

SPONSORS

GOLD

JOHNSON MATTHEY
PQ CORP/ZEOLYST

SILVER

HEL INC

Officers

CHAIR

Anton Petushkov
Zeolyst International

CHAIR-ELECT

Josh Pacheco
Zeolyst International

PAST CHAIR

Torren Carlson
DuPont

TREASURER

Lifeng Wang
Zeolyst International

SECRETARY

Dan Slanac
DuPont

PROGRAM CHAIR

Istvan Halasz
PQ Corp.

ARRANGEMENTS CHAIR

Tzia Ming

DIRECTOR, SPONSORSHIP

Thomas Yeh
Johnson Matthey

DIRECTOR, STUDENT POSTER

Eric Sacia
DuPont

DIRECTOR, MEMBERSHIP

Jacob Dickinson
DuPont

WEBMASTER

Carl Menning
Sentry Data Systems

NATIONAL REPRESENTATIVE

Dion Vlachos
University of Delaware

Catalysis Club of Philadelphia

Thursday, November 10th, 2016

DoubleTree Hotel

4727 Concord Pike Wilmington, DE 19803

Annual CCP Student Poster Contest

And

Professor Ravindra Datta: Unraveling Catalytic Mechanisms and Kinetics: Lessons from Electrical Networks

Fuel Cell Center, Department of Chemical Engineering, Worcester
Polytechnic Institute, Worcester, MA 01609

Social Hour: 5:30 PM

Dinner: 6:30 PM

Meeting: 7:30 PM

Members: \$35.00

Walk Ins & Non-members: \$40.00

Students & Retired Members: \$20.00

Menu (served as a buffet)*

**Selection of 3 entrees: 1) Grilled flank
steak, 2) blood orange salmon, and 3)
vegetable lasagna**

**Buffet also comes with a classic Caesar
salad and a sesame ginger salad, rolls
and butter, chef's choice of desserts,
coffee, tea, iced tea, decaf, and water.*

Meal reservations – Please register
online by **Friday, November 4th** at

[http://catalysisclubphilly.org/
program/meeting-registration/](http://catalysisclubphilly.org/program/meeting-registration/) or

notify your company representative
or our Arrangements Chair Tzia
Ming (tonn@seas.upenn.edu)

Membership - Dues for the 2016-17
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).

Catalysis Club of Philadelphia

Thursday, November 10th, 2016

DoubleTree Hotel

4727 Concord Pike Wilmington, DE 19803



Unraveling Catalytic Mechanisms and Kinetics: Lessons from Electrical Networks

Professor Ravindra Datta

Fuel Cell Center, Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609

Abstract

Catalytic reaction networks, in general, comprise of multiple steps and pathways. While one can now readily predict kinetics of these molecular steps from first principles, there is not yet available a comprehensive framework for: 1) visualizing and analyzing these reaction networks in their full complexity; and 2) unequivocally identifying the germane steps and pathways.

Thus, we have developed an approach called the “Reaction Route (RR) Graph” approach, which allows: 1) direct enumeration of all the pathways as walks on the RR Graph; 2) thermodynamic consistence of step kinetics; 3) elucidation of dominant pathways that contribute materially to the overall flux; 4) identification of bottleneck steps in each of these pathways; and 5) development of explicit rate laws based on the electrical analogy.

The electrical network analogy is based on two aspects of RR Graphs, namely: 1) quasi-steady state (QSS) mass balance of intermediate species, the equivalent of the Kirchhoff’s Current Law (KCL) of electrical circuits; and 2) Hess’s law, or thermodynamic consistence, the equivalent of the Kirchhoff’s Potential Law (KPL), which makes RR Graphs precisely equivalent to electrical networks. Further, we define the step resistance in terms of step kinetics to make the analogy complete. The approach is described with the help of the water-gas shift example.

Biography

Ravi Datta is Professor of Chemical Engineering and Director of WPI Fuel Cell Center. He obtained his Ph.D. degree from the University of California, Santa Barbara, in 1981. From then until 1998, he was a Professor of Chemical Engineering at the University of Iowa, when he moved to WPI, and served as Chemical Engineering Department Head until 2005. Ravi’s research is focused on catalytic and electrocatalytic reaction engineering of Clean Energy, including, fuel cells, hydrogen, renewable fuels, novel catalysts, and catalytic reaction networks. He is a coauthor of 150 papers and 8 patents, and has been a mentor to 25 doctoral students.