

# 2nd International Conference on Reaction Kinetics, Mechanisms and Catalysis RKMC 2021

20 - 22 May 2021 / Online from Budapest, Hungary

## Final Programme

### Thursday / 20 May 2021

Time zone: GMT +2		Oral Session 1 Session Chair: Gábor Lente		
9:00	9:05	Opening remarks	Gábor Lente <i>Conference Chair</i>	University of Pécs HUNGARY
9:05	9:40	From snapshots of working catalysts to mechanisms: Opportunities and limitations of operando spectroscopy	Angelika Brückner <i>Plenary Speaker</i>	Leibniz-Institute for Catalysis GERMANY
9:40	10:15	Hydrogen storage and recovery with the use of chemical hydrogen batteries. Water-soluble N-heterocyclic carbene complexes of Ru(II), and Ir(I) in the forefront	Ferenc Joó <i>Plenary Speaker</i>	University of Debrecen HUNGARY
10:15	10:35	Hydrodeoxygenation of lignin-derived model compounds to produce renewable jet fuel	Mark Martinez-Klimov	Åbo Akademi University FINLAND
10:35	11:00	Coffee Break		
		Oral Session 2 Session Chair: Angelika Brückner		
11:00	11:35	The role of spectroscopy in understanding the nature of the active sites in heterogeneous catalysts: the case of TS-1	Matteo Signorile <i>Plenary Speaker</i>	University of Turin ITALY
11:35	12:10	Oscillatory carbonylation of poly(ethylene glycol)methyl ether acetylene. Improved model of reaction mechanism	Željko Čupić <i>Plenary Speaker</i>	University of Belgrade SERBIA
12:10	12:30	Reaction extent (advancement of reaction): A new general definition	Vilmos Gáspár	Eötvös Loránd University HUNGARY
12:30	14:00	Lunch Break		
14:00	16:00	Poster Session		
		Oral Session 3 Session Chair: Enrico Bibbona		
16:00	16:35	Network structure and dynamics for biochemical reaction networks	David F. Anderson <i>Plenary Speaker</i>	University of Wisconsin USA
16:35	17:10	Biodynamical properties of phosphorylation networks	Maya Mincheva <i>Plenary Speaker</i>	Northern Illinois University USA

17:10	17:45	<b>Motifs of multistationarity in reaction networks</b>	<b>Casian Pantea</b> <i>Plenary Speaker</i>	West Virginia University USA
17:45	18:05	<b>Chemical reaction networks connected by diffusive and convective connections</b>	<b>Katalin M. Hangos</b>	University of Pannonia HUNGARY
18:05	18:25	<b>Static and dynamic absolute concentration robustness</b>	<b>Joshi Badal</b>	California State University San Marcos USA
19:00	20:30	<b>Welcome Session with Coffee / Tea / Beer / Wine</b>		

## Friday / 21 May 2021

<b>Oral Session 4A</b> Session Chair: András Sápi				<b>Oral Session 4B</b> Session Chair: Tibor Nagy			
9:00	9:20	<b>Preparation of Pt electrocatalyst supported by novel, graphite oxide derived Ti(1-x)MoxO2-C type of composites</b>	<b>Ilgar Ayyubov</b> Research Centre for Natural Sciences HUNGARY	<b>High-speed tracking of fast chemical precipitations</b>	<b>Réka Zahorán</b> University of Szeged HUNGARY		
9:20	9:40	<b>Influence of the multifunctional mixed oxide-carbon composite support on the CO tolerance and stability of Pt electrocatalysts</b>	<b>Irina Borbáth</b> Research Centre for Natural Sciences HUNGARY	<b>Solving inverse problems of chemical kinetics by metaheuristic methods</b>	<b>Leniza Enikeeva</b> Novosibirsk State University RUSSIA		
9:40	10:00	<b>Synthesis and characterization of PdNi nanoparticles supported by carbon mixed transition metal oxides for applications in the electrochemical devices</b>	<b>Muhammad Sufaid Khan</b> University of Malakand PAKISTAN				
10:00	10:20	<b>Electrocatalytic hydrogenation of glucose and xylose on highly dispersed carbon fiber supported Au nanocatalysts I</b>	<b>Jay Pee Ona</b> Ábo Akademi University FINLAND	<b>Numerical modeling of precipitate formation in microfluidic system</b>	<b>Paszka Papp</b> University of Szeged HUNGARY		
10:20	10:40			<b>Over-equilibrium as a result of CPE</b>	<b>Vitaliy Trishch</b> National Technical University of Ukraine UKRAINE		
10:40	11:00	<b>Coffee Break</b>					
<b>Oral Session 5A</b> Session Chair: Vilmos Gáspár				<b>Oral Session 5B</b> Session Chair: Stevan Macesic			
11:00	11:20	<b>Lyapunov stability of ring-like compartmental models</b>	<b>Áron Erdélyi</b> Pázmány Péter Catholic University HUNGARY	<b>Co,H-SSZ-13 Zeolite Catalysts Prepared by Solid-Phase Reaction for NO-SCR by methane</b>	<b>Hanna Solt</b> Research Centre for Natural Sciences HUNGARY		
11:20	11:40	<b>Bio-inspired flow-driven chitosan pattern formations</b>	<b>Pawan Kumar</b> University of Szeged HUNGARY				
11:40	12:00	<b>Extensions of detailed balance for not necessarily reversible Markov chain models of reaction networks</b>	<b>Daniele Cappelletti</b> Politecnico di Torino ITALY	<b>Performance of mixed templates incorporated SAPO-34 for Methanol to olefins reaction</b>	<b>Baljinder K. Riyar</b> Indian Institute of Technology Roorkee INDIA		

