

# ISCRE 24 – POSTER SESSION 1

MONDAY, JUNE 13, 2016

5:00 pm to 7:00 pm

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LEACHING PROCESS FOR THE RECOVERY OF VALUABLE METALS FROM SPENT LITHIUM-NICKEL-COBALT-MANGANESE-OXIDE-BASED LITHIUM-ION BATTERIES

Li-Po He, Shu-Ying Sun, Xing-Fu Song and Jian-Guo Yu  
(Paper #10)

KINETICS OF OXIDATIVE CRACKING OF HEXANE TO OLEFINS OVER VOX/CE-AL<sub>2</sub>O<sub>3</sub> IN A GAS PHASE OXYGEN FREE ENVIRONMENT

AbdAlwadood Elbadawi, Muhammad Khan, Shaikh Razzak, Mohammad Hossain and Mohammad Quddus  
(Paper #27)

THE EFFECTS OF SUPPORT ACIDITY ON QUINOLINE AND INDOLE HYDRODENITROGENATION - A DETAILED KINETIC STUDY

Minh Tuan Nguyen, Melaz Tayakout-Fayolle, Fabien Chainet, Gerhard Pirngruber and Christophe Geantet  
(Paper #35)

INSIGHT INTO PT-BI BIMETALLIC CATALYSTS FOR TUNING SELECTIVITY AND IMPROVING STABILITY

Yang Xiao and Arvind Varma  
(Paper #50)

EFFECTS OF PORE NETWORK STRUCTURE ON MULTIPHASE REACTIONS USING A DISCRETE MODELLING APPROACH

Guanghua Ye, Xingui Zhou, Marc-Olivier Coppens and Weikang Yuan  
(Paper #51)

C-O BOND ACTIVATION ON MULTIFUNCTIONAL HETEROGENEOUS CATALYSTS

Alexander Mironenko, Glen Jenness and Dionisios Vlachos  
(Paper #70)

LIGNIN DEPOLYMERIZATION USING NITRATE-INTERCALATED LAYERED  
DOUBLE HYDROXIDE CATALYSTS

Jacob Kruger, Nicholas Cleveland, Shuting Zhang, Rui Katahira, Brenna  
Black, Gina Chupka, Mary Bidy and Gregg Beckham  
(Paper #71)

PALLADIUM SUBNANO-CLUSTERS ON TITANIA FOR SOLAR-LIGHT  
REMOVAL OF NO

Kakeru Fujiwara, Ulrich Müller and Sotiris Pratsinis  
(Paper #78)

HIGHLY EFFICIENT PTFE BIMETALLIC AND PTFE TRIMETALLIC  
NANOCATALYSTS: FROM QUASI-CORE-SHELL STRUCTURE TO NANOALLOY

Hua Zhang, Jinbao Zheng, Nuwei Zhang, Jian-Feng Li and Bing H. Chen  
(Paper #80)

EFFECT OF PARTICLE SHAPE ON FLUID FLOW AND HEAT TRANSFER IN A  
PACKED BED

Karthik G. M. and Vivek Buwa  
(Paper #95)

EFFECT OF METALLIC TYPES ON 2-PROPANOL PHOTOOXIDATION FOR  
PHOTOINDUCED HYDROGEN FORMATION

Rattabal Khunphonoi, Nurak Grisdanurak and Eric Puzenat  
(Paper #104)

KINETICS ANALYSIS FOR ULTRASONIC DEGRADATION OF ORGANIC  
COMPOUNDS

Daisuke Kobayashi and Hideyuki Matsumoto  
(Paper #118)

PATCHED-BIMETALLIC SURFACES AS HIGHLY ACTIVE CATALYSTS

Wei Guo and Dionisios Vlachos  
(Paper #125)

FIRST PRINCIPLES MATERIALS DESIGN: IMPROVED ELECTROCATALYSTS  
FOR OXYGEN REDUCTION

Jeffrey Herron and Manos Mavrikakis  
(Paper #130)

