



CIS-9 

9th Czech - Italian - Spanish Conference on Molecular Sieves and Catalysis

4-7th June 2023. TOLEDO, SPAIN

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SCIENTIFIC CONTRIBUTIONS

Plenary communications

PL-1: *"Beyond classical shape selective effects in zeolite catalysis"*

Avelino Corma

PL-2: *"Open-framework silicates under pressure: compressional behaviour and crystal–fluid interaction"*

G. Diego Gatta

PL-3: *"Enantioselective Synthesis of Cyclic Compounds using Organocatalysis"*

Jan Veselý

Keynote communications

KN-1: *"The transition to a waste based industry"*

Rafael Roldán

KN-2: *"Characterization of porous materials with CO₂ around 195 K"*

Sebastian Ehrling

Oral communications

O-1: *"Chemically activated hydrochars as catalysts for the treatment of HTC liquor"*

Alberto de Mora, José Luis Diaz de Tuesta, María Isabel Pariente, Yolanda Segura, Fernando Martínez

O-2: *"Design of bi-functional Ni-zeolites for ethylene oligomerization: controlling Ni speciation and zeolite properties by one-pot and post-synthetic Ni incorporation"*

Adrián Martínez Gómez-Aldaraví, Cecilia Paris, Avelino Corma, Manuel Moliner, Cristina Martínez

O-3: *"Dealumination of USY as facile method for stabilization of subnanometric metal clusters"*

Ang Li, Muhammad Numan, Yuyan Zhang, Jiří Čejka, Changbum Jo, Michal Mazur

O-4: *"Solventless sustainable synthesis of zeolitic imidazolate frameworks with hydraulic press and high temperature"*

Marta Pérez-Miana, Javier U. Reséndiz-Ordóñez, Joaquín Coronas

O-5: *"Design of Lewis Acid Zeolite Catalysts via Assembly – Disassembly – Organization – Reassembly approach"*

Sarra Abdi, Daniel Rainer, Mariya Shamzhy, Jiří Čejka

O-6: *"Generation of mesoporosity in crystals of zeolite Omega by post-synthesis treatments with surfactants"*

Joaquín Pérez-Pariente, Alejandro Vidal de la Fuente, Amel Mekki, Boudhjer Boukoussa, Marisol Grande, Enrique Sastre, Carlos Márquez-Álvarez, Manuel Sánchez-Sánchez

O-7: *"Nanostructuring of CPPs based on dyes using a new ultra-mini-emulsion technique for an improvement in photo(electro)catalytic applications"*

Sandra Palenzuela Rebella, Teresa Naranjo, Mariam Barawi, Marta Liras, Víctor A. de la Peña O'Shea

O-8: *"Accelerated modelling of supported Pt clusters via reactive machine learning potentials"*

Christopher James Heard, Andreas Erlebach, Lukáš Grajciar, Tereza Benešová

O-9: *"Understanding zeolite-water oxygen exchange under steaming conditions"*

Tereza Benešová, Christopher James Heard

O-10: *"Study of the catalytic activity of GTM-3 chiral zeolite: Expanding the knowledge of the new asymmetric catalyst"*

Ramón de la Serna, Carlos Márquez-Álvarez, Joaquín Pérez-Pariente, Luis Gómez-Hortiguela

O-11: *"Integrated CO₂ capture and methanation over Li/Na-Ru dual function materials"*

Stefano Cimino, Elisabetta Maria Cepollaro, Milena Pazzi, Luciana Lisi

O-12: *"New methods for imaging zeolites at atomic level"*

Zhuoya Dong, Yanhang Ma, Álvaro Mayoral

O-13: *"Basic catalytic synthesis of gamma-lactams over amino-functionalized multiwall carbon nanotubes"*

Niurka Barrios-Bermúdez, Arisbel Cerpa-Naranjo, María Luisa Rojas-Cervantes

O-14: *"Catalytic performances in ethane dehydrogenation in the presence and absence of CO₂ over Co/zeolites materials"*

Safaa Essid, Roman Bulánek

O-15: *"Valorisation of glucose into biofuels and high value-added chemicals using zeolites as catalyst"*

