The Twenty-Third Midwest Undergraduate Computational Chemistry Consortium (MU3C) Conference

July 28th-29th 2014
Iowa State University
Ames, IA

\[ \tilde{H}_{ab} = H^o + H'_{ab} + H''_{ab} \]

\[ + \frac{1}{2} \sum_{\gamma} \left[ \frac{H'_{a\gamma} H'_{b\gamma b}}{E_a^o - E_\gamma^o} + \frac{H'_{a\gamma} H'_{b\gamma b}}{E_b^o - E_\gamma^o} \right] \]

\[ \{\gamma\} \]

Official Conference Hotel: Fairfield Inn and Suites, Ames IA.
Monday 28 July 2014
9:00am Stacey Stoffregen, University of Wisconsin-River Falls
Welcome to the Twenty-Third MU3C Conference

9:05am Michael Esch, Grand Valley State University, Carbonmonoxy
Myoglobin Vibrational Frequency Investigation

9:30am Derek Saxon, Ripon College, Aluminum(III) Isopropoxide
Initiated Polymerization of Gluconolactone

9:55am Dalton Blood, Hope College, Parameterizing Fluorescent
Protein Chromophores for Molecular Dynamics Simulations

10:20am Nathan Vance, Hope College, High-Performance, Low-Cost
Computational Chemistry Infrastructure

10:40am Break

10:55am Richard Edwards Hope College, Using WebMO to Promote
Use of Computational Chemistry in Teaching and Research

11:20am Mark Gordon, Iowa State University, How to do Accurate
Calculations on "Real" Chemistry

12:10pm Lunch

1:30pm Chemistry Department Tour

2:30pm Klaus Ruedenberg, Iowa State University, Three Millennia of
Atoms, Molecules and Bonds, the Growth of Scientific Insights in the
Atomistic Structure of Matter

3:20pm Break

3:35pm John Dood, Hope College, Developing Ion Parameters Using
Shared GPU Accelerator Hardware

4:00pm Panel Discussion: Graduate Student Life and MU3C Faculty
Business Meeting

6:30pm Dinner at Aunt Maude’s, Ames IA

Tuesday 29 July 2014
9:00am Nathan Bamberger and Kit Pavlekovski, Carleton College,
Sodium and Carbon Dioxide Behavior within Al-Substituted Zeolites

9:40am Eliza Green, Carleton College, Manipulating Strong Bonds
through Transition metal-Element Cooperation: A DFT Study

10:05am Katie Blise, Carleton College, Organocatalysts for
Biorenewable Desymmetrization: A Quantum Mechanical Study

10:30am Brian Schumacher, Ripon College, Substitution Effects and
Enantioselectivity in Rhodium Catalyzed Intramolecular Hydroacylation

10:55am Break

11:10am Theresa Windus, Iowa State University, On the Way to High
Accuracy with Decreased Cost

12:00pm Lunch

1:20pm Xueyu Song, Iowa State University, Statistical Mechanics at
Iowa State Chemistry

2:10pm Caroline Kordes, Ripon College, Is Ketene an Intermediate in
the Addition of Imines to Azlactone to Form a Beta-Lactam?

2:35pm Panel Discussion: Faculty Positions at PUIs (Presenters:
Heriberto Hernandez, Amanda Jonsson, Samuel Keasler, Daniela
Kohen, Keith Kuwata, Christopher Lawrence, Will Polik, Joe Scanlon,
Justin Shorb, Jonathan Smith, Erin Speetzen, Stacey Stoffregen, Matt
Zwier)