12:00	12:20	<b>Inference of RNA life-cycle kinetic rates and simultaneous gene clustering from sequencing data</b>	<b>Enrico Bibbona</b>	Politecnico di Torino ITALY	<b>The kinetics of zeolitic imidazolate framework (ZIF-8) formation and synthesis in a confined flow reactor</b>	<b>Edina Balog</b>	University of Szeged HUNGARY
12:20	12:40	<b>Algorithmic construction of reaction networks from delayed kinetic differential equations</b>	<b>Mihály Vághy</b>	Pázmány Péter Catholic University HUNGARY	<b>The use of zeolite-supported nanoparticles of ruthenium dioxide as catalyst of levulinic acid hydrogenation</b>	<b>Valentina G. Matveeva</b>	Tver State Technical University RUSSIA
12:40	14:00	<b>Lunch Break</b>					
<b>Oral Session 6A</b> Session Chair: Katalin Ósz				<b>Oral Session 6B</b> Session Chair: András Tompos			
14:00	14:20				<b>Activity of MgO-SiO<sub>2</sub> catalysts in ethanol-to-butadiene reactions</b>	<b>Blanka Szabó</b>	Research Centre for Natural Sciences HUNGARY
14:20	14:40	<b>Catalytic chain termination by inhibitors in oxidation of unsaturated compounds in the liquid phase and microheterogeneous systems</b>	<b>Ivan V. Tikhonov</b>	P.G. Demidov Yaroslavl State University RUSSIA	<b>The use of polymeric Pd-containing catalysts for selective hydrogenation of phenylacetylene to styrene</b>	<b>Linda Zh. Nikoshvili</b>	Tver State Technical University RUSSIA
14:40	15:00	<b>Multicriteria optimization of gasoline catalytic reforming temperature regime based on a kinetic model with grouped hydrocarbons</b>	<b>Irek Gubaydullin</b>	Institute of Petrochemistry and Catalysis of Russian Academy of Sciences RUSSIA	<b>Hydroisomerization of hexane over Pt-modified Beta-Bentonite extrudates shaped catalysts: synthesis, catalysis, reaction mechanism</b>	<b>Narenda Kumar</b>	Åbo Akademi University FINLAND
15:00	15:20	<b>Methanol photocatalytic reforming reaction over alkali-doped graphitic carbon nitride</b>	<b>Emília Tálás</b>	Research Centre for Natural Sciences HUNGARY	<b>Catalyst development for the direct synthesis of hydrogen peroxide</b>	<b>Christoph Schmidt</b>	Åbo Akademi University FINLAND
15:20	15:40	<b>Investigation of the efficiency of BiOI/BiOCl composite photocatalysts using UV, cool and warm white LED light sources - photon efficiency, toxicity, reusability, matrix effect, and energy c</b>	<b>Tünde Alapi</b>	University of Szeged HUNGARY	<b>Exploring the reaction mechanism of the direct synthesis of hydrogen peroxide with transient studies and FTIR-ATR</b>	<b>Ole Reinsdorf</b>	Åbo Akademi University FINLAND
15:40	16:00	<b>Effect of Ag, Ca, and Fe on photocatalytic activity of ZnO nanoparticles to remove textile dyes under sunlight irradiation</b>	<b>Meriem Kouhail</b>	Mohammadia School of Engineers MOROCCO	<b>Phase composition and activity of Zr-Zn-O catalysts in the reaction of conversion ethanol</b>	<b>Tahmina Taghiyeva</b>	Azerbaijan State Oil and Industry University AZERBAIJAN
16:00	16:30	<b>Coffee Break</b>					
<b>Oral Session 7A</b> Session Chair: Gábor Lente				<b>Oral Session 7B</b> Session Chair: Ágnes Szegedi			
16:30	16:50	<b>Investigation of the dynamical properties of the mechanism regulating the formation of reactive oxygen species in rhizosphere</b>	<b>Stevan Mačević</b>	University of Szeged HUNGARY	<b>Hydrodeoxygenation of lignin-derived guaiacol on supported Pd and Ni catalysts using neat and phosphorus-modified <math>\gamma</math>-alumina supports</b>	<b>Gyula Novodárszki</b>	Research Centre for Natural Sciences HUNGARY
16:50	17:10	<b>Kinetics and mechanism of action of triterpenoids</b>	<b>Elena Nikolaevna Schvareva</b>	Ufa State Petroleum Technological University RUSSIA	<b>Mesoporous catalysts for co-processing of biomass and petroleum</b>	<b>Antonina A. Stepacheva</b>	Tver State Technical University RUSSIA

