## **OCTOBER 2010 NEWSLETTER**

The three hundred ninety second meeting of the American Chemical Society Susquehanna Valley Section will be held on Wednesday, October 13, 2010 in Mcgowan Center (third floor of the Bevevino Library) on the Misercordia University campus. The meeting will begin at 7:30 PM and will be preceded by dinner at 6:00 PM at Leggio's restaurant (formerly Pickett's Charge). The speaker will be Dr. Adriana Dinescu from Wilkes University.

# "From Transition Metal Chemistry to Molecular Simulation of Enzymes"

Dr. Adriana Dinescu Assistant Professor of Chemistry Wilkes University

Numerous enzymatic reactions are controlled by the chemistry of transition metals. The main reasons why transition metals are the essential constituent of many catalytic systems include their ability to stabilize diverse geometries, variable coordination numbers, a variety of ligand types, multiple oxidation states, and different spin states. While my previous work has been directed to enzyme dynamics and electronic properties of transition metal complexes, most recent interests lie in applying computational methods to examine reaction pathways for bio-inspired water gas shift reaction (WGSR). Carbon monoxide dehydrogenase catalyzes a similar reaction and its active site includes an unprecedented heterometal Cu-Mo cluster. I will present some of my work on transition metal chemistry, including electronic structure studies of biomimetic Cu-Mo complexes and their application to WGSR.

Adriana Dinescu received her B.Eng. in Chemistry from Polytechnic University of Bucharest in Romania. Working under the guidance of Tom Cundari, she received her Ph.D. in computational inorganic chemistry from the University of North Texas in 2007. Following postdoctoral work with Michael Benson and Aurora Clark at Idaho National Laboratory, she spent one year teaching general chemistry at Butler University in Indiana. Adriana Dinescu

joined the Chemistry Department at Wilkes University in 2009. Her research interests include modeling and simulation of bioinorganic systems and their applications to energy efficient catalysis.

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### **DINNER:**

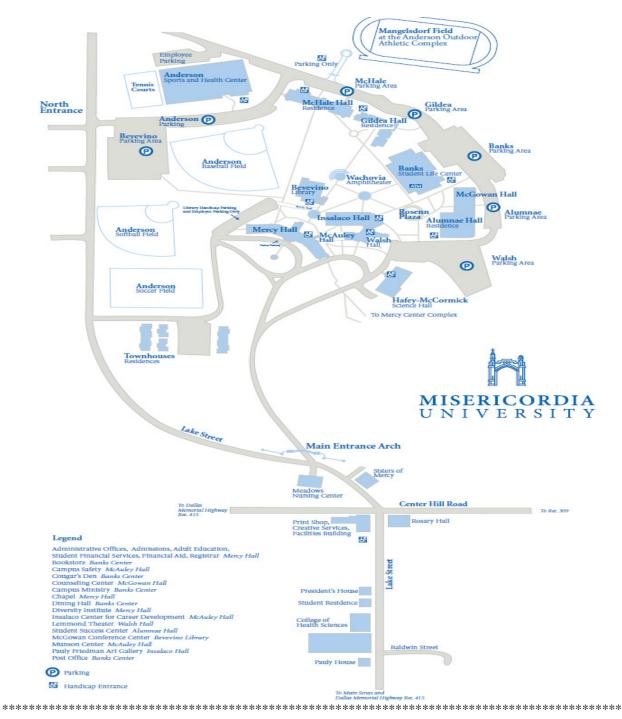
Dinner will be at Leggio's Restaurant (formerly Pickett's Charge, 1092 Route 315, Plains Township) at 6:00 PM., following cocktails at 5:30 PM. Ordering will be from the menu and RSVP should be to Helen Bogdon at 570-674-6378 or <a href="https://leggios315.com/">https://leggios315.com/</a>

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## **DIRECTIONS TO MISERICORDIA UNIVERSITY:**

#### From Route 80 East

Take exit 260 to Route 81 North. Take exit 170B Wilkes-Barre. Exit ramp merges with Route 309 North. Stay on 309 for 9 miles into Dallas. In Dallas, continue on Route 309 North. Where Route 309 veers toward the right (just past the Dallas Shopping Center), continue straight on Route 415 for 1/4 mile to the second light (stay in right lane). At this light, bear to the right onto Lake Street. Follow Lake Street for 1/2 mile, past Center Hill Road. The College entrance arch is on your right. Campus map can be found at <a href="http://misericordia.edu/directions/Map.pdf">http://misericordia.edu/directions/Map.pdf</a>.



#### **ACS Elections**

Ballots for President-Elect, 2011 were mailed on Sept. 24 to all ACS members eligible to vote as of Aug. 16. You may still vote by the traditional paper or online <a href="https://www.vres.us/webapps/vwr2035.pgm">https://www.vres.us/webapps/vwr2035.pgm</a> with your member account number and Personal PIN that were included in your ballot package. The voting deadline is November 12, 2010. Two candidates will vie for the office of president-elect of the American Chemical Society for 2011 in this fall's election. They are Luis A. Echegoyen, the Robert A. Welch Chair in Chemistry at the University of Texas, El Paso and Bassam Z. Shakhashiri, a professor of chemistry at the University of Wisconsin, Madison. Information regarding each of these candidates can be found at <a href="http://pubs.acs.org/cen/acsnews/88/8836electionC1.html">http://pubs.acs.org/cen/acsnews/88/8836electionC1.html</a> and <a href="http://pubs.acs.org/cen/acsnews/88/8836electionC2.html">http://pubs.acs.org/cen/acsnews/88/8836electionC2.html</a>, respectively. The successful candidate will serve as ACS president in 2012 and as a member of the ACS Board of Directors from 2011 to 2013.

Section Web Page: http://course.wilkes.edu/SusquehannaValleyACS/