Benjamín Torres-Olea, Antonio Pérez-Merchán, Cristina García-Sancho, Juan Antonio Cecilia, Ramón Moreno-Tost, Pedro Jesús Maireles-Torres

O-16: *"Catalytic utilization of a system comprising hydrosilane, B(C₆F₅)₃, and transition metal complex"*

Michal Horáček, Vojtech Varga, Martin Lamač, Jan Merna, Jiří Pinkas

O-17: *"Influence of the synthesis method of Cu-Y catalysts for the gas phase oxidative carbonylation of methanol to dimethyl carbonate"*

Marino M. Álvarez, Jennifer Cueto, Pablo Marín, Salvador Ordóñez, David P. Serrano

O-18: *"Hydroxyapatite modified with copper for biofuel synthesis"*

Daniel Alejandro Valdivieso-Vera, Iván Alonso Santos-López, María Olga Guerrero-Pérez, Isabel Barroso-Martín, Enrique Rodríguez-Castellón, Gerardo Antonio Flores-Escamilla, Brent Edward Handy, Jorge Guillermo Huerta-Muñoz, José Julián Cano-Gómez, Luis Hernández-Adame

O-19: *"Study of ceria-based materials for CO₂ capture and their functionalization with ruthenium for methane production"*

Andrea Rizzetto, Samir Bensaid, Raffaele Pirone, Marco Piumetti

O-20: *"Influence of bulky functional groups in cycloaddition reaction catalyzed by Zn-URJC-13"*

Jesús Tapiador, Pedro Leo, Gisela Orcajo, Guillermo Calleja

O-21: *"Influence of synthesis conditions of Co/SiC and TiC-SiC on H₂ production from NH₃"*

Marina Pinzon, Paula Sánchez, Antonio de Lucas-Consuegra, Ana R. de la Osa, Amaya Romero

O-22: *"SU-101 for the removal of pharmaceutical active compounds by the combination of adsorption/photocatalytic processes"*

Antonio J. Chacón-García, Sara Rojas, Erik Svensson-Grape, Tom Willhammar, Andrew K. Inge, Yolanda Pérez, Patricia Horcajada

O-23: *"New efficient catalysts based on LDH for synthesis of sandalwood-type fragrances"*

Iva Paterova, Martina Slana, Olga Gorlova

O-24: *"3D printed Pt-ZSM5/Geopolymer as catalyst for H₂-SCR"*

Elisabetta Maria Cepollaro, Stefano Cimino, Luciana Lisi, Domenico Caputo, Marco D'Agostini, Paolo Colombo, Giorgia Franchin

Q-25: *“Propane dehydrogenation over Pt and Ga-containing MFI zeolites with modified acidity and textural properties”*

Adriana Souza de Oliveira, María del Mar Alonso-Doncel, Jennifer Cueto, Martin Kubů, Jiří Čejka, David P. Serrano, Rafael Ángel García-Muñoz

Q-26: *“Valorization of End of Life Tyres by pressurized catalytic pyrolysis over nanocrystalline ZSM-5 zeolite”*

Francisco Miguel González-Pernas, David P. Serrano, Inés Moreno, Patricia Pizarro

Q-27: *“Hierarchical zeolites for dimethyl ether conversion into light olefins (DTO): synthesis, characterization, and catalytic performance”*

Emanuele Giglio, Giorgia Ferrarelli, Fabio Salomone, Elena Corrao, Massimo Migliori, Samir Bensaid, Raffaele Pirone, Girolamo Giordano

Q-28: *“Hydrodeoxygenation of cyclohexanone dimer for the production of high-density aviation fuels over Al₂O₃-Nb₂O₅-supported Ni/Re catalysts”*

María Ventura, Eduardo Gaya, Marisa B. Navas, Sara Jerez, Marcelo E. Domine, Marta Paniagua, Gabriel Morales, Juan A. Melero

Q-29: *“Understanding the changes in lignocellulose catalytic pyrolysis when shifting from batch to continuous reaction systems”*