KINETICS FOR METHYLATION OF 2-METHYLNAPHTHALENE OVER ZSM-12  
WITH DIFFERENT CRYSTAL SIZES

Gaku Watanabe, Yuta Nakasaka, Taichi Taniguchi, Takuya Yoshikawa,  
Teruoki Tago and Takao Masuda  
(Paper #138)

COMPOSITION EFFECTS OF PTSB ALLOY ON BASE-FREE OXIDATION OF GLYCEROL

Hua Dong, Xuezhong Duan, Jiaqi Lei, Gang Qian and Xinggui Zhou  
(Paper #143)

GUIDELINES FOR OPTIMAL DOSING STRATEGIES FOR REACTIONS OF ALDEHYDES AND AMMONIA

Emanuele Moiola, Leo Schmid, Peter Wasserscheid and Hannsjörg Freund  
(Paper #154)

POTENTIAL OF A LOOP REACTOR FOR THE OXIDATION OF HYDROCARBON MIXTURES OVER A CRXO<sub>3</sub> CATALYST - IMPORTANCE OF THE REACTION KINETICS

Gregor Kiedorf, Tanya Wolff, Andreas Seidel-Morgenstern and Christof Hamel  
(Paper #158)

CERIUM-ZIRCONIUM-PRASEODYMIUM OXIDE CATALYSTS FOR CO OXIDATION

Marco Piumetti, Samir Bensaid, Nunzio Russo and Debora Fino  
(Paper #167)

EXPERIMENTAL AND SIMULATION STUDY OF DIMETHYL ETHER SYNTHESIS FROM SYNGAS ON A COMMERCIAL CU/ZNO/AL<sub>2</sub>O<sub>3</sub> CATALYST

Karla Herrera Delgado, Johannes Abeln, Till Henrich and Jörg Sauer  
(Paper #172)

SOLVENT EFFECTS ON THE HYDROFORMYLATION OF LONG CHAIN OLEFINS

Martin Gerlach, Max Lemberg, Reni Grauke, Gabriele Sadowski, Andreas Seidel-Morgenstern and Christof Hamel  
(Paper #178)

AMMONIA OXIDATION: A DFT STUDY

Johanna Espach, Jane Mugo and Glenn Jones  
(Paper #185)

CURING KINETICS OF EPOXIDIZED VEGETABLE OIL AND A GREEN HARDENER BASED ON NON-ISTHERMAL DSC METHOD

Zhenhao Xi, Yahua Chen, Ling Zhao and Weizhen Sun  
(Paper #199)

BIOMASS OXIDATION TO FORMIC ACID IN AQUEOUS MEDIA USING POLYOXOMETALATE CATALYSTS – BOOSTING FA SELECTIVITY BY IN-SITU EXTRACTION

Jakob Albert, Jenny Reichert and Peter Wasserscheid  
(Paper #200)

CHARACTERIZATION OF MICROSTRUCTURED REACTORS FOR  
DEHYDROGENATION OF LIQUID ORGANIC HYDROGEN CARRIERS

Martin Cholewa and Peter Pfeifer (Michael Belimov, presenter)

*(Paper #205)*

DEACTIVATION OF IR-RE ALLOY CATALYST IN GLYCEROL  
HYDROGENOLYSIS

Li Leng, Xin Ren, Jinghong Zhou and Xinggui Zhou

*(Paper #207)*

FACILE SYNTHESIS OF N-DOPED CARBON COATED LITHIUM ZINC  
TITANATE PARTICLES TOWARDS ENHANCED PERFORMANCE IN LITHIUM-  
ION BATTERY APPLICATIONS

Chi Chen

*(Paper #215)*

ENHANCED METATHESIS OF ETHYLENE AND 2-BUTENE ON TUNGSTEN  
INCORPORATED ORDERED MESOPOROUS SILICATES

Jian-Feng Wu, Anand Ramanathan, William K. Snavely, Andrzej Rokicki and  
Bala Subramaniam

