



The 8th Federation of European Zeolite
Associations (FEZA) Conference

FEZA2021

VIRTUAL | 5 - 9 July 2021
www.fezaconference.org



Scientific Programme

All times are BST

Monday 5 July 2021

8:30 Welcome and Introduction

8:45 Plenary Lecture: Xiaodong Zou: The impacts of electron crystallographic methods for structural studies of porous materials

9:55 Parallel session 1: Novel Materials and Structural Methods 1/3

09:55 Andreas Erlebach Reactive Neural Network Potentials for Zeolites with Density Functional Theory Accuracy

10:10 Takuya Hikino Synthesis of microporous titanosiloxane materials using cage siloxane as building blocks

10:25 Hwajun Lee PST-33: THE LAST MEMBER OF THE 4-LAYER ABC-6 FAMILY OF ZEOLITES

10:40 Yuki Sada Extracting the synthesis–structure relationship hidden behind the elaborate synthesis of zeolites by a data-driven approach

10:55 Q&A

9:55 Parallel session 2: Advanced Characterisation and Operando Spectroscopies 1/3

09:55 Nick Pellens The role of water during zeolite formation in hydrated silicate ionic liquids

10:10 Monica Jimenez-Ruiz Evidence of Hydronium Formation in Water–Chabazite Zeolite Using Inelastic Neutron Scattering Experiments and ab Initio Molecular Dynamics Simulations

10:25 Yi Luo Application of 3D electron diffraction techniques in developing novel zeolite materials

10:40 Gwilherm Nenert In-situ and ex-situ investigation of the Deca-Dodecasil 3 Rhombohedral zeolite for noble gas capture

10:55 Q&A

9:55 Parallel session 3: Probing Synthetic Methodologies 1/1

09:55 Michael Thorne Mechanochemical Synthesis of Mixed Metal, Mixed Linker Glass-Forming Metal–Organic Frameworks and Their Properties

10:10 Hamish Hei-Man Yeung In situ insights into the crystallisation of metal–organic frameworks

10:25 Joseph Barker The Structure, Synthesis and Properties of the Carboxyethylphosphonate Metal–Organic Framework BIRM-1.

10:40 Glen Smales Following the formation of Zeolites and MOFs in-situ

10:55 Q&A

11:25 Keynote lecture: Alessandro Turrina: Synthesis of small pore zeolite catalysts via co-templating approach

13:30 Plenary lecture: Svetlana Mintova: Mastering Zeolite Synthesis: Challenges and Opportunities

14:45 Keynote lecture: Celine Chizallet: Atomistic simulation of intricate aluminosilicate catalysts

15:30 Parallel session 1: New Synthetic Methods and Post-Synthetic Modification 1/4

15:30 Heloise Oliveira Pastore 2D-3D-3D transformation: ferrierite and omega zeolites from Na-RUB-18 layered silicate

15:45 Maksym Opanasenko Vapour-phase-transport technique for the synthesis of new zeolites by assembly-reassembly method

16:00 Mariame Akouche Synthesis of embryonic zeolites with controlled physicochemical properties

16:15 Mariya Shamzhy A combination of ADOR strategy and isomorphous substitution for the synthesis of model zeolite catalysts to examine pore size-activity relationship

16:30 Q&A

15:30 Parallel session 2: Catalytic Properties 1/1

15:30 Sam Ivko Dispersible Microporous Polymers as Supports for Carbonylation Catalysts

15:45 Michiel Dusselier MOF-derived zeolite hybrid catalysts for CO₂ to olefins and fine chemical catalysis

16:00 Matteo Miceli Iron/Metal-Organic Framework (Fe-MOF)-based electrodes for direct nitrogen reduction reaction to ammonia in mild conditions

16:15 M. Melero Sulfide Organic Polymers (SOPs) as efficient heterogeneous catalysts for esterification, thioesterification and amidation reactions

16:30 Q&A

15:30 Parallel session 3: Gas Adsorption, Separation and Storage 1/2

15:30 Anouk L'Hermitte Porous boron nitride - Moving up the scale for use in molecular separations

15:45 Stefano Brandani Measurements of CO₂ kinetics in a flexible zeolite using the Zero Length Column method