17:10	17:30	<b>Hydrolysis-oxidation of starch in the presence of solid and soluble heteropoly acid catalysts for the production of formic acid</b>	<b>Nikolay Gromov</b>	Boreskov Institute of Catalysis SB RAS RUSSIA	<b>Hydrolytic oxidation of cellobiose in the presence of a Pt-containing polymeric catalyst</b>	<b>Oleg V. Manaenkov</b>	Tver State Technical University RUSSIA
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## Saturday / 22 May 2021

### Oral Session 8 Session Chair: Ferenc Joó

9:00	9:35	<b>How can metal-support interactions affect the catalytic performance?</b>		<b>Aleksey Vedyagin</b> <i>Plenary Speaker</i>		Boreskov Institute of Catalysis RUSSIA
9:35	10:10	<b>Catalysis tailoring: from the nanostructures and molecular level understanding to the industrial applications</b>		<b>András Sápi</b> <i>Plenary Speaker</i>		University of Szeged HUNGARY
10:10	10:30	<b>Effect of metal-acid sites location and proximity in shaped catalyst on their catalytic behaviour in n-hexane hydroisomerization</b>		<b>Zuzana Vajglova</b>		Åbo Akademi University FINLAND

### Coffee Break

### Oral Session 9 Session Chair: Vilmos Gáspár

11:00	11:20	<b>Microkinetics of butanol formation via ethanol coupling reactions over MgO-Al<sub>2</sub>O<sub>3</sub> mixed oxide catalyst</b>		<b>Tibor Nagy</b>		Research Centre for Natural Sciences HUNGARY
11:20	11:40	<b>Effect of the reductive treatment on the state and electrocatalytic behavior of Pt in catalysts supported on Ti<sub>0.8</sub>Mo<sub>0.2</sub>O<sub>2</sub>-C composite</b>		<b>Christina Silva</b>		Research Centre for Natural Sciences HUNGARY
11:40	12:00	<b>Kinetics of flax processing waste pyrolysis</b>		<b>Yury V. Lugovoy</b>		Tver State Technical University RUSSIA
12:00	12:20	<b>Kinetic study of the oxidation of iodide ion by dicyanobis(phenanthroline)iron(III) in aqueous-organic solvent medium</b>		<b>Rozina Khattak</b>		Shaheed Benazir Bhutto Women University PAKISTAN
12:20	12:40	<b>Multicriteria optimization of the catalytic reaction for the synthesis of benzyl butyl ether based on the kinetic model</b>		<b>Kamila Koledina</b>		Institute of Petrochemistry and Catalysis of Russian Academy of Sciences RUSSIA

### Lunch Break

### Oral Session 10 Session Chair: Gábor Lente

14:30	14:50	<b>Silica coating for Pd/C catalysts: compromising active phase protection and accessibility</b>		<b>Sophie Hermans</b>		UCLouvain BELGIUM
14:50	15:10	<b>Base-catalyzed aldol condensation of propanal with cinnamaldehyde followed by hydrogenation</b>		<b>Iva Paterova</b>		UCT Prague CZECH REPUBLIC
15:10	15:30	<b>Mechanism and kinetics of platinum nanocatalyst degradation during the oxygen evolution reaction through in situ Transmission Electron Microscopy</b>		<b>Rui Filipe Serra Maia</b>		University of Pennsylvania USA

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15:30	15:40	<b>Closing remarks</b>	<b>Gábor Lente</b> <i>Conference Chair</i>	University of Pécs HUNGARY
17:00	18:00	<b>Virtual Sightseeing</b>		

The Organizers reserve the right to make changes in the Conference programme