

# 6<sup>th</sup> International Flame Chemistry Workshop

## Expertise for Changing Times

August 15<sup>th</sup> – August 19<sup>th</sup>, 2022

### Day 1: Low-temperature oxidation

Session Chair and Discussion Leader: Brandon Rotavera

- 6:30-6:45 Login
- 6:45-6:50 Nils Hansen (Sandia)
- 6:50-7:05 *Recent progress of autoxidation chemistry by advanced mass spectrometry*  
Zhandong Wang (USTC Hefei)
- 7:05-7:20 *Underestimated concentration of ketohydroperoxides in n-butane low-temperature oxidation by the SVUV-PIMS diagnosis: a theoretical study on the photoionization cross section*  
Feng Zhang (USTC Hefei)
- 7:20-7:35 *Exploring the highly oxygenated intermediates formation in alkylcyclohexanes cool flame chemistry: Unraveling the structure effects and chemical mechanisms*  
Jiabiao Zou (KAUST)
- 7:40-7:55 *Chemical kinetics of cyclic ether species profiles*  
Nicholas Dewey (University of Georgia)
- 7:55-8:10 *Time-resolved quantification of ROO, OOQOOH, KHP in dimethyl ether oxidation*  
David Couch (Sandia)
- 8:10-8:25 *Systematically Derived Thermodynamic Properties for Alkane Oxidation*  
Sarah Elliott (Argonne)
- 8:25-9:00 Discussions

### Day 2: Theory and Uncertainty in Mechanism Development

Session Chair and Discussion Leader: Mani Sarathy

- 6:45-7:00 Login
- 7:00-7:15 *Automated calculation of prompt effects in kinetic mechanisms using statistical models: the case of butene flame chemistry*  
Luna Pratali Maffei (Politecnico di Milano)
- 7:15-7:30 *OptEx: An integrated experimental design and data clustering framework for combustion kinetic model optimization*  
Bin Yang (Tsinghua University)
- 7:30-7:45 *Generation of hybrid chemistry models by parameter optimization using indirect experiments*  
Torsten Methling (DLR)

- 7:50-8:05 *Laminar flame speed predictions using artificial neural networks and its comparison with detailed chemical kinetic mechanisms*  
Shashank Sakleshpur Nagaraja (KAUST)
- 8:05-8:20 *Comparison of the performance of ethylene combustion mechanisms based on large number of indirect measurements*  
Boyang Su (ELTE Eotvos Lorand University)
- 8:20-8:35 *Adaptive Dimension Reduction of Parameter Space in Uncertainty Quantification of Reaction Mechanism*  
Chengcheng Liu (Tsinghua University)
- 8:35-9:00 Discussions

### **Day 3: Particle Growth: Nanoparticles and PAHs**

*Session Chair and Discussion Leader: Bin Yang*

- 6:30-6:45 Login
- 6:45-7:00 *Gas-Phase Kinetics of Silanes and Siloxanes*  
Sebastian Peukert (University of Duisburg-Essen)
- 7:00-7:15 *Unraveling combustion chemistry of silicon-based flame synthesis precursors: Insight into similarities and differences from hydrocarbon counterparts*  
Yuyang Li (Shanghai Jiao Tong University)
- 7:15-7:30 *Elementary chemistry of siloxanes and silanols: challenges and opportunities*  
Robert Tranter (Argonne)
- 7:30-7:45 *Reactions of the Precursors for the Spray-Flame Synthesis of Nanoparticles in Partial Spray Evaporation*  
Munko Gonchikhyapov (University of Paderborn)
- 7:45-8:00 Discussions
- 8:00-8:15 *The unique chemistry of aromatic  $\pi$ -diradical soot precursors*  
Jacob Martin (Curtin University)
- 8:15-8:30 *Competition between unimolecular/bimolecular reactions of allylic radicals and their relevance in flames*  
Jaeyoung Cho (Argonne)
- 8:30-8:45 *A detailed kinetic model for aromatics formation from small hydrocarbon and gasoline surrogate fuel combustion*  
Raymond Langer (RWTH Aachen)
- 8:45-9:00 Discussions

#### Day 4: Nitrogen Chemistry

Session Chair and Discussion Leader: Raghu Sivaramakrishnan

- 6:45-7:00 Login
- 7:00-7:15 *Investigating Amine Oxidation with Computational Chemistry and Photoionization Mass Spectrometry: Insight into the Reactivity of C-centered and N-centered Radicals*  
Sommer Johansen (Sandia)
- 7:15-7:30 *An experimental and modeling work on the oxidation of ammonia-based fuel blends at intermediate temperatures and atmospheric pressure*  
Xiaoyu He (PTB)
- 7:30-7:45 *Plasma Assisted Ammonia Combustion - An Exploration*  
Wenting Sun (Georgia Tech)
- 7:50-8:05 *Probing the Gas-phase Kinetics of HTPB Composite Propellants Combustion: A High-level Theoretical Study*  
Yang Li (Northwestern Polytechnical University, China)
- 8:05-8:20 *Shock tube measurements of chemical weapon simulants at high temperature*  
Ramees Khaleel Rahman (UCF)
- 8:20-9:00 Discussions

#### Day 5: Multi-Physics Phenomena

Session Chair and Discussion Leader: Wenting Sun

- 6:45-7:00 Login
- 7:00-7:15 *Pulsed discharges development in chemically active media*  
Andrey Starikovskiy (Princeton University)
- 7:15-7:30 *Kinetic Studies of Excited Singlet Oxygen Atom O(1D) Reactions with Dimethyl Ether*  
Hongtao Zhong (Princeton University)
- 7:30-7:45 *Experimental and Computational Studies of Supercritical Combustion Chemistry of Low-Carbon Gaseous Fuels*  
Hao Zhao (Peking University)
- 7:50-8:05 *Low-Temperature Plasma-Assisted Chemical Looping Combustion, kinetic insights into methane oxidation with NiO vs. CuO*  
Christopher Burger (Princeton University)
- 8:05-8:20 *Low-temperature reforming of biomass tar into syngas using highly active catalysts*  
Jie Ren (USTC)
- 8:20-8:35 *Theoretical and experimental study of Li-ion battery thermal runaway*  
Peng Zhao (Tennessee)
- 8:35-9:00 Discussions