16:00 Maxime Debost CHA zeolite nanocrystals free of organic templates for selective CO₂ capture

16:15 Hanjun Fang A Transferable Force Field for Predicting Adsorption and Diffusion of Hydrocarbons and Small Molecules in Silica Zeolites with Coupled Cluster Accuracy

16:30 Niels De Witte Assessment of the adsorption step duration and purge flowrate on the performance of demand-driven PSA units

16:45 Q&A

Tuesday 6 July 2021

8:30 Parallel session 1: Catalytic Properties 1/5

08:30 Luc Cornelis Jacobus Smulders Hydroisomerization of n-heptane over Pt/SAPO molecular sieves: The impact of metal-acid proximity

08:45 Takahiko Moteki Reaction mechanism and effect of zeolite framework structure for CO-assisted methane conversion into C1/C2 oxygenates over supported Rh catalyst

09:00 Zahra Asgar Pour Synthesis of hierarchical, macroscopic and bead-shaped Lewis acid zeolites by hydrothermal treatment and subsequent post-synthesis techniques

09:15 Nan Wang Molecular elucidating of an unusual growth mechanism for polycyclic aromatic hydrocarbons in confined space

09:30 Sen Wang Increase of alkene-based cycle contribution in MTO processes by regulating aluminium locations in zeolite lattice sites

09:45 Q&A

8:30 Parallel session 2: New Synthetic Methods and Post-Synthetic Modification 2/4

08:30 Zhendong Liu Development of Ultrafast Methods for Post-synthesis Modifications of Zeolites

08:45 Michiel Dusselier One-pot synthesis of iron containing SSZ-13 zeolites with record methanol productivity in methane oxidation

09:00 Angélique Simon-Masseron DEVELOPMENT OF ZEOLITE/POLYMER BASED COMPOSITE VIA PHOTOPOLYMERIZATION AND APPLICATION IN THE FIELDS OF 3D PRINTING AND ADSORPTION

09:15 Santiago Leon Computational screening of structure-directing agents for the synthesis of pure silica ITE zeolite

09:30 Wenhua Fu Preparation of Hierarchical IWR Zeolites Based on Reassembly of Building Units

09:45 Q&A

8:30 Parallel session 3: Gas Adsorption, Separation and Storage 1/1

08:30 Christopher Marsh Ammonia Capture in a Robust Aluminium Metal-Organic Framework Decorated with Free Carboxylic Acid Moieties

08:45 Paul Iacomi MOFs for siloxane capture: from high throughput screening to experimental validation

09:00 Pengbo Lyu Ammonia capture via an unconventional reversible guest-induced metal-linker bond dynamics in a highly stable Metal-Organic Framework

09:15 Mi Tian Nanoporous polymer-based composites for enhanced hydrogen storage

09:30 Ozgur Yazaydin Modeling of Gas Transport through Polymer/MOF Interfaces: A Microsecond-Scale Concentration Gradient-Driven Molecular Dynamics Study

09:45 Q&A

10:15 Keynote lecture: Yi Li: High throughput computations and databases of zeolites

11:10 Plenary lecture: Simon Weston: Porous Materials Research at ExxonMobil: Zeolites, MOFs and CO₂ Capture

13:30 Keynote lecture: Kim Jelfs: Computational discovery of porous molecular materials

14:25 Keynote lecture: Wilhelm Schwieger: Hierarchically-ordered zeolites: preparation concepts and potential applications

15:20 Parallel session 1: Catalytic Properties 2/5

15:20 Karoline Kvande Methane to methanol conversion over Cu-zeolites - structure performance relationships

15:35 Naonobu Katada Strong Brønsted Acid Site Accessible from Large 12-ring Pore in YFI Type (YNU-5) Zeolite

15:50 Ben Dennis-Smith Promotion of zeolite-catalyzed methanol dehydration to DME by organic additives

16:05 Cristina Martínez CO₂ hydrogenation to chemicals: adjusting final product distribution by selecting zeolite structure and crystal size

16:20 Gerhard Pirngruber Shape selectivity effects in the conversion of multicyclic naphthenes