Maurizio Pagano, Jennifer Cueto, Héctor Hernando, Inés Moreno, David P. Serrano

Q-30: *“Sorption enhanced DME synthesis via direct CO₂ hydrogenation over 3D hybrid zebra materials”*

Giuseppe Bonura, Serena Todaro, Giosuè Giacoppo, Alessandro Cajumi, Catia Cannilla, Enrico Catizzone, Giorgia Ferrarelli, Massimo Migliori, Girolamo Giordano, Francesco Frusteri

Q-31: *“Direct Hydrogenation of CO₂ to Valuable Hydrocarbons via Fischer-Tropsch Route over Tandem Zeolite-Based Catalysts”*

Raúl Murciano, Sara Escorihuela, José Manuel Serra, Agustín Martínez

Q-32: *“Ethyl levulinate ketalization with glycerol promoted by zeolites”*

Vincenzo Russo, Francesco Taddeo, Rosa Vitiello, Rosa Turco, Riccardo Tesser, Martino Di Serio

Q-33: *“Green hydrogen production by thermochemical water splitting based on mixed cerium oxides shaped as reticulated porous structures”*

Alejandro Pérez, María Orfila, María Linares, Javier Marugán, Raúl Sanz, Raúl Molina, Juan Ángel Botas

Q-34: *“Recovery of strategic metals using mesoporous activated carbon as sorbent”*

Naby Conte, José María Gómez, María Mercedes Lobete, Eduardo Díez, Araceli Rodríguez, Laura Castro, Jesús Ángel Muñoz

Flash-Oral communications

F-1: *“Synthesis of porous materials from primary oily sludge and their application as CO₂ adsorbents.”*

Sara Jerez, Silvia Favero, María Ventura, María Isabel Pariente, Magda Titirici, Juan A. Melero

F-2: *“Generation of mesoporosity in USY zeolite with high Si/Al atomic ratio by a modified surfactant-templating approach”*

Cristina Molina, Albina Abdrasilova, Gema Gómez-Pozuelo, Laura Briones, Juan Ángel Botas, David P. Serrano, Ángel Peral, José María Escola

F-3: *“Optimisation of the synthesis of La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O₃ perovskite by reactive grinding and its structural shaped for green hydrogen production by thermochemical water splitting”*

Alejandro Pérez, Elisa Díaz-Correas, María Orfila, María Linares, Javier Marugán, Raúl Sanz, Raúl Molina, Juan Ángel Botas

F-4: *“Encapsulation of additives in thermoresistant materials synthesised by green methods for application in textile fibers”*

Cristina Pina, César Rubio, Elena Piera, Miguel A. Caballero, Carlos Téllez

F-5: *“Zeolite/geopolymer composites with hierarchical porosity manufactured by 3D printing for application in CO₂ capture processes”*

Mariana Schneider, Regina de Fatima Peralta Muniz Moreira, Agenor de Noni Júnior, Dachamir Hotza, Mar Calzado, Olga Guerrero Pérez, Enrique Rodríguez-Castellón

F-6: *“Single-atom Pt catalyst supported on Ce-MOFs for the low temperature CO oxidation reaction”*

Benjamin Bohigues, Sergio Rojas-Buzo, Davide Salusso, Avelino Corma, Manuel Moliner, Silvia Bordiga

F-7: *“Green Sustainable Synthesis of Covalent Organic Framework TpPa-1”*

Iñigo Martínez-Visus, Matías Ulcuango, Beatriz Zornoza, Joaquín Coronas, Carlos Téllez

F-8: *“Covalent Organic Frameworks Based on BODIPY and BOPHY Dyes for Artificial Photosynthesis”*

Teresa Naranjo, Tania Mazuelo, Miguel Gómez-Mendoza, Felipe Gándara, Marta Liras, Victor de la Peña O’Shea

F-9: *“Pyridinium-based quaternary OSDA for TON-type zeolites and their structure determination using cRED”*

Daniel N. Rainer, Michal Mazur, Russell E. Morris, Jiří Čejka

F-10: *“The catalytic activity of 2D material-supported catalysts: a micro spectroscopic study at the single active site level”*

