

WORKSHOP on "WATER IN ZEOLITES"



Liblice, September 19-22, 2021

Sunday – September 19, 2021

14.00		Bus – Prague Airport (Terminal 2) – Liblice Castle
16.00-18.00		Registration
18.00-18.10		Opening Ceremony
	Chair: Jiří Čejka	
18:10-19:00	PL1	How water acts on reacting molecules in zeolites - toward a molecular understanding J.A. Lercher
19:00-19:50	PL2	The role of EM (TEM, STEM & SEM) for study of the crystal growth, crystal defects and surface termination of zeolites A. Mayoral
20:00		Welcome (Garden) Party

Monday - September 20, 2021

	Chair: Petr Nachtigall	
9:00-9:50	PL3	The effects of solvents on adsorption energies, and the effect of pH on activation barriers, at the liquid / solid interface C.T. Campbell
9:50-10:25	KN1	Next generation quantum chemistry of water in acidic zeolites J. Sauer
10:25-10:50		Coffee Break & Posters
	Chair: Lukáš Grajciar	
10:50-11:10	OP1	Operando modelling of Germanosilicate hydrolysis <u>C. Heard</u> , M. Jin, L. Grajciar, P. Nachtigall
11:10-11:30	OP2	Theoretical Study of Zeolite Hydrolysis under Alkaline Conditions <u>M. Jin</u> , M. Liu, P. Nachtigall, L. Grajciar, C.J. Heard
11:30-11:50	OP3	The influence of defects on zeolite hydrolysis barriers M. Liu
11:50-12:10	OP4	A theoretical study of graphene oxide and zeolites behavior for water treatment D.M. Cid Perez
12:15-14:00		Lunch
	Chair: Michal Mazur	
14:00-14:50	PL4	About the aluminum coordination in zeolites and their role in forming acid sites J. van Bokhoven
14:50-15:25	KN2	Water in ADOR transformation of zeolites M. Opanasenko
15:25-15:45	OP5	Towards understanding the role of rare earth ions in the prevention of dealumination in zeolite Y <u>K. Stanciakova</u> , S. Simko, J. Louwen, R.E.Bulo, E.T.C. Vogt, B.M. Weckhuysen
16.00		Guided Tour to Lobeč Brewery
20:00		Dinner

Tuesday - September 21, 2021*Chair: David Kubička*

9:00-9:50	PL5	Solvent Effects on Intermolecular MPVO and Cycloaddition Reactions in Zeolites with Different Intrapore Polarity Y. Roman-Leschkov
9:50-10:10	OP6	Zeolitic materials for the adsorption heat pumps <u>W. Schwieger</u> , R. Herrmann, A. Kuhnt, E. Pleißner, S. Sathyanath, M. Hartmann
10:10-10:30	OP7	Water content effect of zeolites in the chlorine retention capacity from plastic pyrolysis oils A. Romero
10:30-10:55		Coffee Break & Posters
<i>Chair: Maksym Opanasenko</i>		
10:55-11:15	OP8	Water Adsorption Studies on a Series of Demetallated Faujasite Zeolites <u>K. Peikert</u> , J. Kenvin
11:15-11:35	OP9	Water vapor adsorption and pore size analysis on various modified MCM41 J. Adolphs
11:35-11:55	OP10	Water Vapor Adsorption on Zeolites at different temperatures <u>V. Martis</u> , J. Willkomm, A. Lieb
11:55-12:15	OP11	ADORable zeolites in Water-vapour adsorption: insight into the disassembly of germanosilicates M. Kubů, <u>O. Veselý</u> , J. Čejka
12:15-14:00		Lunch
<i>Chair: Mariya Shamzhy</i>		
14:00-14:35	KN3	Reactive neural network potentials for zeolites (and water) with DFT accuracy L. Grajciar
14:35-14:55	OP12	Computational study of T-atom vacancies in MSE zeolite framework P.S. Petkov, <u>G.N. Vayssilov</u>
14:55-15:15	OP13	Interaction of Water with H-MFI in the Low-Loading Regime Studied by Highly Accurate QM:QM Methods <u>H. Windeck</u> , F. Berger, J. Sauer
15:15-15:45		Coffee Break & Posters
<i>Chair: Wilhelm Schwieger</i>		
15:45-16:05	OP14	The importance of steaming in catalyst equilibration prior to testing P. Diddams
16:05-16:25	OP15	Catalytic properties of (MO _x @Nb and Nb)-zeolites based catalyst in the oxidation of glucose and HMF M. E. Fergani, N. Candu, P. Granger, <u>V. I. Parvulescu</u> , S. M. Coman

16:25-16:45

OP16

On the effect of water on hydrotalcite-derived catalysts
and their activity in aldol condensation
D. Kubička, V. Korolova, O. Kikhtyanin

17:00-18:30

*Round-table Discussion***18.30-18.40*****Closing Remarks******19:00******Farewell Dinner*****Wednesday - September 22, 2021*****9:00******Bus - Liblice Castle - Prague Airport***

POSTERS

1. Influence of alcohol in the synthesis solution on the ZSM-5 crystallisation and membrane properties
H. Richter, A. Simon, I. Voigt
2. Unraveling role of Ca-hydroxo clusters in MTH reaction by use of step-response approach
A. Liutkova
3. On the Role of Ions in the Formation of Zeolites
S. Prodinge
4. Mechanistic insights on the water-zeolite synergy in the conversion of biomass-derived guaiacol
M. Bocus, E. Van den Broeck, Y. Liao, B.F. Sels, V. Van Speybroeck
5. The influence of water on nuclear magnetic resonance properties in zeolites
S. Vanlommel, A.E.J. Hoffman, V. Van Speybroeck
6. Computational study of the structure and stability of iron species in MFI-type zeolite
I.Z. Koleva, H.A. Aleksandrov, R. Nikolova, G.N. Vayssilov
7. Catalytic performance of Fe-modified derivatives of 2D MWW-type zeolites in DeNO_x process
A. Jankowska, A. Kowalczyk, M. Rutkowska, W. Mozgawa, L. Chmielarz
8. Copper modified (Al,Ti)-ferrierite zeolite and its delaminated derivatives (ITQ-6) as active catalysts for NH₃-SCR process
A. Świąt, A. Kowalczyk, M. Rutkowska, U. Diaz, L. Chmielarz
9. Theoretical study of zeolite-water interactions under streaming conditions
T. Benešová, C. Heard, P. Nachtigall
10. The effect of water treatment on the properties of pure silica CHA zeolite
K. Gołębek, M. Shamzhy, Q. Yue, J. Čejka
11. In-situ techniques for tracking the metal-silanols interactions in 2D zeolite precursor
A. Li, S. Abdi, B. Šmíd, M. Mazur
12. Lewis acid isorecticular zeolites: synthesis, characterization and catalytic applications
S. Abdi, P. Rani, M. Kubů, M. Shamzhy, J. Čejka
13. Interpretation of ²⁷Al MAS NMR results based on ab initio molecular dynamics: effects of temperature and water loading
C. Lei
14. Understanding Germanosilicate Hydrolytic (In)stability based on Germanium Distributions derived using Neural Network Potentials
I. Saha, L. Grajciar, A. Erlebach, C.J. Heard, P. Nachtigall
15. Identification of collective variables using neural networks
M. Šípka, L. Grajciar, M. Pavelka

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