16:35 Q&A

15:20 Parallel session 2: Adsorption and Ion Exchange 1/1

15:20 Ozgul Agbaba Sener Oligomerization of Acetylene to Unsaturated C₄ Compounds under Pressurized Conditions

15:35 Ivan George Clayson The ion-exchange mechanism of catalytic transition metals into H-CHA

15:50 Jean Daou Influence of the compensating cation nature on the water adsorption properties of zeolite and their associated composite material forms

16:05 Veselina Georgieva Tuning CO₂ Adsorption of Merlinoite via Cation Exchange

16:20 Maura Mancinelli Ag-exchanged FAU-type zeolite for the removal of perfluoroalkyl substances (PFAS) from water: a combined in situ synchrotron X-ray diffraction and thermal analysis/isotope ratio mass spectrometry study.

16:35 Q&A

15:20 Parallel session 3: Physical Properties and the Role of Defects 1/2

15:20 Christopher J Heard OPERANDO MODELLING OF ZEOLITE HYDROLYSIS: SOLVATION, DEFECTS AND pH EFFECTS

15:35 Susan Henkelis Luminescent Properties of DOBDC MOFs: the Role of Free Hydroxyls

15:50 Jessica Rimsza Energetics and Structure of Ag-Water Clusters Formed in Mordenite

16:05 Michael Fröba Nanoconfinement of water and an ionic liquid solution in mesoporous host materials

16:20 Bruno Alonso Weak CH...O hydrogen bonds in as-synthesized zeolites: investigation of a widespread and often neglected intermolecular interaction

16:35 Q&A

Wednesday 7 July 2021

8:30 Parallel session 1: Catalytic Properties 3/5

- 08:30 Jannick Vercammen Shape Selective C-H Activation of Aromatics to Biaryllic Compounds Using Molecular Palladium in Zeolites
- 08:45 Mercedes Boronat A Theoretical Parameter Connecting Cavity Architecture, Confined Hydrocarbon Pool Species, and Olefin Distribution in the Methanol-to-Olefin Reaction Catalyzed by Small-Pore Cage-Based Zeolites
- 09:00 Christopher Parlett Spatially orthogonal chemical functionalization of a hierarchical pore network for catalytic cascade reactions
- 09:15 Xiaolei Fan Structured Silicalite-1 Encapsulated Ni Catalyst Supported on SiC Foam for Catalytic Dry Reforming of Methane
- 09:30 Max L. Bols Metalloenzymes vs. Metallozeolites: Exploiting the Similarities and the Differences
- 09:45 Q&A

8:30 Parallel session 2: Disordered and Amorphous Materials 1/1

- 08:30 Emily Meekel Correlated Linker Disorder in Metal-Organic Frameworks
- 08:45 Rustem Valiullin Advanced characterisation of disordered mesoporous solids
- 09:00 Irene Bechis Structure prediction of amorphous Metal-Organic Frameworks
- 09:15 Alice Mary Bumstead Investigating the Melting Behaviour of Polymorphic Zeolitic Imidazolate Frameworks
- 09:30 Q&A

8:30 Parallel session 3: Gas Adsorption, Separation and Storage 2/2

- 08:30 Mingzhe Sun Transition metal cation-exchanged SSZ-13 zeolites for CO₂ capture and separation from N₂
- 08:45 Michael Badawi Use of atomistic simulations and machine learning perturbation theory to design optimized zeolite formulations for selective trapping applications
- 09:00 Vladimir Martis Variation in water vapor and CO₂ adsorption equilibrium on MOFs and Zeolites due to outgassing conditions
- 09:15 Dina G. Boer Binderless zeolite beads with hierarchical porosity for selective CO₂ adsorption
- 09:30 Jin Shang Revisit the molecular sieving behaviour in zeolite LTA for high-performance gas separation
- 09:45 Q&A

10:15 Keynote lecture: Neil Champness: MOFs to control reaction processes: A journey through complex structures

11:10 Keynote lecture: Veronique van Speybroeck: Towards modeling spatiotemporal processes within nanoporous materials

13:30 Plenary lecture: Manuel Moliner: Designing microporous materials for target catalytic applications

14:35 Karena Chapman: Porous materials as a platform for nanoparticle formation

15:30 Parallel session 1: New Synthetic Methods and Post-Synthetic Modification ¾

