



September 13–17, 2021

CLEERS Virtual Workshop

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HOSTED AND COORDINATED BY
OAK RIDGE NATIONAL LABORATORY

UNDER THE GUIDANCE OF
DOE ADVANCED ENGINE CROSSCUT TEAM

WITH SUPPORT FROM
DOE VEHICLE TECHNOLOGIES OFFICE

AGENDA

MONDAY, SEPTEMBER 13, 2021

11:00 a.m.	Welcome and Introduction	
11:05 a.m.	Invited Presentation: Continuing Progress Towards 2027 Low NOx Targets – Update on Demonstration Efforts at SwRI	Christopher Sharp, Southwest Research Institute
11:55 a.m.	Close-coupled SCR: An Approach to Meet Ultra-Low NOx Requirements for Heavy-Duty Diesel Engines	John Kasab, AVL Powertrain Engineering Inc.
12:20 p.m.	Break	
12:50 p.m.	Comparative Evaluation of Ammonium Carbamate and UWS Based SCR System for Diesel Engine NOx Reduction Under WHTC	Hassan Raza, Korea Institute of Machinery and Materials
1:15 p.m.	Can a Heat Exchanger Improve the Cold-start Performance of a PNA-SCR System for NOx abatement?	Petr Koci, University of Chemistry and Technology, Prague, Czech Republic
1:40 p.m.	Detailed Hydrocarbon Speciation of GDI Cold-start Exhaust Emissions and Use of HC-traps on Current Light-duty Trucks	Melanie DeBusk, Oak Ridge National Laboratory
2:05 p.m.	Break	
2:35 p.m.	Panel Discussion: Aftertreatment Catalyst Durability: Information Gaps and Future Needs	Tom Pauly, Umicore Danan Dou, John Deere Alissa Recker, Daimler Christine Lambert, Ford Motor Co.
4:15 p.m.	End of first day sessions	

AGENDA

TUESDAY, SEPTEMBER 14, 2021

11:00 a.m.	Welcome and Introduction	
11:05 a.m.	Stuart Daw Memorial Presentation: Novel Structured Low-Temperature Oxidation Catalysts for Future Emission Control Applications	Eleni Kyriakidou, University at Buffalo
11:55 a.m.	Support surface modification induced highly stable precious metal catalyst for efficient CO oxidation	Fudong Liu, University of Central Florida
12:20 p.m.	Break	
12:50 p.m.	Elucidation of Active Sites for Low-Temperature CO Oxidation over Ceria Supported Copper Catalysts that are 100% Regenerable After SO ₂ Poisoning	Carlos Garcia Vargas, Washington State University; Pacific Northwest National Laboratory
1:15 p.m.	Tailoring the Local Environment of Pt in Single-Atom Pt ₁ /CeO ₂ Catalysts for Robust Low-Temperature CO Oxidation	Dong Jiang, Washington State University
1:40 p.m.	Hydrothermally Stable Ceria/Alumina Supports for Exhaust Emission Control	Hien Pham, University of New Mexico
2:05 p.m.	Break	
2:35 p.m.	Low Temperature Automotive Exhaust Abatement Catalysts with High OSC and Thermal Stability	Devendra Pakhare, Pyrochem Catalyst Company
3:00 p.m.	Exploring the Reactivity of Single Atom Doped MxOy Catalysts for NO Reduction in TWC Applications	Konstantin Khivantsev, Pacific Northwest National Laboratory
3:25 p.m.	Versatile Halloysite-supported Core@shell Nanoparticle for the Elimination of Automotive Exhaust Pollutants	Wei Jing Li, University of Michigan
3:50 p.m.	A Novel, Smaller Honeycomb for Significant PGM Saving	Mansour Masoudi, Emissol, LLC
4:15 p.m.	End of second day sessions	

