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Wednesday, October 16th, 2019
Clarion Hotel, 60 Cottontail Ln, Somerset, NJ 08873

Professor Srinivas Rangarajan

Department of Chemical & Biomolecular Engineering
Lehigh University

Developing kinetic models to elucidate the mechanism of large and complex catalytic systems

Heterogeneous catalysis is a prominent means to upgrade carbon sources to chemicals and energy carriers. Designing an “optimal” catalyst is an open multi-faceted problem requiring analysis and decision making at multiple levels – from understanding molecular events to elucidating complex reaction mechanisms, identifying suitable catalysts, and optimizing reactor performance. My research, in this context, brings disparate yet complementary computational tools from systems engineering, informatics, and ab initio computational chemistry for detailed modeling and design of heterogeneous catalytic processes.

In this talk, I will focus on some of these facets. Several catalytic processes tend to be complex in that the underlying reaction system comprises of several hundred to thousands of species and reactions, thereby precluding a manual analysis that is comprehensive and error-free. Therefore, first, I will present our rule-based computational tool, Rule Input Network Generator (RING), to construct and analyze the mechanism of such complex reaction networks. RING can construct an exhaustive network of all plausible reactions and species of a system and identify reaction pathways forming a specific product through rule-based queries and "prune" out energetically infeasible pathways. I will demonstrate the utility of this tool through examples involving mechanism identification in polyol conversion over transition metals. Designing optimal catalysts require mathematical tools to identify catalytic parameters in conjunction with inputs from (and feedback to) experiments and computational chemistry. Therefore, in the second part, I will present new methods that leverage nonlinear optimization to rigorously identify active sites and surface environment of catalysts under working conditions using statistically validated models. Finally, I will present ongoing activity in my group to bridge these two facets of research, through concepts such as active machine learning, optimization, and Bayesian inference.

Speaker Bio:

Srinivas is a P.C. Rossin Assistant Professor in the Department of Chemical & Biomolecular Engineering at Lehigh University, Bethlehem, PA. He previously was a postdoctoral research scholar working with Profs. Manos Mavrikakis and Christos Maravelias. He obtained his PhD in Chemical Engineering at the University of Minnesota in 2013 under the supervision of Profs. Prodromos Daoutidis and Aditya Bhan. Srinivas is originally from India and did his undergraduate studies at the Indian Institute of Technology, Madras. His research interests include complex network analysis, microkinetic modeling, computational heterogeneous catalysis, and applications of machine learning and optimization in reaction mechanism discovery and modeling. His research has been recognized with the ACS Petroleum Research Fund Doctoral New Investigator Award and the AIChE CAST division's David Smith Jr Graduate Publication Award.

Dinner is a buffet, and includes		Members	**$40**
a choice of beef, chicken or fish		Non-members	**$50**
Social Hour (Cash Bar)	6:00 PM	Students	**$25** (***Student Members*** **= $10**)
Dinner	7:00 PM	Retired/Post-Doc/Unemp.	**$40** (***Members*** **= $30**)
Presentation	7:45 PM	Annual Membership Dues	**$35 (*Students* = $15)**

Deadline for dinner reservations is **4:00 p.m. Friday, October 11th, 2019**

To make your reservation, fill out the online form. With the exception of extreme circumstances, anyone not canceling reservations by the above deadline will be billed for dinner regardless of attendance.

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