- 15:30 Lichen Liu Generation of Subnanometric Metal Clusters in Zeolites and Their Evolution Behavior Under Reaction Conditions
- 15:45 Josip Bronic Influence of postsynthesis treatments on acid site strength of ZSM-5
- 16:00 Yu Liang Multivalent Cations Function as Accelerants and Structure-directing Agents of Zeolite Crystallization
- 16:15 Heng Dai Two- and Three-Dimensional Finned Zeolite Catalysts
- 16:30 Run Zou Selective demetalization of amphiphilic zeolites in oil/water emulsion
- 16:45 Q&A

15:30 Parallel session 2: Dynamic materials 1/1

- 15:30 Bonity Lutton-Gething New insight into the thermoresponsive behaviour of MIL-53 MOFs revealed by in-situ single crystal X-ray diffraction
- 15:45 Muslim Dvoyashkin Exploration of n-Butane Diffusion in Highly-Flexible Mesoporous Metal-Organic Framework DUT-49 using the Pulsed Field Gradient NMR
- 16:00 Catherine Walshe Synthesis and postsynthetic modification of flexible scandium metal-organic frameworks
- 16:15 Jenny G. Vitillo Tuning the gate opening in zeolitic imidazolate frameworks by metal substitution
- 16:30 Derya Bessinger Fast-Switching Vis-IR Electrochromic Covalent Organic Frameworks⁸³⁶
- 16:45 Q&A

15:30 Parallel session 3: Advanced Characterisation and Operando Spectroscopies 2/3

- 15:30 Eddy Dib The location of defects in zeolites probed by solid state NMR
- 15:45 Sophie Helena Van Vreeswijk Nanoscale Visualization of Carbon and Magnesium Clusters in Zeolites Active in the Methanol-to-Olefins Process
- 16:00 John P. S. Mowat Structural Analysis of Faulting in the Triclinic Zeolite UZM-55 and the new Polymorph: UZM-55FM
- 16:15 Cameron M Rice Fast Room-Temperature Lability of CHA Framework - 17O Solid-state Nuclear Magnetic Resonance Spectroscopy
- 16:30 Ines Lezcano-Gonzalez Confined species shaping the lifetime of zeolite catalysts for methanol conversion
- 16:45 Q&A

Thursday 8 July 2021

08:30 Parallel session 1: Energy Applications 1/1

- 08:30 Ciara Byrne Probing Zeolitic Imidazolate Frameworks (ZIFs) for heat storage applications
- 08:45 Petra Agota Szilagyi Development of a new class of adaptable free-standing hydroxide-ion exchange membranes based on metal-organic frameworks for alkaline fuel cells
- 09:00 Michelle Åhlén CO₂ and SF₆ adsorption on mixed-linker ZIF-7-8s: The effect of linker substitution on gas uptake and selectivity¹⁵⁷
- 09:15 Anna-Caroline Lavergne-Bril Selective Cobalt precipitation for the synthesis of precursors for cathode materials of li-ion batteries
- 09:30 Guillaume Maurin Computational guided discovery of novel MOFs for Water-Adsorption Driven Heat allocation
- 09:45 Q&A

08:30 Parallel session 2: Ion Exchange and Other Applications 1/1

- 08:30 Magdalena Malgorzata Lozinska The unique effect of copper cations on the flexibility of zeolite Rho causes exsolution
- 08:45 Martin Jendrlin Ion-selective pencil: towards a zeolite-based multi-sensor system for precision agriculture
- 09:00 Antony Nearchou A nuclear clean-up act - microporous silicates for decontamination of radioactive waste streams
- 09:15 Minkee Choi Design of effective zeolite-based ion-exchangers for radioactive Cs⁺ and Sr²⁺ capture
- 09:30 Jennifer Readman Structural studies of titanium and zirconium silicate ion-exchange materials for the treatment of nuclear waste.
- 09:45 Q&A

08:30 Parallel session 3: New Synthetic Methods and Post-Synthetic Modification 4/4