AGENDA

WEDNESDAY, SEPTEMBER 15, 2021

11:00 a.m.	Welcome and Introduction	
11:05 a.m.	Invited Presentation: Modeling Emission Catalyst Systems for Gasoline Applications	Manish Sharma, BASF
11:55 a.m.	What Really Matters In Three Way Catalyst Light-off?	Andrew "Bean" Getsoian, Ford Motor Co.
12:20 p.m.	Break	
12:50 p.m.	Reactivity of Novel High-performance Fuels on a Commercial Three-way Catalyst for SI/ACI Engine Emissions Control	Sreshtha Sinha Majumdar, Oak Ridge National Laboratory
1:15 p.m.	Methane Oxidation on Structured Pt/Pd + Mixed Metal Oxide Spinel: Mechanistic Origins of Conversion Enhancement During Feed Modulation	Michael Harold, University of Houston
1:40 p.m.	Exhaust Gas After-treatment of Hydrogen Combustion Engines by Elective Catalytic Reduction with Hydrogen	Michael Borchers, Institute for Chemical Technology and Polymer Chemistry
2:05 p.m.	Break	
2:35 p.m.	Poster Session: Lightning Round	
3:20 p.m.	Break	
3:30 p.m.	Poster Session: Room Discussion	
4:15 p.m.	End of third day sessions	

AGENDA

THURSDAY, SEPTEMBER 16, 2021

11:00 a.m.	Welcome and Introduction	
11:05 a.m.	Comparison of Pd/LTA and Pd/SSZ-13 as Passive NO _x Adsorbers (PNA)	Louise Olsson, Chalmers University of Technology
11:30 a.m.	Single Atom Ru on CeO ₂ : Effective and Stable PNA/RNA Material	Janos Szanyi, Pacific Northwest National Laboratory
11:55 a.m.	Pd-dilution Approaches for Highly Efficient Passive NO _x Adsorbers	Pranaw Kunal, Oak Ridge National Laboratory
12:20 p.m.	Break	
12:50 p.m.	Analytical Models for Particulate Filter Backpressure Prediction	Tim Watling, Johnson Matthey
1:15 p.m.	Investigation of Diesel Particulate Filter Design Parameters to Improve Filtration Performance under Various Test Cycles	Zhuqi Wang, NGK Automotive Ceramics USA
1:40 p.m.	Impact of Catalyst Zoning and Permeability on performance of a Diesel Oxidation Catalyst Filter Through Device Scale Modeling	Ken Rappe Pacific Northwest National Laboratory
2:05 p.m.	Break	
2:35 p.m.	Degradation Modes on Diesel Oxidation Catalysts	Rama Krishna Dadi, Cummins
3:00 p.m.	An Efficient Solution of Developing Reduced-order Models for Monolith Reactors with Dual-layered Washcoat and Micro-kinetics	Mingjie Tu, University of Houston
3:25 p.m.	Urea Water Solution Selective Catalyst Reduction Mixer Multi-objective Optimization	Mihai Chiruta, Cummins Emission Solutions
3:50 p.m.	End of fourth day session	

