



French-German Adsorption Conference

October 24 – 26th 2023

ECPM - Strasbourg

Program



Tuesday October 24th

13 :30 *Welcome coffee break*

14 :00 – 14 :15 *Opening remarks*

14 :15 : *Liquid adsorption session*

14 :15 – 15 :00 Gabriele Iffland (BASF SE)
Industrial Applications of Liquid Phase Adsorption

15:00 – 15:20 S. Gravelle, Separation of water and ethanol mixtures by nanoporous organosilica; a molecular dynamics study

15:20 – 15:40 J.W. Lee, Double-Layer Simulated Moving Bed Chromatography for Ternary Separations: Langmuir Isotherms

15:40 – 16:00 M. Fiedler, A molecular dynamics approach to calculate protein adsorption data

16 :00 – 16 :20 Coffee break

16 :20 : *Characterization Science session*

16 :20 – 16 :40 A. Galarneau, Characterization of carbon monolith for wastewater treatment under flow

16 :40 – 17 :00 C. Cuadrado Collados, Quantitative Assessment of Hydrophilicity/Hydrophobicity in Mesoporous Silica by Combining Adsorption, Liquid Intrusion and Solid-State NMR spectroscopy

17:00 – 17:20 O. Osta, The impact of the pore wall hydrophobicity on the density of confined water: A combined nitrogen and water sorption study.

17 :20 – 17 :40 M. Benamar, Understanding the evolution of microporosity during hierarchization treatments of side pocket containing zeolites

17:40 – 18 :00 A. Kahlal, Towards a DFT approach to Mechanical Properties in Nanoporous Materials

18:00 – 20:00 Poster session



Wednesday October 25th

- 08:40 – 09:25** **Carlos Nieto-Draghi (IFP Energies Nouvelles)**
A new class of descriptors for nanoporous materials and its applications to Classification and CO₂ gas adsorption into zeolites
- 09:25 TSA – processes session
- 09:25 – 09:45** **B. Claessens**, Cation-exchanged LTA Zeolites for the Separation of Propane and Propylene
- 09:45 – 10:05** **M. Roehnert**, Binary adsorption of light hydrocarbons on zeolites at low temperatures
- 10 :05 – 10 :25** **I. Bezverkhy**, D₂/H₂ separation by adsorption in zeolites under cryogenic conditions: understanding the mechanism from experiment and molecular simulation
- 10 :25 – 10 :45** **N. Braunschweig**, Adsorption Chiller for Industrial Application
- 10 :45 – 11 :00** *Coffee break*
- 11 :00 : Gas adsorption session**
- 11:00 - 11:20** **G. Salazar Duarte**, Hidden Adsorption – TSA in industrial gas processing plants
- 11:20 - 11:40** **M.T. Rozaini**, Shaping of HKUST-1 for CO₂ capture from biogas
- 11:40 - 12:00** **Y. Xiong**, Transition metal-exchanged GIS zeolites for CO₂/CH₄ separation
- 12:00 - 12:20** **N. Kofmann**, Direct Air Capture with solid amine sorbents: understanding the effect of water on process performance
- 12:20 – 12:40** **Y. Magnin**, Carbon Capture in Metal-Organic Frameworks from wet flue gases
- 12:40 - 14:20** *buffet – poster session*
- 14:20: CO₂ adsorption session
- 14:20 - 14:40** **R. Morales Ospino**, Chitosan-based activated carbons for CO₂ capture and biogas upgrading
- 14:40 - 15:00** **K.A. Zervidi**, A hybrid system for capturing CO₂ directly from the air
- 15:00 - 15:20** **V. Selmert**, Electrospun Carbon Nanofibers as Selective Adsorbent for the Separation of CO₂
- 15:20 - 15:40** **R. Pinto**, Effective microwave-assisted regeneration of MOF/graphene oxide composites for post-combustion CO₂ capture



French – German Adsorption conference

15:40 - 16:00 **D. Chakraborty**, MOFs as sustainable sorbents for CO₂ capture solutions

16 :00 – 16 :15 Coffee break

16 :15 : Transport and kinetics session

16:15 -17: **Christian Bläker (University of Duisburg-Essen)**
Methods for Characterization of Activated Carbons, Zeolites and Silica Gels"

17 :00 – 17:20 **S. Dutta**, Mediation of water vapour transport in nanopores via salt solutions: thermodynamic and kinetic study

17 :20 – 17:40 **R. Denoyel**, Impact of tortuosity and surface diffusion on transport through porous media

17 :40 – 18:00 **H.O. Rubiera Landa**, An Efficient Implementation of Maxwell-Stefan Theory for Modeling Gas Separation Processes

18 :00 – 18:20 **A . Grim**, Improvement of axial dispersion estimation in porous media for gases under pressure: Experimental and modelling methods

18 :20 : End of the day

20 :00 : Dinner



Thursday october 26th

09:00 :

09:00 – 09:45 **Cécile Lutz (Arkema)**
Zeolithes for sustainable development

09:45 – 10:05 **S.Ehrling (3P)**, The limits of surface and pore volume characterization

10:05 – 10:25 **Micromeritics**, Title to be announced

10 :25 – 10 :45 **J. Dowd (SM)**, Vapour Adsorption Studies of Porous Materials

10 :45 – 11 :00 *Coffee break*

11 :00 : Liquid adsorption and recycling session

11:00 - 11:20 **A. Seidel - Morgenstern**, Frontal analysis method for determining adsorption isotherms