Iryna Danylo, Lukáš Koláčný, Pavlíčková Vladimíra Svobodová, Silvie Rimpelová, Tomáš Hartman, Martina Pitínová, Martin Veselý

F-11: *“Crystal-fluid interactions in natural erionite-group zeolites under compression”*

Tommaso Battiston, Paolo Lotti, Davide Comboni, G. Diego Gatta

F-12: *“Comparative removal of PFAS from water by adsorption on natural and synthetic zeolites”*

Maura Mancinelli, Claudia Belviso, Lutz Ahrens, Annalisa Martucci

F-13: *“LTA Zeolites to Sorption Enhanced Methanation in a Ni-Fe/ γ -Al₂O₃ catalytic fluidized bed reactor”*

Irene de Matías, Paúl Durán, Víctor Daniel Mercader, Pablo Aragüés-Aldea, Eva Francés, Javier Herguido, José Ángel Peña

F-14: *“Modelling of temperature-programmed reduction of metal oxide catalysts considering the particle size distribution effect”*

Jhonny Villarroel-Rocha, Antonio Gil

F-15: *“Enhanced CO₂ methanation cyclic SERP process with Ni5A and Ni13X as catalyst”*

Andrés Cañada-Barcala, Rubén Calero-Berocal, Gonzalo Pascual-Muñoz, Marcos Larriba, Vicente Ismael Águeda-Maté, José Antonio Delgado-Dobladez

F-16: *“MWW-type zeolites supported ammonium-tagged Hoveyda-Grubbs catalyst: activity and selectivity in acyclic diene metathesis of α,ω -dienes”*

Martin Kubů, Michal Mazur, Naděžda Žilková, Hynek Balcar

F-17: *“Preparation of functionalised tetrahydropyrans catalysed by isorecticular zeolites”*

Anastasia Kurbanova, Martin Nigrini, Kinga Gołąbek, Ondřej Veselý, Jan Veselý, Jiří Čejka

F-18: *"Physicochemical changes of BN during oxidative dehydrogenation of propane"*

Sajad Mehran, Knotkova Katerina, Slang Stanislav, Rubes Miroslav, Bulanek Roman

F-19: *"Cu-Mn oxides prepared by SCS procedure as catalysts for the total oxidation of VOCs under dry and wet conditions"*

Clarissa Cocuzza, Enrico Sartoretti, Chiara Novara, Fabrizio Giorgis, Samir Bensaid, Nunzio Russo, Debora Fino, Marco Piumetti

F-20: *"Redox and non-redox catalysts for propylene ODH with CO₂"*

Daniel Ballesteros-Plata, Juan Antonio Cecilia, Isabel Barroso-Martín, Enrique Rodríguez-Castellón, Antonia Infantes-Molina

F-21: *"New catalysts for Baeyer-Villiger oxidation of β -cyclocitral"*

Olga Gorlova, Iva Paterová, Petra Přibyllová

F-22: *"Acetalization of glycerol with benzaldehyde using copper-based MOF"*

Elena García-Rojas, Pedro Leo, Gisela Orcajo, Carmen Martos

F-23: *"Platinum-based graphene-like aerogels doped with boron in Hydrogen Evolution Reaction"*

Javier Cencerrero, Amaya Romero, Ana Raquel de la Osa, Antonio de Lucas-Consuegra, Paula Sánchez

F-24: *"The influence of the PtRu/C morphology on the ethanol electro-reforming product distribution"*

Alberto Rodríguez-Gómez, Fernando Dorado, Paula Sánchez, Antonio de Lucas-Consuegra, Ana Raquel de la Osa

F-25: *"Ru supported on Mg/Al hydrotalcites for phenol hydrogenation"*

Nadia Benmebirouk-Pareja, Isabel Barroso-Martín, Maia Montaña, Daniel Ballesteros-Plata, Juan Antonio Cecilia, Antonia Infantes-Molina, Enrique Rodríguez-Castellón

F-26: *"Insights into the influence of feed impurities on catalyst performance in the solvent-free dimerization of renewable levulinic acid"*