*(Paper #222)*

MULTI-TECHNIQUE APPROACHES TO STUDY DIFFUSION PHENOMENA IN  
VACUUM GAS OIL HYDROTREATING

Svetan Kolitcheff, Antoine Hugon, Jan Verstraete, Elsa Jolimaitre and  
Melaz Tayakout-Fayolle

*(Paper #225)*

SYNGAS PRODUCTION FROM STEAM AND DRY REFORMING OF METHANE  
OVER NI-BASED CATALYST IN MICROCHANNEL REACTOR: CFD MODELING  
WITH ELEMENTARY KINETICS

Chenxi Cao, Nian Zhang and Yi Cheng

*(Paper #233)*

THE ROLE OF THE SUPPORT AND REACTION CONDITIONS ON THE VAPOR  
PHASE HYDRODEOXYGENATION OF M-CRESOL OVER PT/TIO<sub>2</sub> AND PT/C  
CATALYSTS

Glen Ferguson, Michael Griffin, Daniel Ruddy, Mary Bidy, Gregg Beckham  
and Joshua Schaidle

*(Paper #264)*

OPTIMIZATION AND KINETIC STUDY OF 5-HYDROXYMETHYL FURFURAL (HMF) OXIDATION TO 2,5-FURANDICARBOXYLIC ACID (FDCA) WITH COBALT/MANGANESE/BROMIDE CATALYST

Xiaobin Zuo, Amit Chaudhari, Kirk Snavely, Fenghui Niu, Daryle Busch and Bala Subramaniam

*(Paper #274)*

LIGNIN DEPOLYMERIZATION INTO AROMATIC MONOMERS OVER NOVEL ZIRCONIUM INCORPORATED MESOPOROUS SILICATES

Kakasaheb Nandiwale, Andrew Danby, Anand Ramanathan, Raghunath Chaudhari and Bala Subramaniam

*(Paper #283)*

INVESTIGATING SILANE THERMAL DECOMPOSITION WITH AUTOMATIC MECHANISM GENERATION

Belinda Slakman and Richard West

*(Paper #285)*

ENHANCED REACTION STABILITY OF METAL-MODIFIED ZSM-5 FOR UPGRADING OF BIOMASS PYROLYSIS VAPORS

Matthew Yung, Calvin Mukarakate, Kristiina Iisa, Alexander Stanton, Richard French and Kimberly Magrini

*(Paper #286)*

DESIGN SPECIFICATIONS FOR A POROUS COMPOSITE LSM/YSZ CATHODE FOR SOLID OXIDE FUEL CELLS

Aayan Banerjee and Olaf Deutschmann

*(Paper #287)*

IDENTIFICATION OF ACTIVE SITES ON TRANSITION METAL CATALYSTS

Marcel Nunez and Dionisios Vlachos

*(Paper #307)*

CATALYST-SCALE MODELING OF NON-SPHERICAL PARTICLE SHAPES FOR THE GAS-PHASE FISCHER-TROPSCH SYNTHESIS

Arvind Nanduri and Patrick L. Mills

*(Paper #309)*

PROCESSES FOR THE PRODUCTION OF OXYGENATE FUELS FROM RENEWABLES

Joerg Sauer, Ulrich Arnold, Ludger Lautenschuetz and Dorian Oestreich (Karla Herrera Delgado, presenter)

*(Paper #311)*

MODELING TRANSPORT-KINETICS INTERACTIONS IN COMMERCIAL CATALYST SHAPES FOR SO<sub>2</sub> OXIDATION TO SO<sub>3</sub>

Anuradha Nagaraj and Patrick Mills

*(Paper #313)*

LIQUID-PHASE MECHANISM GENERATION FOR APPLICATION TO FUEL OXIDATION

Belinda Slakman, Karl Chatelain, Arij Ben Amara, Laurie Starck, Mickael Matrat, Laurent Catoire, Andre Nicolle and Richard West