11:20 – 11:40 **S. Asad**, New Carbamoyl Surface-modified ZrO₂ Nanohybrids for selective Au Extraction from E-Waste

11 :40 - 12:00 **C. Plait**, Mesoporous adsorbent for palladium recovery: synthesis, characterization and adsorption properties

12:00 – 12:10 **Closing remarks**

12 :10 : lunch box and departure



Posters

1. Partially Mg-exchanged GIS for optimized CO₂/CH₄ and CO₂/N₂ separations, J. Al Atrach, Y. Xiong, I. Golub, E. B. Clatworthy, R. Guillet-Nicolas, V. Valtchev
2. Evaluation of CO₂-CH₄ separation performances by clay-based adsorbent materials for biogas up-grading, A. El. Azrak, D. Grekov, L. Truche, P. Pré
3. Efficiency of metal-loaded zeolite Y in dye degradation, H. Benaouda, N. Bouchiba
4. Preparation and Characterization of ion-exchanged offretite zeolites with copper, silver and zinc for antibacterial applications, I. Bouledjouad, D. Dari, F. Djafri, F. Bennabi
5. Immersion Microcalorimetry to study the sulfur-carbon interaction, M-V Coulet, L. Gourmelen, R. Denoyel
6. Hydrogen isotopes separation by selective adsorption on FAU zeolites: influence of Si/Al ratio and cationic composition, C. Coutier, C. Cabaud, J-P. Bellat, I. Bezverkhyy
7. Quantification of Water and Silanol Species on Various Silicas by IR Spectroscopy, J.P. Debs, A. Travert, F. Thibault-Starzyk, P. Ghesquière, N. Malicki
8. Radon adsorption in purely siliceous zeolites: Grand Canonical Monte Carlo simulation study, S. Lyu, I. Deroche, T. Örs, J.-L. Paillaud
9. Molecular Simulation of Acoustic Response of Fluid Adsorption in Nanoporous Materials, L. Didier, A. Sam, R. Venegas, B. Coasne
10. Measurements of thermal effects during intrusion and extrusion of electrolyte solutions in pure silica zeolites, C. Dirand, I. Bezverkhyy, J-P. Bellat
11. Determination of Microporous and Mesoporous Surface Areas and Volumes of Mesoporous Zeolites by Corrected t-plot Analysis, L. Desmurs, A. Galarneau, C. Cammarano, V. Hulea
12. Structural and Energetic Characterization of Silica-Alumina Gels, L. Gehrke, C. Bläker, C. Pasel, D. Bathen
13. Energy consumption of VSA carbon capture; from lab scale to a pilot plant, M. Gholami, J. F. M. Denayer
14. Gas by Molecular Separation Trapdoor mechanism in multicationic zeolites, C. Grimaud, A. Tuel, C. Daniel, D. Farrusseng
15. Textural analysis of various biochar using several probe gases, M. Guilmont, E. Ghomri, C. Vaultot, Y. Le Brech, N. Thevenin, R. Gadiou



French – German Adsorption conference

16. Enhancing gas adsorption through HKUST-1 hybridization with activated carbons, L. Jimenez-Lopez, R. Morales, V. Fierro, A. Celzard
17. Study of glycine behavior in a comet, Y. Kviring, Y. Kviring, J. Simon, M. Salazar
18. Molecular dynamics simulation of glycine in contact with ice, Y. Kviring, JM. Simon, JM Salazar
19. Design of an unprecedented filtration device based on an elastic adsorbent for the adsorption intensification process of metal ions, M. Masquelier, C. Gourmand, L. Jierry and C. Bertagnolli
20. Extruding diffusion constants from your extrudates: pore geometry and adsorbate kinetics, S. R. McIntyre, E. Hunter-Sellars, P. A. Sáenz-Cavazos, A. R. Houghton, D. R. Williams
21. Recent developments in molecular Density Functional Theory: towards a more versatile tool for the characterization of nanoporous materials, C. Miqueu, R. Labeyrie, A. Barthes
22. Competitive CO₂/H₂O Dynamic Column Breakthrough of CALF-20 under Adiabatic Conditions, Tai Nguyen, Sabereh Rezaei, Kasturi Nagesh Pai, Andrew Liu
23. Correlation between gas storage capacity and surface area in MOFs?, M. Perbet, R. Morales, A. Celzard, V. Fierro, E.A. Quadrelli, D. Farrusseng
24. Investigation of catalytic COS formation on zeolites, S. Pfeifer, C. Pasel, C. Bläker, T. Eckardt, J. Eggebrecht, D. Bathen
25. Impact of airborne nanoparticles on workers' health: a new method based on Krypton gas adsorption, O. Rastoix, S. Merouane, C. Vallieres, D. Rousset
26. Sieving of H₂ and its isotopes by zeolites: Molecular simulations achievements and failures. J. Marcos Salazar, G.C.Q da Silva, J.M. Simon
27. Aspects of a novel sensitive method for meso-macropore analysis based on nitrogen adsorption at the triple point temperature (63 K) M. Terlinden, F. Kleitz, M. Thommes
28. Development and application of a novel pore network model for physisorption characterization, J. Söllner, M. Thommes
29. CPO-27(Ni) pelletization: Impact on structural, textural, and thermal properties, G. Trierweiler Gonçalves, L. Michelin, L. Josien, J.-L. Paillaud, G. Chaplais
30. Frontal analysis method with fractional sampling technique using a tandem HPLC system, S. Zarei, J. W. Lee, A. Seidel-Morgenstern