# Combining Multiscale Physics and Data to Enable Predictive Modeling of Complex Reacting Systems in Energy, Propulsion, and the Environment

***Michael P. Burke***
*Columbia University*

## Monday, March 14th, 2022
## 12:30 PM

## MAE Special Seminar Series

**Understanding and being able to predict the outcomes of complex reaction systems would be invaluable to varied scientific and engineering disciplines – ranging from enabling future energy, aerospace, and chemical processing technologies to understanding the Earth's climate and the potential origins of life beyond Earth. Yet, unraveling and making predictions of complex reaction systems are notoriously challenging tasks. I outline an overall approach that overcomes those challenges by combining (1) ab initio computational studies of historically missing physics and chemistry, (2) data-driven modeling that integrates data and physics from multiple scales, and (3) optimal design of experiments and theoretical calculations. I will then highlight one of these three elements in depth, focusing on our ab initio theoretical studies of non-equilibrium phenomena induced by reactions in combustion and propulsion and by photons in the Earth's atmosphere – both of which feature vibrationally excited reactants relevant to "vibrational ladder climbing" in plasmas. Finally, I will describe how these theoretical calculations, in general, can be combined with experimental data via multiscale data-driven modeling and, more broadly, how automation of our overall approach can create "robotic scientific communities" capable of autonomous scientific inquiry and self-improving simulations of reacting systems.**

**Michael P. Burke is an Associate Professor of Mechanical Engineering at Columbia University, where he also holds affiliate appointments in Chemical Engineering and the Data Science Institute. Prior to joining Columbia in 2014, Burke earned his Ph.D. in Mechanical and Aerospace Engineering in 2011 at Princeton University, where he was a Wallace Memorial Honorific Fellow, and he worked as a Director's Postdoctoral Fellow in the Chemical Sciences and Engineering Division at Argonne National Laboratory. Burke is a recipient of the National Science Foundation's CAREER award, the Combustion Institute's Research Excellence Award, the Combustion Institute's Hiroshi Tsuji Early Career Researcher Award, and the American Chemical Society's PRF Doctoral New Investigator Award. His publications have been featured in the "News and Views" section of Nature Chemistry, selected as the Feature Article in Combustion and Flame, and chosen for the Distinguished Paper Award at the 31st International Symposium on Combustion.**

PRINCETON
Mechanical & Aerospace Engineering