**Program**

**4th International Workshop on Flame Chemistry**

[www.princeton.edu/~yju/4th\_flame\_chemistry\_workshop.html](http://www.princeton.edu/~yju/4th_flame_chemistry_workshop.html)

**July 28th + 29th 2018, Trinity College Dublin, Ireland**

**Saturday, July 28th 2018**

8:00-8:30 am Registration + Breakfast

8:30-8.35 am Welcome: N. Hansen

**Session 1: Collisional and Transport Effects**

Chair: Nicole Labbe (University of Colorado Boulder, USA)

Invited Talk:

8:35-9:00 am *Collision parameters for alcohols, peroxides, and highly-branched hydrocarbons*

Ahren Jasper (Argonne National Laboratory, USA)

Contributed Talks:

9:00-9:15 am *H2O and CO2 kinetic effect on C/H sub-mechanisms in diluted combustion*

Pino Sabia (Instituto di Ricerche sulla Combustione, IRC-CNR, Naples, Italy)

9:15-9:30 am *Multi-component reactive pressure-dependent chemistry*

Mike Burke (Columbia University, USA)

9:30-10:00 am Discussions

10:00-10:30 am Coffee Break

**Session 2: PAH and Soot Formation (a joint session with the ISF workshop)**

10:30-10:50 am *What is current knowledge in PAH chemistry - Mechanism point of view: Understanding PAH chemistry: challenges for mechanism development*

Tiziano Faravelli (Politecnico di Milano, Italy)

10:50-11:10 am *What is current knowledge in PAH chemistry - Elementary reaction point of view* Stephen Klippenstein, Argonne National Laboratory, USA

11:10-11:30 am *Potential validation experiments*

Nils Hansen, Sandia National Laboratories, USA

11:30-12:30 pm Discussions

12:30-14:00 pm Lunch Break

**Session 3: Large Scale Computing and a priori Mechanism Generation**

Chair: Phil Westmoreland (North Carolina State University, USA)

Invited Talks:

14:00-14:25 pm *Automation of rate constant calculation: status and perspectives*

Carlo Cavalotti (Politecnico di Milano, Italy)

Contributed Talks:

14:25-14:40 pm *Automated reaction mechanism construction: Overview & current status*

Mengjie Liu (Massachusetts Institute of Technology, USA)

14:40-14:55 pm *Building large and accurate kinetic models using Genesys*

Ruben van de Vijver (Sandia National Laboratories, USA)

14:55-15:10 pm *Comparing the results and performance of chemical kinetic modeling software*

Raymond Langer (RWTH Aachen, Germany)

15:10-15:25 pm *Experimental and comparative modeling study of high temperature and very high pressure cyclohexane, methylcyclohexane, and 6-bromo-1-hexene pyrolysis*

Kenneth Brezinsky (University of Illinois Chicago, USA)

15:25-15:40 pm *ChemConnect2: Cloud-based repository of inter-linked combustion data backed with chemical knowledge*

Edward Blurock (Lund, Sweden)

15:40-16:10 pm Discussions

15:55-16:20 pm Coffee Break

**Session 4: Warm Flame and Plasma- and Ozone-assisted Combustion Chemistry**

Chair: Frederique Battin-Leclerc (CNRS Nancy, France)

Invited Talk:

16:20-16:45 pm *Warm flames and HO2 chemistry*

Yiguang Ju (Princeton University, USA)

Contributed Talks:

16:45-17:00 pm *Ozone-assisted ethylene oxidation at low-temperatures*

Aric Rousso (Princeton University, USA)

17:00-17:15 pm *Highly oxidized products from rapid alkane autoxidation*

Zhandong Wang (KAUST, Saudi Arabia)

17:15-17:45 pm Discussion

18:00-20:00 pm Dinner

**Sunday, July 31st 2016**

8:00-8:30 am Registration + Breakfast

**Session 5: Transformative Experimental Tools**

Chair: Kenneth Brezinsky (University of Illinois Chicago, USA)

Invited Talk:

8:30-8:55 am *Absorption diagnostics for chemical kinetic studies*

Aamir Farooq (KAUST, Saudi Arabia)

Contributed Talks:

8:55-9:10 am *A high-pressure, turbulent flow reactor for autoignition chemistry research*

Yi Yang (University of Melbourne, Australia)

9:10-9:25 am  *Shock Tube imaging of flame propagation at variable temperature and pressure*

Alison Ferris (Stanford University, USA)

9:25-9:40 am *Detection of intermediates formed in the oxidation of fuels using cavity ring-down spectroscopy*

Olivier Herbinet (CNRS Nancy, France)

9:40-9:55 am *X-ray diagnostics for flames: from fields to particles*

Robert Tranter (Argonne National Laboratory, USA)

9:55-10:10 am *Flame-sampling mass spectrometry for the investigation of PAH formation*

Lena Ruwe (Bielefeld University, Germany)

10:10-10:40 am Discussions

10:40-11:00 am Coffee Break

**Session 6: Combustion Chemistry at Low-Temperatures**

Chair: Matteo Pelucchi (Politecnico di Milano, Italy)

Invited:

11:00-11:25 am *Low-temperature chemistry of oxygenated molecules, what do we know?*

Zeynep Serinyel (CNRS Orleans, France)

Contributed Talks:

11:25-11:40 am *The kinetics influencing the propensity of n-butanol and its blends with a gasoline surrogate to knock and super knock*

Alison Tomlin (Leeds University, Great Britain)

11:40-11:55 am *Revisiting the autoignition mechanisms of hydrocarbons and oxygenated fuels*

Zhandong Wang (KAUST, Saudi Arabia)

11:55 am-12:10 pm *Using mechanism generators to probe THF combustion chemistry*

Phil Westmoreland (North Carolina State University, USA)

12:10-12:25 pm *Autoignition in IC engines*

Peng Zhao (Oakland University, USA)

12:25-12:40 pm *A critical evaluation of rate constants for syngas combustion kinetics*

Ultan Burke (NUI Galway, Ireland)

12:40-13:10 pm Discussions

13:10-13:15 pm Final Discussions/Conclusions

13:15 pm Adjourn