Professor Pinjing Zhao  
North Dakota State University

Nickel-Mediated Alkyne and Amine Transformations for Greener Catalysis

Alkynes and amines are ubiquitous small-molecule building blocks in modern chemical synthesis. In particular, their diverse interactions with transition metal complexes make them attractive targets in metal-catalyzed transformations. In this presentation Dr. Zhao will describe his group’s recent studies on nickel-mediated stoichiometric and catalytic transformations of alkynes and amines towards synthetic applications. Compared to existing methods using precious metal-based catalysts, these new catalytic reactions provide distinctive benefits of using earth-abundant nickel catalyst, high atom efficiency, and significantly reduced energy inputs that contribute to the advancement of green chemistry. The unique features of current catalytic systems are attributed to novel reaction pathways via ligand-enabled nickel interactions with alkyne and amine molecules for selective and low-energy substrate activations.

4:00 PM – Bruggeman Conf. Rm. - Biotech Building  
(Refreshments at 3:45 PM)
Modeling the electrochemical double layer:

Challenges and new approaches.

Kathleen Schwarz
National Institute of Standards and Technology
Rockville, Maryland

Abstract Globally, significant resources are consumed by the seemingly disparate challenges of controlling metal deposition, electrocatalysis, and corrosion. These problems seem particularly unrelated when considering their differing economic drivers and technical needs. However, despite the specific differences between these challenges, all of them are fundamentally driven by the same need for prediction and control of electron and ion transfer reactions at charged, heterogeneous interfaces. These reactions can strongly depend on the interfacial properties due to local electric fields and solvation effects. Characterizing these interfacial properties, the properties of the electrochemical double layer, remains a significant open problem for computational electrochemistry. In this talk, I will describe how we have developed and benchmarked improved continuum models for the electrochemical double layer, with the most promising of these models implemented in our open-source and freely accessible software package, JDFTx. Specifically, I will describe our progress towards the development of continuum solvation models that capture the correct magnitude and voltage-dependence of the capacitance of the double layer. I will then illustrate how we have applied these models to investigate formic acid oxidation reaction mechanisms and probe the capacitance behavior of metallic surfaces with surface adsorbates.
Biosketch: Dr. Schwarz received her bachelors in chemistry from Washington University in St. Louis, and her PhD in Chemistry at Cornell University. Following her PhD, she was a National Research Council Postdoctoral Associate at the National Institute of Standards and Technology (NIST). Dr. Schwarz is currently a Research Chemist at NIST. She is interested in developing and applying computational approaches to understand the properties of electrochemical interfaces.
DEPARTMENT OF CIVIL & ENVIRONMENTAL ENGINEERING

SEMINAR

“The Roles and Responsibilities of Future Engineers Towards Sustainability”

Wednesday, February 13, 2019

JROWL-2C14

1:00 – 2:00

Dr. Raphael Rodrigues

Research Professor

ABSTRACT:
The dynamic transformations our society is undergoing due to population growth and resources consumption is constantly questioning conventional Engineering practices. How can the next generation of engineers prepare themselves to break existing paradigms and include these variables in their projects? What is so-called "sustainable development" and how did this term become part of Engineering? This talk will take a global perspective, presenting the overlap of Environmental Engineering with other Engineering areas and it will also be open for debate and discussion.

BIO:
Prof. Raphael Rodrigues attended the University of Sao Paulo (USP), in Brazil, where he received his B.S. in Environmental Engineering graduating with Highest Honors in 2011. He subsequently started his Ph.D., focusing his research on advanced water treatment technologies using modified ultrafiltration membranes. His research results led him to a fellowship at Harvard School of Engineering and Applied Sciences in 2013. After returning to Brazil and finishing his Ph.D., Raphael joined the Faculty of USP for two years, being recognized as one of the most innovative professors of his department. Raphael also has experience as a technical auditor for Sao Paulo's Environmental Protection Agency and also as environmental consultant developing engineering projects such as wastewater treatment plants retrofit, water reuse, rainwater harvesting, and water treatment units.

Refreshments will be served
A Theoretical Study of Schwarzites and Linear Carbon

Pure carbon structures contain a wealth of information and potential properties, we focus on two, long linear carbon chains and Schwarzites. Long linear carbon chains, a one dimensional sp hybridized carbon chain, have been observed to be encapsulated by a carbon nanotube. Together this system produces a resonant Raman signal from 1770-1860 cm\(^{-1}\), known as the C-mode. The origin of this signal is still under scrutiny. We explore the nature of Raman activity in long linear carbon chains through the use of first principles density functional theory and identify the effect of exact exchange in calculations using hybrid functionals. With exact exchange the most intense Raman active mode, the longitudinal optical mode, converges, with respect to length, to 1831 cm\(^{-1}\), within the range of reported measurements of the C-mode. Also the electronic gap converges, with respect to length, to 1.8 eV, near the known resonance energy.

Schwarzites are sp\(^2\), or hexagonal, triply periodic minimal carbon surfaces with negative Gaussian curvature from the introduction of 7-, 8-, 9-, and 10-membered rings. Recently theoretical impregnation of zeolites, simulating the templating processes, has produced Schwarzites.

We present first principles and classical dynamics calculations of electronic and vibronic density of states calculations to establish a connection between the theoretical structures proposed to the experimentally obtained materials. We identify the theoretical structures as energetically and dynamically stable, graphitic in nature, and semimetallic.