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Catalysis Club of Philadelphia

Thursday, September 15th, 2016

DoubleTree Hotel

4727 Concord Pike Wilmington, DE 19803

CCP Awardee: Dion Vlachos

In Silico Prediction of Materials for Energy Applications

*Elizabeth Inez Kelley Professor of Chemical & Biomolecular Engineering and
Professor of Physics at the University of Delaware; Director of the Catalysis
Center for Energy Innovation (CCEI)*

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*

Vegetable Lasagna

Airline Breast of Chicken – white wine sauce, lump crab imperial and baby vegetables

Mushroom Stuffed Flank Steak – local Kennett Square mushroom medley roasted with goat cheese and herbs, rosemary whipped potatoes, sautéed green beans, and sherry reduction

**All dinners served with a salad, rolls and butter, chef's choice of desserts, coffee, tea, iced tea, decaf, and water.*

Meal reservations – Please register online by **Friday, Sept. 9th** at

<http://catalysisclubphilly.org/>

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

notify your company representative or Treasurer

(Lifeng.wang@pqccorp.com) or Chair

(anton.petushkov@pcorp.com)

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).

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In Silico Prediction of Materials for Energy Applications



Dion Vlachos

Elizabeth Inez Kelley Professor of Chemical & Biomolecular Engineering and Professor of Physics at the University of Delaware; Director of the Catalysis Center for Energy Innovation (CCEI)

Abstract

In this talk, the need for new materials in various energy domains will be discussed. Multiscale simulation will then briefly be introduced as an enabling technology to address diverse engineering topics. A specific application of multiscale simulation is the prediction of macroscopic behavior from first principles. A more impactful avenue of research is how one could use multiscale modeling in reverse engineering for predicting new materials for production of energy and chemicals and energy storage. We will demonstrate how descriptor-based modeling can enable such a search of novel materials with emergent behavior and assess this framework with experiments. An outstanding question is how reliable and robust are model predictions in comparing to data and our quest for searching new materials. We will demonstrate this methodology for the specific example of ammonia decomposition for hydrogen production for fuel cells and briefly touch upon renewable chemicals and fuels from lignocellulosic biomass.

Speaker Bio

catalysisclubphilly.org

Dionisios (Dion) G. Vlachos is the Elizabeth Inez Kelley Professor of Chemical & Biomolecular Engineering and Professor of Physics at the University of Delaware and the Director of the Catalysis Center for Energy Innovation (CCEI), an Energy Frontier Research Center (EFRC) funded by the Department of Energy (DOE). He obtained a five-year diploma in Chemical Engineering from the National Technical University of Athens, Greece in 1987, his M.S. and Ph.D. from the University of Minnesota in 1990 and 1992 respectively, and spent a postdoctoral year at the Army High Performance Computing Research Center in Minnesota. After that, Dr. Vlachos joined the University of Massachusetts as an assistant professor, was promoted to an associate professor in 1998 and joined the University of Delaware in 2000. He was a visiting fellow at Princeton University in the spring of 2000, a visiting faculty member at Thomas Jefferson University and Hospital in the spring of 2007 and the George Pierce Distinguished Professor of Chemical Engineering and Materials Science at the University of Minnesota in the fall of 2007.

Professor Vlachos is the recipient of the R. H. Wilhelm Award in Chemical Reaction Engineering from AIChE and is an AAAS Fellow. He also received a NSF Career Award and an Office of Naval Research Young Investigator Award. He is a member of AIChE, ACS, the Combustion Institute, MRS, the North American Catalysis Society (NACS) and the Society for Industrial and Applied Mathematics (SIAM).

Dr. Vlachos' main research thrust is multiscale modeling and simulation along with their application to catalysis, crystal growth, portable microchemical devices for power generation, production of renewable fuels and chemicals, catalyst informatics, detailed and reduced kinetic model development and process intensification. He is the corresponding author of more than 340 refereed publications with nearly 10,000 citations and has given over 200 plenary lectures, keynote lectures and other invited talks. Professor Vlachos has served as an executive editor of the Chemical Engineering Science journal and also served or currently serves on the editorial advisory board of ACS Catalysis, Reaction Chemistry & Engineering, Industrial and Engineering Chemistry Research, Applied Catalysis A: General, Proceedings of the Combustion Institute, the Open Energy and Fuels Journal, the Journal of Nano Energy and Power Research and the Journal of Chemical Engineering & Process Technology.