Catalysis Club of Philadelphia

Thursday November 15th, 2012
DoubleTree Hotel
4727 Concord Pike Wilmington, DE 19803

Designing and Probing Photovoltaic and Photocatalytic Materials

Jason B. Baxter
Department of Chemical and Biological Engineering
Drexel University

AND

A DFT study of the acid-catalyzed conversion of 2,5-dimethylfuran and ethylene to p-xylene

Nima Nikbin
Department of Chemical and Biomolecular Engineering
University of Delaware
(Student Talk, 15 minutes)

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

Chicken Marsala smothered with Sweet Mushroom Marsala, served with Creamy Risotto & Asparagus

Baseball Sirloin served with Pesto Whipped Potatoes, Baby Carrots & a Madeira Sauce

Vegetarian: Mediterranean Purse Roasted Vegetables, Cous Cous, Asiago Cheese Stuffed in a flakey Purse served with Ratatouille

Vegan: vegetable phyllo triangle, served with tomato relish.

Meal reservations - Please notify your company representative or Jacob Weiner (jlweiner@udel.edu, phone: 302.831.2213) by ***Thursday November 8th***.

Company Representatives – We would like to encourage you to make meal/meeting reservations to your company representative.

Membership - Dues for the 2012-13 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).

Designing and Probing Photovoltaic and Photocatalytic Materials

Jason B. Baxter
Department of Chemical and Biological Engineering
Drexel University, Philadelphia, PA

Abstract:
The sunlight incident on the earth provides 10,000 times more power than is needed to meet global demand. However, converting this energy into electricity or fuels efficiently and cost effectively remains a great challenge. Nanostructured solar cells present opportunities to inexpensively convert sunlight to electricity through the use of architectures tailored on the nanometer to micrometer length scale. Planar solar cells are subject to opposing constraints where thick films are required for light absorption while thinner films are desirable for efficient charge separation. Extremely thin absorber (ETA) solar cells can decouple these constraints by using a thin absorber at the interface between highly structured p- and n-type layers. In this talk, I will describe our work on ETA solar cells that use a thin CdSe coating on a ZnO nanowire array to absorb light and inject electrons into the oxide. Rational design of these architectures requires control over morphology and microstructure of the materials, as well as knowledge of material properties such as photoexcited carrier lifetimes and mobilities. Our approach utilizes a combination of solar cell measurements and ultrafast transient absorption spectroscopy to understand the effects of CdSe thickness, annealing conditions, and interfacial treatments on the dynamics and efficiency of charge carrier separation, and ultimately on the solar-to-electric energy conversion efficiency. These studies provide guidelines for architecture design and materials selection for ETA solar cells.

Speaker Bio:
Jason B. Baxter is an Assistant Professor in the Department of Chemical and Biological Engineering at Drexel University in Philadelphia, PA, where he began in 2007. He received his B.S. from the University of Delaware in 2000 and his Ph.D. from the University of California Santa Barbara in 2005, both in chemical engineering. From 2005-2007, he was an ACS Alternative Energy Postdoctoral Fellow at Yale University. His research interests are in designing and fabricating semiconductor nanomaterials for solar energy conversion and in understanding ultrafast photophysics in these systems. He received the NSF CAREER Award in 2009.

A DFT study of the acid-catalyzed conversion of 2,5-dimethylfuran and ethylene to p-xylene

Nima Nikbin
Department of Chemical and Biomolecular Engineering
University of Delaware, Newark, DE
(Student Talk, 15 minutes)

Abstract:
In this paper we present the detailed mechanism for the conversion of DMF and ethylene to p-xylene. The mechanism was calculated by gas-phase DFT (Density-Functional Theory) for the uncatalyzed, the Brønsted acid-catalyzed and the Lewis acid-catalyzed reaction. The conversion consists of Diels-Alder cycloaddition and subsequent dehydration of the cycloadduct, an oxa-norbornene derivative. Even though the DMF-ethylene cycloaddition is thermally feasible, we find that Lewis acids can further lower the activation barriers by decreasing the HOMO-LUMO gap of the addends. The catalytic effect may be significant or negligible depending on whether the Diels-Alder reaction proceeds in the normal or the inverse electron-demand direction. We find that Brønsted acids are extremely effective at catalyzing the dehydration of the oxa-norbornene derivative, which, according to our calculations, cannot proceed uncatalyzed. On the other hand, we find that Brønsted acids do not catalyze the cycloaddition. Although strong Lewis acids like Li^+ can catalyze the dehydration, our calculations indicate that relatively elevated temperatures would be required as they are not as effective as Brønsted acids. We argue that the specific synthetic route to p-xylene is kinetically limited by the Diels-Alder reaction when Brønsted acids are used and by the dehydration when a Lewis acid is used, with the latter being slower than the former. Finally, we adduce experimental data that corroborate the theoretical predictions: we observe no activity in the absence of a catalyst and a higher turnover frequency to p-xylene in the Brønsted acidic zeolite HY than in the Lewis acidic zeolite NaY.