*(Paper #331)*

COMPOSITION AND REACTION MODELING FOR THE SIMULATION OF LIGNIN CONVERSION

Maria Lopez-Abelairas, Luis Pereira de Oliveira, Nadège Charon and Jan J. Verstraete

*(Paper #334)*

EFFECTS OF SODIUM NITRITE ON STRUCTURE AND THERMAL PROPERTIES OF LiNO<sub>3</sub>-NaNO<sub>3</sub>-KNO<sub>3</sub> MOLTEN SALT FOR ENERGY STORAGE

Ze Sun, Xinmei Yang, Haiou Ni, Guimin Lu and Jianguo Yu

*(Paper #346)*

A MECHANISTIC INVESTIGATION OF SURFACE SITES ON TRANSITIONAL ALUMINA MATERIALS

Minje Kang, Joseph F. DeWilde and Aditya Bhan

*(Paper #358)*

SELECTIVE DEHYDROGENATION OF ETHANOL ON NiCu NANOPARTICLES AND NANOPOROUS NiCu

Junjun Shan, Hang Li, Jianchao Ye, Nare Janvelyan, Jilei Liu, Juergen Biener, Cynthia Friend and Maria Flytzani-Stephanopoulos

*(Paper #362)*

A UNIFIED AROMATIC HYDROGENATION KINETIC MODEL ACCOUNTING FOR RING SUBSTITUENTS

Naghme Fatemi, Kenneth Toch and Joris W. Thybaut

*(Paper #376)*

MECHANISTIC INSIGHTS INTO THE HYDROGENOLYSIS OF ACIDS OVER Pd-Re CATALYTIC SURFACES

Ashwin Chemburkar and Matthew Neurock

*(Paper #380)*

ELECTROCATALYTIC REDUCTION OF CO<sub>2</sub> BY METAL/IONIC LIQUID  
INTERFACES: THEORETICAL INSIGHTS

Stuart Winikoff and Matthew Neurock

*(Paper #382)*

ELECTROCATALYTIC PERFORMANCES OF PHOSPHORUS DOPED CARBON  
SUPPORTED PALLADIUM TOWARD FORMIC ACID OXIDATION

Jianding Li, Qifeng Tian and Shiyue Jiang

*(Paper #385)*

MECHANISTIC INSIGHTS INTO FACET-DEPENDENT CH<sub>4</sub> FORMATION OF  $\eta$ -  
Fe<sub>2</sub>C FISCHER-TROPSCH CATALYST

Nan Song, Bingxu Chen, Xuezhi Duan, Gang Qian, De Chen and Xinggui Zhou

*(Paper #389)*

DEVELOPMENT, TESTING AND EXPERIMENTAL RESULTS EVALUATION OF  
A MEMBRANE REACTOR FOR SOLAR STEAM REFORMING USING MOLTEN  
SALTS AS HEAT TRANSFER FLUID

Alessio Gentile, Barbara Morico, Gaetano Iaquaniello, Alberto Giaconia  
and Giampaolo Caputo

*(Paper #395)*

RATE-BASED DESIGN OF EXPERIMENTS USING CONTINUOUS-FLOW  
REACTORS

Chris Hone, Richard Bourne and Frans Muller

*(Paper #406)*

DIRECT CATALYTIC CONVERSION OF METHANE TO METHANOL AND  
ACETIC ACID USING MOLECULAR OXYGEN IN AN AQUEOUS MEDIUM OVER  
RH/ZSM-5 AND IR/ZSM-5

Mengwei Li, Junjun Shan and Maria Flytzani-Stephanopoulos

*(Paper #414)*

MATERIALS AND CHEMICALS FROM RENEWABLE AND WASTE CARBON  
SOURCES: REACTION ENGINEERING AND SPECTROSCOPY

Michael Timko

*(Paper #433)*