CATALYSIS CLUB OF PHILADELPHIA
Promoting Catalytic Science and Technologies

Catalysis Club of Philadelphia

7pm, Thursday, May 7th, 2020

Virtual Monthly Meeting

Skype link shared after registration

Speaker: Prof. Srinivas Rangarajan

Lehigh University, Chemical and Biomolecular Engineering

Next-generation mechanistic modeling techniques for complex catalytic reaction networks

Officer Election Results

Vote here

Meeting Schedule:
Meeting .....7:00 PM

Meeting Fees:
Free to all who register

Menu
What is in your fridge!

Meeting etiquette
Please remember to mute your microphone and arrive early to solve any technical issues

Online registration – Please register online by **Wednesday, *May 6th*** at http://catalysisclubphilly.org/webinar-registration/ or notify or Chair Jacob Dickinson (Jacob.G.Dickinson@dupont.com)

A Skype meeting invite will be provided on May 7 to all those who register.

Membership - Dues for the 2019-20 season will be $25.00 ($5.00 for the local chapter and $20.00 for the national club). Dues for students, post-docs and retirees will be $10.00 ($5.00 for local club and $5.00 for national club).

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Prof. Srinivas Rangarajan

Next-generation mechanistic modeling techniques for complex catalytic reaction networks

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Abstract: Several catalytic processes tend to be complex in that the underlying reaction system comprises of several hundred to thousands of species and reactions. Building and analyzing such reaction networks manually is cumbersome and error-prone. Further, developing detailed mechanistic models, as is done routinely for small reaction systems, is computationally intractable. Research in my group focuses on developing scalable techniques to study such complex reaction networks.

In this talk, I will present a 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. Using polyol conversion as an example, I will demonstrate how RING can be used, in a near-automated fashion, to obtain compact microkinetic models that are consistent with experiments.