

# COMBUSTION WEBINAR

## *Advances in Theoretical Chemical Kinetics for Combustion*

**Speaker:** Dr. Stephen Klippenstein, Argonne National Lab

**Time:** Feb. 20<sup>th</sup> 2021

*10 am EST; 4 pm Paris; 11 pm Beijing.*

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COMBUSTION  
WEBINAR



**Biography:** Stephen Klippenstein received a B.Sc. from Univ. of British Columbia in 1983 and a Ph.D. from Caltech in 1988, working under the direction of R. A. Marcus (of electron transfer and RRKM theory fame). Currently, he is a Distinguished Fellow at Argonne National Lab. He is a Combustion Fellow, an APS Fellow, and was awarded the Zeldovich Gold Medal by the Combustion Institute in 2018, and the Polanyi Medal by the Gas Kinetics Group of the Faraday Division of the Royal Society of Chemistry in 2020. His research focusses on the development and application of high accuracy methods for predicting the kinetics and dynamics of gas phase reactions. He has developed transition state theory methods, master equation methods for connecting microscopic dynamics to the phenomenological rate coefficients required for kinetic modelling, and kinetic and dynamic treatments for prompt and roaming reactions.

**Abstract:** Chemical models for combustion commonly rely on tens of thousands of parameters describing the transport, thermochemistry, and kinetics for all the species involved in the transformation from fuel to products and pollutants. We will survey a number of recent advances in theoretical kinetics aimed at improving the accuracy of the data that underpins these models. A variety of topics will be briefly touched upon including: (i) automation of high-level theoretical procedures in order to increase the volume of high accuracy data produced, (ii) methods for improving the accuracy of predicted heats of formation, (iii) methods for predicting partition functions, (iii) a new simple physical model for predicting tunneling, (iv) the master equation and well-merging, (v) the role of stereochemistry, (vi) energy transfer and the 2-dimensional master equation, and (vii) non-thermal reaction kinetics. Illustrative examples of the significance of these theoretical advances will be provided throughout the talk.



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