

## Catalysis Club of Philadelphia

Thursday October 15<sup>th</sup>, 2015

DoubleTree Hotel

4727 Concord Pike Wilmington, DE 19803

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## Engineering Molecular Transformations over Supported Metal Catalysts for the Sustainable Conversion of Biomass-Derived Intermediates to Chemicals and Fuels

Matthew Neurock

*Shell Professor of Chemical Engineering and Materials Science,*

*University of Minnesota, Minneapolis, MN.*

**Social Hour: 5:30 PM**

**Dinner: 6:30 PM**

**Meeting: 7:30 PM**

**Members: \$35.00**

**Walk Ins & Non-members: \$40.00**

**Student & Retired Members: \$20.00**

### *Menu\**

**Seared Yellow Fin Tuna** – (cucumber wasabi-teriyaki glaze, sautéed spinach with jasmine rice);

**Pesto Roasted Chicken Breast** – (sun-dried tomato risotto and sautéed broccolini);

**Grilled Vegetable Ravioli** – (grilled vegetables blended with ricotta, mozzarella, parmesan, fontina, and pecorino romano cheeses wrapped in basil pasta);

*\*All dinners served with wedge salad (Iceberg lettuce, applewood bacon, onions, grape tomatoes, chives, tarragon with blue cheese dressing), rolls and butter, chef's choice of desserts, coffee, tea, iced tea, decaf, and water.*

**Meal reservations** - Please notify your company representative or

Alex Mironenko ([alexmir@udel.edu](mailto:alexmir@udel.edu))

by **Thursday October 8<sup>th</sup>**, or register online:

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

**Membership** - Dues for the 2015-16 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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### Engineering Molecular Transformations over Supported Metal Catalysts for the Sustainable Conversion of Biomass-Derived Intermediates to Chemicals and Fuels



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Minneapolis, MN.*

Future strategies for energy production will undoubtedly require processes and materials that can efficiently convert sustainable resources such as biomass into fuels and chemicals. While nature's enzymes elegantly integrate highly active centers together with adaptive nanoscale environments to control the catalytic transformation of molecules to specific products, they are difficult to incorporate into large scale industrial processes and limited in terms of their stability. The design of more robust heterogeneous catalytic materials that can mimic enzyme behavior, however, has been hindered by our limited understanding of how such molecular transformations proceed over inorganic materials. The tremendous advances in ab initio theoretical methods, molecular simulations and high performance computing that have occurred over the past two decades provide unprecedented ability to track these transformations and how they proceed at specific sites and within particular environments. This information together with the unique abilities to follow such transformations spectroscopically is enabling the design of unique atomic surface ensembles and nanoscale reaction environment that can efficiently catalyze specific

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molecular transformations. This talk discusses recent advances in computational catalysis and their application to engineering molecular transformations for the conversion of biomass into chemicals and fuels. We will discuss the active sites, mechanisms and nanoscale reaction environments involved in specific bond making and breaking reactions important in the conversion of biomass-derived intermediates into chemicals and fuels and the design of 3D environments necessary to carry out such transformations.