Marta Paniagua, Gabriel Morales, Juan A. Melero, Daniel García

F-27: *"Application of bimetallic PtCo, PtMo and PtMn catalysts in perhydrobenzyltoluene dehydrogenation"*

Kevin Alconada, Victoria Laura Barrio

F-28: *"Catalytic reduction of chlorates by platinum catalysts"*

Adrián Plá-Hernández, Antonio Eduardo Palomares-Gimeno, Fernando Rey

F-29: *"Catalytic upgrading of lignin-derived bio-oils over ion-exchanged H-ZSM-5 zeolites"*

María Inés Ávila, Laura Briones, Gema Gómez-Pozuelo, José María Escola, David P. Serrano, Ángel Peral, Juan Ángel Botas

F-30: *"New insights about the effect of acidity of ZSM-5 zeolite on dehydration of methanol and ethanol"*

Giorgia Ferrarelli, Enrico Catizzone, Massimo Migliori, Girolamo Giordano

F-31: *"Microwave assisted synthesis of Pd@MOF composites for catalytic hydrogenation of olefins under ambient conditions"*

Ignacio D. Lemir, Carlos Fernandez-Ruiz, Raul M. Guerrero, Yolanda Pérez, Patricia Pizarro, David P. Serrano, Patricia Horcajada

F-32: *"Investigation of the Fe role in paraffin cracking over Al-free Fe-ZSM-5 zeolites"*

Anastasia Kurbanova, Dominika Zákutná, Kinga Gołąbek, Ming-Feng Hsieh, Jan Přeč

F-33: *"Xylose hydrogenation promoted by Ru/SiO₂ sol-gel catalyst: from batch to continuous operation"*

Vincenzo Russo, Benedetta Anna De Liso, Henrik Grénman, Kari Eränen, Francesco Taddeo, Antonio Aronne, Martino Di Serio, Tapio Salmi

Poster communications

P-1: *"Synthesis of inorganic-pillared titanium carbides (MXenes)"*

Pavla Eliášová, Oleh Dvorenchenko

P-2: *"The Effect of Copper Loading on Selected MOFs: Sustainable Synthesis and Photocatalytic Behaviour"*

Nejat Redwan Habib, Abi M. Tadesse, Raquel Sainz, Manuel Sánchez-Sánchez, Isabel Díaz

P-3: *"Decomposition of methanol-water solution over heterojunction photocatalysts"*

Vendula Meinhardová, Lada Dubnová, Kamila Kočí, Libor Čapek

P-4: *"Synthesis and asymmetric catalytic activity of GTM-4 chiral zeolite materials prepared with benzyl-containing ephedrine derivatives"*

Luis Gómez-Hortigüela, Ramón de la Serna, Jaime Jurado-Sánchez, Joaquín Pérez-Pariente

P-5: *"Inversion of chirality in GTM-4 enantio-enriched zeolite driven by a minor change of the structure-directing agent"*

Ramón de la Serna, Itziar Arnaiz, Carlos Márquez-Álvarez, Joaquín Pérez-Pariente, Luis Gómez-Hortigüela

P-6: *"Plasma jet sputtering as a perspective tool for the preparation of Co-Cu-Mn oxides: effect of preparation conditions on properties and oxidation activity"*

Květa Jirátová, Martin Čada, Roman Perekrestov, Jana Balabánová, Martin Koštejn, Jaroslav Maixner, Pavel Topka, Zdeněk Hubička, František Kovanda

P-7: *"Sustainable synthesis of ZIF-8 at room temperature from aqueous mixtures having the exact stoichiometric Zn/linker ratio"*

M. Asunción Molina, Jorge Rodríguez-Campa, M. Rosa Flores Borrell, Manuel Sánchez-Sánchez

P-8: *"13X zeolite-chitosan composite-based aerogels for CO₂ removal"*

Enrica Luzzi, Martina Salzano de Luna, Giovanni Filippone, Paolo Aprea, Domenico Caputo

P-9: *"From geopolymers to zeolites: synthesis and characterization of foamed FAU-X monoliths"*