- 08:30 Hao Xu Structural Stabilization and Diversity of Germanosilicates
- 08:45 Raquel Simancas Synthesis and catalytic performance of the P-modified Al- and Ga-containing ITQ-52 zeolite
- 09:00 Dongil Kwon Fine-tuning the molecular sieving properties of aluminosilicate zeolites by post-synthesis functionalization of the interior surface for light olefin/paraffin separation
- 09:15 Bert Sels Isomerization of unsaturated fatty acids with hierarchical ZSM-5
- 09:30 Q&A

10:15 Keynote lecture: Sharon Ashbrook: Exploiting Isotopic Enrichment in NMR Spectroscopy

11:10 Plenary lecture: Stefan Kaskel: Understanding responsivity of metal-organic frameworks

13:30 Keynote lecture: Unni Olsbye: Site-structure-performance correlations in zeolite- and MOF-based catalysts

14:25 Parallel session 1: Industry Discussion session

14:25 Sohail Abdo Zeolite-based technologies for societal needs KEYNOTE

14:55 Silke Sauerbeck New Zeolites – The Long and Winding Road from Lab to Production

15:10 Timothy Johnson Fast optimisation of MOF syntheses – bespoke, budget, in-situ monitoring to guide production

15:25 Eduard L Kunkes Zeolite Crystallization via Staged Addition of Reagents

15:40 Ray O.K. Ozdemir Developing Markets for Titanium Metal Organic Frameworks

15:55 Guoping Hu The industrialisation process of an ionic liquidic zeolite (ILZ) adsorbent for coal seam gas purification

16:10 Q&A

14:25 Parallel session 2: Catalytic Properties 4/5

14:25 Ruixue Zhao Impact of extra-framework clusters in zeolites on alkane cracking

14:40 Hiromi Yamashita Hollow Titanosilicate Nanospheres Encapsulating PdAu Nanoparticles for H₂O₂-mediated One-pot Oxidation Reaction

14:55 Reisel Millán Diffusion of [Cu(NH₃)₂]⁺ complexes in Cu-CHA catalysts under NH₃-SCR-NO_x reaction conditions: insights from AIMD simulations FEZA21-OR-018

15:10 Hongjun Park Mesoporous zeolites as versatile support for metal catalysts in industrially relevant reactions

15:25 Q&A

14:25 Parallel session 3: Binding, Sensing and Separating Guests 1/1

14:25 Tina M. Nenoff Direct Electrical Detection of Target Environmental Gases by a Zeolite and MOF Based Sensors

14:40 Michael Tiemann A CuO@KIT-6 Silica Nanocomposite for Highly Selective H₂S Gas Sensing

14:55 Dana Medina-Tautz Energy efficient ultrahigh flux separation of oily pollutants from water with superhydrophilic nanoscale metal-organic framework architectures

15:10 Annika Möslin Unravelling the Guest Encapsulation in Metal-Organic Frameworks via Infrared Nanospectroscopy

15:25 Q&A

15:55 Parallel session 2: Novel Materials and Structural Methods 2/3

15:55 Benjamin Yuhas Synthesis and Characterization of Novel Small-Pore (Silico)Aluminophosphates

16:10 Shreya Sathyanath Hydrothermal Transformation of Diatoms into Zeolite Chabazite-Diatom Composite and Testing in Ammonia - Selective Catalytic Reduction (SCR) Applications

16:25 Gregory J. Lewis Synthesis and Characterization of ZnAPO/SAPO-58 and ZnAPO-63 with New Zeotype Topologies

16:40 Mervyn Shannon JMZ-11: A Set of Non-Stochastic Intergrowths in the CHA-GME System with the Distinctive Feature of a Prominent "sfw-GME" Tail

16:55 Q&A

15:55 Parallel session 3: Computational Prediction of Structure and Properties 1/1

15:55 François-Xavier Coudert Systematic exploration of physical properties of nanoporous materials properties: combining quantum calculations, classical simulations, and machine learning

16:10 Steven Bennett Discovery of Synthesizable Organic Materials

16:25 Andrew Tarzia High-throughput structure prediction of metal-organic cages

16:40 Rama Oktavian Computational Characterisation and Screening of Zr-Oxide Metal Organic Frameworks for CO₂ Capture

