas Adsorption in COF-108 with C60 Impregnation.** Yujun Zhu, Jianhai Zhou, Jun Hu, Honglai Liu, Ying Hu, East China University of Science and Technology
- P-1057 **Synthesis of Hydrotaicites using Polymer Template and their CO₂ Adsorption Capacities.** Hee Jin Jang, Ki Bong Lee, Sung Hyun Kim, Korea University
- P-1058 **Two Components of Chloride Anion Exclusion Volume in Montmorillonitic Soils.** Tamara Polubesova¹, Mikhail Borisover², ¹The Hebrew University of Jerusalem; ²The Volcani Center ARO
- P-1059 **Mixed Theoretical and Experimental Study of Breathing in MIL-53(Al).** Aurélie Ortiz¹, Marie-Anne Springuel-Huet², François-Xavier Coudert¹, Alain H. Fuchs¹, Anne Boutin³, ¹CNRS & Chimie ParisTech; ²UPMC; ³Ecole Normale Supérieure
- P-1060 **Computational Exploration of Functionalized Porous Zr Terephthalate MOF for Membrane Based Adsorption Applications.** Dong Wu¹, Qingyuan Yang², Chongli Zhong², Guillaume Maurin³, ¹Institut Charles Gerhardt Montpellier UMR 5253 CNRS; ²State Key Laboratory of Organic-Inorganic Composites Beijing University of Chemical Technology; ³Université Montpellier 2
- P-1061 **Multicomponent Chiral Separations by Multicolumn and Simulated Moving Bed Adsorption Processes.** António E. Ribeiro¹, Nuno S. Graça², Alexandre P. Ferreira², Alírio E. Rodrigues², Luis S. Pais¹, ¹Polytechnic Institute of Bragança; ²University of Porto
- P-1062 **Adsorptive Desulfurization of Hydrocarbon Fuels using Mixed Oxide Supported Silver Adsorbents: Effect of Surface Acidity at Ambient Conditions.** A. H. M. Shahadat Hussain, Bruce J. Tatarchuk, Auburn University

Multicomponent Chiral Separations by Multicolumn and Simulated Moving Bed Adsorption Processes

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In the last decades, the direct resolution of enantiomers by liquid chromatography using chiral stationary phases (CSPs) has become a very popular technique. Due to the development of new and more stable CSPs and also by exploring and developing new and more efficient modes of operation, the use of chiral liquid chromatography, from the analytical scale through high-performance liquid chromatography (HPLC) to the preparative and industrial scales through simulated moving bed (SMB) technology, has gained a renewed interest.

The chiral separation process is a complex task, governed by several different interactions between the chiral solutes, the solvent and the CSP. In a preparative point of view, and when considering the choice of the mobile phase (solvent) composition, a high selectivity of the enantiomers should not be the only goal to be aimed, as it is frequently followed at analytical scale. Besides the choice of a CSP with high loading capacity, a high solubility of the solutes in the solvent and low retention times should also be taken into account, in order to improve the preparative process performance, as it was extensively explained for the separation of chiral non steroidal anti-inflammatory drugs [1-4].

This work will extend the study of these topics to multicomponent chiral separations. The separation of nadolol stereoisomers will be used as case study. Nadolol is a non-selective beta-adrenergic receptor antagonist (β -blocker) pharmaceutical drug, widely used in the treatment of cardiovascular system diseases [5]. Its chemical structure has three stereogenic centres which allows for eight possible stereoisomers. However, the two hydroxyl substituents on the cyclohexane ring are fixed in the cis-configuration which precludes four stereoisomers [6].

The separation of nadolol stereoisomers on CHIRALPAK[®] AD at both analytical and preparative scales was recently reported by Ribeiro et al. [7]. CHIRALPAK[®] AD is, nowadays, the most used commercially available CSP. It is an amylose-based CSP and is produced by physical coating of the chiral polymer on a matrix. However, due to their coated nature, this CSP can only be used with a limited range of solvents such as the polar solvents (e.g. acetonitrile, alcohols) or non-polar solvents (e.g.

alkanes) in combination with some polar components as modifiers (mainly alcohols). Immobilization of a polysaccharide-derivative on the support is an evolutionary strategy to make a CSP compatible with the whole range of organic solvents, which will consequently extend its application scope. CHIRALPAK® IA is a CSP containing amylose 3,5-dimethylphenylcarbamate immobilized onto silica gel [8].

This work will present a complete methodology concerning experimental, modelling and simulation results. Both the CHIRALPAK® AD and CHIRALPAK® IA CSP will be evaluated. The selection of the proper CSP/solvent combination for preparative operation will be fully study taking into account the screening strategy proposed by Zhang et al. [9]. Additional results include the measurement of nadolol stereoisomers solubilities, equilibrium adsorption data and fixed bed (breakthroughs) experiments. The complete screening of CSP/solvent combination will lead to the choice of the better solutions for the separation of nadolol stereoisomers, considering the target component or components to be obtained. Simulation and experimental results will be presented for the multicomponent separation of nadolol stereoisomers by multicolumn and Simulated Moving Bed adsorption processes.

References:

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