Assunta Campanile, Barbara Liguori, Carlo Gravino, Claudio Ferone, Lara Gigli, Paolo Aprea, Domenico Caputo

P-10: *"Synthesis of ZSM-5 zeolite in the presence of long-chain surfactants: from mesophases to nanocrystals and dendritic nanoarchitectures"*

María del Mar Alonso-Doncel, Elena A. Giner, David P. Serrano

P-11: *"Synthesis of pure silica zeolites with low content in organic structure directing agents"*

José Valero, Susana Valencia, Fernando Rey, Eduardo Pérez-Botella

P-12: *"Pair Distribution Function (PDF) studies on Enzyme@MOF composites"*

María Asunción Molina, Alicia Manjón-Sanz, Isabel Díaz, Enrique Sastre, Rosa M. Blanco, Manuel Sánchez-Sánchez

P-13: *"Binuclear iron sites for the activation of small molecules. Structural-functional dependency"*

Kinga Mlekodaj, Agnieszka Kornas, Dominik K. Wierzbicki, Jiri Dedeczek, Stepan Sklenak, Radim Pilar, Mariia Lemishka, Edyta Tabor, Hana Jirglová

P-14: *"Influence of the framework topology of small pore Ag-containing zeolites on the adsorption of ethene"*

Fernando Rey, Alessandra de Marcos-Galan, Gabrielli Almeida, Joaquín Martínez-Ortigosa, José Alejandro Vidal-Moya, Germán Sastre, Mónica Jiménez-Ruiz, Teresa Blasco

P-15: *"Synthesis, characterization and performances of perovskites-based materials for Solid Oxide Fuel Cell's anode"*

Melodj Dosa, Alessandro Monteverde, Andrea Felli, Marta Boaro, Leonardo Duranti, Elisabetta Di Bartolomeo, Marco Piumetti

P-16: *"Analysis of the active sites in the oxidative dehydrogenation of ethane over Fe-FER"*

Lucie Smoláková, Lada Dubnová, Tomáš Matys Grygar, Milan Pouzar, Libor Čapek

P-17: *"Performance of nickel-manganese and nickel-cobalt-manganese mixed oxide catalysts in ethanol total oxidation"*

Timur Babii, Květa Jirátová, Jana Balabánová, František Kovanda

P-18: *"Effect of manganese addition on the oxidation activity of Ni-Cu and Ni-Co mixed oxides"*

Timur Babii, Květa Jirátová, Jana Balabánová, Martin Koštejn, Jaroslav Maixner, František Kovanda

P-19: *"Laccase@MOF biocatalyst for BPA degradation in aqueous phase. Kinetic aspects"*

María Asunción Molina, Rosa M. Blanco, Manuel Sánchez-Sánchez, A. Meneses-Jácome

P-20: *"VOCs catalytic oxidation for indoor air purification"*

Nadia Grifasi, Samir Bensaid, Nunzio Russo, Debora Fino, Marco Piumetti

P-21: *"Biogas dry reforming over Ni/organosilicon-derived monoliths"*

Máira Mallmann, Emanuelle Acosta, Luisa Isago, André Fragnani, Regina Moreira

P-22: *"Dendritic ZSM-5 zeolites as promising catalysts to obtain jet fuel intermediates through furfural – cyclopentanone aldol condensation"*

Daniel de la Calle, Jennifer Cueto, María del Mar Alonso-Doncel, Elena A. Giner, Rafael A. García-Muñoz, David P. Serrano

P-23: *"Nanosponge and Nanosheet Al/Ga-MFI Zeolites Performance in the Catalytic Pyrolysis of Biomass and Plastics"*

Francisco Artillo, Yuyan Zhang, María del Mar Alonso-Doncel, Michal Mazur, Patricia Pizarro, Květa Kalíková, Jiří Čejka, David P. Serrano

P-24: *"Carrageenan-DFNS catalysts for biomass conversion to alkyl levulinates"*

Mahdi Abdulmohsin Jazea Alsalmim, Alireza Najafi Chermahini, Antonio Pineda, Rafael Luque, Carolina Vargas