16:55 Q&A

Friday 9 July 2021

08:30 Parallel session 1: Physical Properties and the Role of Defects 2/2

08:30 Christine Kirschhock Dynamics of a flexible GIS framework tuned by Al-distribution and cation-guest interaction

08:45 Michael Fischer DFT-based molecular dynamics elucidate the dynamic behaviour of fluoride anions in all-silica zeolites

09:00 Mollie Trueman CrystalGrower: Modelling the Crystallisation of Porous Materials

09:15 Santhosh Matam Dynamics and Reactivity of Methanol in zeolite H-ZSM-5

09:30 Q&A

08:30 Parallel session 2: Structural Characterisation 1/1

08:30 Zhehao Huang Revealing Structural Details of Nanoporous Materials by Rotation Electron Diffraction Methods

08:45 Patricia Scheurle MOF-74(M) films obtained through vapor-assisted conversion - impact on crystal orientation and optical properties

09:00 Emma Helen Wolpert Emergence of topologically protected phases in framework materials

09:15 Peter Behrens Selective photochemical postsynthetic reactions of metal-organic frameworks containing the benzophenonedicarboxylate linker

09:30 Q&A

08:30 Parallel session 3: Catalytic Properties 5/5

08:30 Laura Löbber Study of Ni-exchanged FAU, MFI and CHA catalysts shows impact of zeolite properties on the activity of Ni single sites for selective butene dimerization

08:45 Stefan Nastase Computational studies on the early stages of the Methanol to Hydrocarbons and related processes

09:00 Yong Yuan Understanding the Correlation between Ga Speciation and Propane Dehydrogenation Activity on Ga/H-ZSM-5 Catalysts

09:15 Pieter Cnudde How acidity influences light olefin diffusion in H-SAPO-34 zeolites

09:30 Q&A

10:00 Parallel session 1: Novel Materials and Structural Methods 3/3

10:00 Alvaro Mayoral Direct Atomic-Level Imaging of Zeolites by Electron Microscopy: From Oxygen bridges to Extra-framework Light Cations, including Iron Framework Atoms and Bimetallic Compounds

10:15 Przemyslaw Rzepka Exploiting resonant X-ray powder diffraction at the Al K edge to locate aluminum in zeolite frameworks

10:30 Jung Cho Disorder in non-cage Containing Zeolites

10:45 Teresa Blasco Spectroscopic evidence on the changes in the F-Si bonding and the local structure of silicon atoms in highly crystalline pure silica RTH-type zeolite

11:00 Q&A

10:00 Parallel session 2: MY SCHEDULE

10:00 Agnes Szegedi Nanosized zeolite Beta based drug formulation for the simultaneous release of silver and sulfadiazine

10:15 Simon M. Vornholt Evaluating and Understanding the Performance of MOF- Polymer Composites for Medical Device Applications

10:30 Heng Zhao The intracellular fate of metal organic frameworks and maghemite nano-objects and the application for inflammatory diseases theranostics

10:45 Samuel Valable Assessment of nanosized zeolites to counteract hypoxia induced radio-resistance in glioblastoma

11:00 Q&A

10:00 Parallel session 3: Advanced Characterisation and Operando Spectroscopies 3/3

10:00 Jiaxu Liu Dual-beam Fourier Transform Infrared Spectrometer: Applications and Potentials in Zeolite Catalysis

10:15 Chiara Negri Structure and reactivity of mobilized Cu-oxygen pairs and their role in the low temperature NH₃-Selective Catalytic Reduction

10:30 Frédéric Blanc Zeolites Heterogeneous Catalysts Caught in the Act by (Dynamic Nuclear Polarisation) Magic Angle Spinning NMR

10:45 Carlos Bornes Unravelling the structure of acid sites in trimethylphosphine oxide adsorbed HZSM-5 using ¹H-³¹P HETCOR NMR

11:00 Q&A

11:30 Lauren McHugh: FEZA PhD Prize BZA Founders Award Lecture: Toxic Gas Adsorption and Water Stability in MOFs and MOF-Activated Carbon Composite Materials

13:30 Plenary lecture: Christopher Jones: The Critical Role of Porous Materials in Carbon Dioxide Capture from Air, Negative Emissions Technologies and Climate Stabilization

14:35 Poster Prizes / Closing Remarks