Preliminary Program MODEGAT VII 2022

Monday, September 12, 2022

Time		Topic	Presenter		Title
09:00-10:00		SCR	Tronconi / Nova	Enrico / Isabella	**Plenary**: The NH3-SCR redox cycle over Cu-CHA catalysts: Insights from transient kinetic analysis
10:00-10:25		SCR	Han	Joonsoo	Effect of SOx and framework Al density on N2O formation over Cu-CHA during NH3 selective catalytic reduction
10:25-10:55					*coffee break*
10:55-11:20		SCR	Bjerregaard	Joachim	Low temperature sulfur poisoning of Cu-CHA during NH3-SCR studied by DFT calculations
11:20-11:45		SCR	Suarez-Corredor	Andres	A data-driven modeling framework to develop an NH3 adsorption model for a vanadium-based SCR catalyst.
11:45-12:10		SCR	Kuntz	Christian	Coupling of liquid and surface chemistry in urea SCR systems
12:10-13:10					*lunch*
13:10-13:35		SCR	Chen	Echo	Model based optimization of SCR catalyst systems with a twin-dosing ammonia strategy
13:35-14:15		AI	Werfel	Johannes	**Keynote:** Vehicle Application of an AI-based Catalyst Model with Online Adaptation
14:15-15:30					*poster session with coffee*
15:30-16:30		NEW	Koltsakis	Grigoris	**Plenary**: Adding an electron to the equation: From catalyst- to battery modelling
16:30-17:10		NEW	Banerjee	Aayan	**Keynote**: Integrated Multiscale Modeling of Solid Oxide Electrodes, Cells, Stacks, and Systems
17:10-17:35		NEW	Deutschmann	Olaf	CO2 Emission Reduction in Steel Industry: Dry Reforming of Coke Oven Gas and Blast Furnace Gas
19:00					*dinner*

Tuesday, September 13, 2022

Time		Topic	Presenter		Title
09:00-10:00		Filter	Koci	Petr	**Plenary**: Modeling of three-way catalysts and particulate filters
10:00-10:25		Filter	Iliev	Oleg	On pore scale simulation of reactive flows in catalytic filters
10:25-11:00					*coffee break*
11:00-11:25		Filter	Watling	Timothy	Simulating Catalytic Reaction and Soot Oxidation in Coated Particulate Filters: A Simplified Modelling Framework
11:25-11:50		Filter	Samuels	Callum	Direct Permeability Estimation in Particulate Filters
11:50-12:15		Filter	Placha	Maria	Pore-scale modelling of soot deposits and their impact on catalytic filter performance
12:15-13:30					*lunch*
13:30-14:10		PNA	Olsson	Louise	**Keynote**: Kinetic modeling of CO influence on passive NOx adsorption
14:10-14:35		PNA	Bounechada	Djamela	Pd-exchanged chabazites as effective Passive NOx Adsorbers (PNAs): a novel transient kinetic analysis
14:35-15:00		OPT	Sjöblom	Jonas	Robust parameter estimation methodology for heterogeneous catalytic reactors
15:00-15:30					*coffee break*
15:30-15:55		Fund	Das	Srashtasrita	Chemical Gradients in Pt/Al2O3 and Cu-SSZ-13 Emission Control Catalysts Revealed by Operando XAS-tomography
15:55-16:20		System	Glatz	Thomas	Virtual Test Bed – What does this mean for Aftertreatment Modeling?
16:20-16:45		System	Karamitros	Dimitrios	Modelling challenges for post EU VI heavy-duty engines
16:45-17:15					*coffee and farewell*

This schedule may be subject to change.

last edit: 08.09.2022