P-25: *"Catalytic pyrolysis of solid recovered fuel (SRF) over n-ZSM-5 zeolite leading to light olefins and low-chlorine oil"*

Gemma Pérez, Jennifer Cueto, Marta Paniagua, Gabriel Morales, Juan Antonio Melero, David P. Serrano

P-26: *"Combination of Al and Zr sites in zeolite catalysts for cascade transformation of furfural to γ -valerolactone"*

Roman Barakov, Nataliya Shcherban, Mariya Shamzhy, Jiří Čejka, Maksym Opanasenko

P-27: *"Properties and catalytic activity of Ga and Zn modified ZSM-5 zeolites"*

Luis F. Aguilar, Julia Aguilar-Pliego, Misael García-Ruiz, Marisol Grande, Carlos Márquez-Álvarez, Enrique Sastre

P-28: *"Hydration Of Materials Having Different Glass/CsAlSi₅O₁₂ Ratio After Six Years At Room Temperature And 55% Relative Humidity"*

Guido Cerri, Antonio Brundu

P-29: *“Recycling strategies dealing with zeolitic imidazolate frameworks applied to the CO₂/N₂ separation with membranes”*

Víctor Berned-Samatán, Lidia Martínez-Izquierdo, Rafiul Hasan, Carlos Téllez, Joaquín Coronas

P-30: *“Selective oxidation of Methane into Methanol with molecular O₂ using Cu_n nanoclusters within CHA models: A computational Study”*

Mario Gallego, Mercedes Boronat, Avelino Corma



Crystal-fluid interactions in natural erionite-group zeolites under compression

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In the last two decades many studies showed that hydrostatic compression is able to enhance or induce the intrusion of molecules (or solvated ions) into the structural nano-cavities of microporous materials, pointing out that this is a viable way to promote a mass transfer from fluids to structurally-incorporated molecules. A full understanding of this phenomenon in natural or synthetic zeolites might expand the number of their utilizations, *e.g.* tailoring of new materials, as catalysts in industrial processes [1,2]. In addition, this phenomenon bears an intrinsic relevance also in Earth Sciences, as zeolites may act as fluid carriers in the upper Earth crust, *e.g.* during the early subduction of oceanic sediments or altered basalts.

In this scenario, we focused on three natural zeolites, structurally characterized by six-membered rings of tetrahedra and belonging to the large group of ABC-6 open-framework materials: erionite, offretite and bellbergite. Erionite is a quite common zeolite in nature, where it forms in basaltic vugs, crystallizing from hydrothermal fluids. It shows an ERI-type framework, made by the repetition of AABAAC sequences of 6-membered rings of tetrahedra layers. Offretite (OFF framework type) shows an AAB sequence and is commonly intergrown with erionite, due the easy occurrence of stacking faults at B and C positions of the 6-membered rings layers. Bellbergite is a rather uncommon zeolite in nature, more famous for its synthetic counterparts [3], and shows an EAB framework with ABBACC sequence.

The crystal-fluid interactions during compression were investigated by means of *in situ* single-crystal X-ray diffraction, which allows to focus the study on the effects that interaction has on the crystal structure of zeolites. The experiments were performed at the ID15B beamline of the European Synchrotron Radiation Facility, using diamond anvil cells to apply hydrostatic pressures on the investigated samples and using different pressure-transmitting fluids: namely, the non-penetrating silicone oil and daphne oil 7575 and potentially penetrating methanol:ethanol:water 16:3:1 mixture, ethanol:water 1:1 mixture, methanol, distilled H₂O and liquid Ne. As *non-penetrating* are intended those fluids which molecules have a kinetic diameter larger than the free diameter of the open-framework of the zeolite and, therefore, cannot be pressure-intruded into the crystal structure. The compressional experiments in non-penetrating fluids provide, therefore, a benchmark to which compare the behavior of the same microporous compound in a potentially penetrating fluid.