AGENDA

FRIDAY, SEPTEMBER 17, 2021

11:00 a.m.	Welcome and Introduction	
11:05 a.m.	Invited Presentation: The Reduction Half Cycle in the Low-T NH ₃ -SCR of NO _x over Cu-CHA Catalysts: Transient Kinetic Analysis and Mechanistic Study	Enrico Tronconi, Politecnico di Milano
11:55 a.m.	Temperature Dependence of Oxidation and Reduction Kinetics during NO _x Selective Catalytic Reduction with NH ₃ on Cu-Chabazite Zeolites	Siddarth Krishna, Purdue University
12:20 p.m.	Break	
12:50 p.m.	Development of Coupled Models for NH ₃ Capacity and SCR on Cu-SSZ-13 at Various Aging Conditions and Temperatures	Austin Ladshaw, Oak Ridge National Laboratory
1:15 p.m.	Multi-scale Modeling Approach to the Nature of Active Sites for a Vanadium-based SCR Catalyst NH ₃ Adsorption Studies	Andres Felipe Suarez Corredor, Scania CV AB, and Chalmers University of Technology
1:40 p.m.	A Comparative Study between Real-world and Accelerated Lab Aging of Cu/SSZ-13 SCR Catalysts	Feng Gao, Pacific Northwest National Laboratory
2:05 p.m.	Break	
2:35 p.m.	Impact of Field Aging on the Redox Half Cycles of NH ₃ -Selective Catalytic NO _x Reduction over a Commercial Cu-SSZ-13 Monolith Catalyst	Dhruba Jyoti Deka, Oak Ridge National Laboratory
3:00 p.m.	Kinetic Model for NH ₃ Solvation, Reduction and Re-oxidation of Active Copper Sites in Cu-SSZ-13 as a function of Hydrothermal Aging	Rohil Daya, Cummins Inc.
3:25 p.m.	Aging of Cu-exchanged Zeolite SCR Catalysts under Lean, Stoichiometric, and Rich Gas Compositions Relevant to Gasoline Applications	Calvin Thomas, Oak Ridge National Laboratory
3:50 p.m.	The Role of the Oxide Component in Hybrid Ceria-manganese Oxide/Cu-SSZ-13 Catalysts in Low-temperature Selective Catalytic Reduction of NO _x by Ammonia via Transient Experiments	Tahrizi Andana, Pacific Northwest National Laboratory
4:15 p.m.	End of fifth day sessions	

POSTER SESSION

WEDNESDAY, SEPTEMBER 15, 2021

SELECTIVE CATALYTIC REDUCTION #1	
Clarification of the NO _x Chemistry and Mechanism of No Reduction with Ammonia (SCR) on Zeolite Catalysts	Konstantin Khivantsev, Pacific Northwest National Laboratory
Influence of ZCuOH, Z ₂ Cu, and Extra Framework Cu _x O _y Species in Cu-SSZ-13 on N ₂ O Formation during the Selective Catalytic Reduction of NO _x with NH ₃	Arthur Shih, Purdue University/Leiden University
SELECTIVE CATALYTIC REDUCTION #2	
How Cu-SSZ-13 Oxidation Activity Affects the Extent of Sulfur Poisoning	Yu-Ren Chen, University of Virginia
Catalytic Urea Decomposition at Low Temperature for NH ₃ -SCR	Lai Wei, University of Virginia
Kinetic Modeling of Hydrothermal Aging on Cu-SSZ-13 for NH ₃ -SCR	Lai Wei, University of Virginia
Insights into the Impacts of Palladium on the SCR and AMOX Performance over Cu/SSZ-13 Catalyst	Yiqing Wu, Pacific Northwest National Laboratory
LOW TEMPERATURE TRAPS	
Understanding the Role of Reaction Conditions and Zeolite Properties on Cation Speciation and Interconversion Between Cations and Nanoparticles in Pd/Zeolites	Keka Mandal, University of Virginia
Effects of Pd Particle Size and Water Pressure on the Structural Transformation of Pd Nanoparticles to Mononuclear Pd(II) Cations in CHA Zeolites	Trevor Lardinois, Purdue University
THREE-WAY CATALYSTS AND METHANE OXIDATION CATALYSTS	
Approaches to Integrating Catalytic Aerogel Materials into Three-way Catalytic Converters	Bradford Bruno, Union College
Investigating the Effects of SO ₂ on Pt-Pd + Mn _{0.5} Fe _{2.5} O ₂ Spinel Dual Layer Catalysts during Lean/Rich Cycling Conditions for Emission Control in Natural Gas Engines	Natalia Diaz Monrenegro, University of Virginia
Rh Catalyst Structural Changes during CO Oxidation	Silvia Marino, University of Virginia
OXIDATION CATALYSTS AND SYSTEMS	
Improved Low Temperature CH ₄ Oxidation over Pd/H-LTA with Si/Al > 8	Tala Mon, University at Buffalo
Fuel Source and Catalyst Aging Effects on N ₂ O Formation in a Diesel Oxidation Catalyst	Carlos Weiler, University of Virginia; Dr. Epling's Lab
An Exhaust Catalyst Simulator (ExhCatSim)	Zhiming Gao, Oak Ridge National Laboratory

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