Among the investigated natural samples, erionite resulted to be the one with the highest magnitude of adsorption, as shown by Figure 1. The new adsorbed molecules act as “pillars” within the framework nanocavities, decreasing the compressibility of the structure, as it is clear comparing the unit-cell *vs.* pressure evolution of erionite compressed in silicone oil and methanol:ethanol:water (16:3:1) mixture, respectively (Figure 1). The obtained results also allow to conclude that the magnitude of the intrusion for a given zeolite is strictly related to the H₂O content of the hydrous *P*-transmitting fluids, where the largest is the water fraction, the highest the magnitude of the intrusion and (sometimes) the lower the pressure at which it occurs. A comparison of the crystal-fluid interactions under pressure in natural erionite and in other synthetic zeolites (*e.g.* SiO₂-ferrierite [4]), points out that the observed magnitude of intrusion in this study is surprisingly high for a natural zeolite, characterized by channels and cages already filled by extraframework cations and molecules. These results suggest that natural zeolites, despite being intrinsically less inclined to show pressure-induced crystal-fluid interaction with respect to synthetic ones, should not be *a priori* excluded as targets for the tailoring of new materials by exploiting hydrostatic compression, especially when a modest temperature is also applied. Moreover, the obtained results also suggest that the role of zeolites as fluid carriers or fluid moderators in the geological processes occurring in the upper Earth crust deserves a more comprehensive characterization for a full understanding.

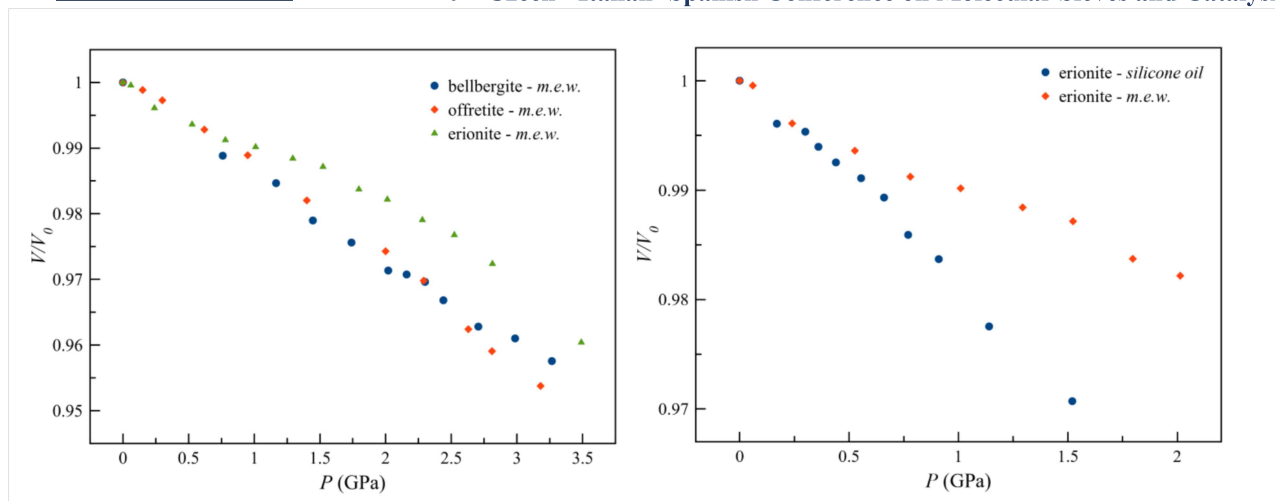


Figure 1. (Left). High-pressure evolution of the unit-cell volumes (normalized to their ambient-conditions values) of natural erionite, offretite and bellbergite. (Right). Compressional evolution of normalized (to ambient-conditions values) unit-cell volumes of natural erionite in the non-penetrating silicone oil and in the penetrating methanol:ethanol:water (16:3:1, *m.e.w.*) mixture.

Acknowledgements: ESRF is acknowledged for the provision of beamtime. The Italian Ministry of Education (MUR) is acknowledged for the support through the projects “PRIN2017—Mineral reactivity, a key to understand large-scale processes” (2017L83S77) and “Dipartimenti di Eccellenza 2023-2027”.

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