Computational Chemistry

Jackson State University

G. Hill
J. Leszczynski
T. V. Shahbazyan
M.-J. Huang
J. D. Watts

University of Mississippi

S. Davis
R. J. Doerksen
J. Ritchie
G. Tschumper
R. M. Wadkins

University of Southern Mississippi

Y. Zhang

Goals

- Recruit and retain top notch faculty to assure critical mass of computational chemists for Mississippi to become a national leader in the computational sciences.

- Attract and train undergraduate, graduate and post doctoral students in state-of-the-art computational research

- Increase opportunities for underrepresented groups to participate in innovative computational chemistry research.

- Build a national and international presence in the computational sciences through the competitive research, involvement in editorial activities, organization of national and international meetings.

Strategies

- Investment in Human Capital – Hire faculty member at USM
- Provide challenging research projects and financial support for students and post-docs
- Involve minority students from high schools and small colleges in research projects
- Organize national and international collaboration
- Collaborate on organization of meetings and grant proposals
- Publish and edit books and international journals

Strategies: Advising and Mentoring

Success Story – Dr. Glake Hill

Yanov, I.; Palacios, J. J.; Hill, G.,
Journal of Physical Chemistry A, **2008,**
112, 2069-2073.

Crucial steps:

Recruitment to Computational Chemistry Summer Institute

Enrollment into Ph.D. Program - graduation

Award to attend 52nd Nobel Laureate Meeting

University of California Office of the President Post-Doctoral Award (one year at the UC Berkeley)

Faculty position at JSU

Collaboration with the former Ph.D. advisor on grant applications and research projects

NSF Career Award Application

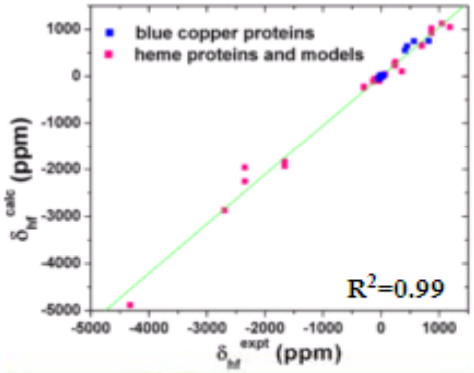
New Faculty Member at USM

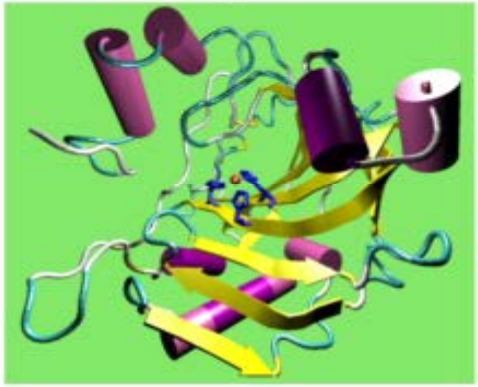
Welcome to Yong Zhang's Group

Computational, Biophysical, and Bioinorganic Chemistry

Assistant Professor, Department of Chemistry and Biochemistry

- Home





High Accuracy Calculations of Spectral Properties

- Predictions of NMR, EPR/ENDOR, Mössbauer properties
- Assistance in experimental spectra assignment
- Elucidation of unusual spectra, structures, and properties in biomolecules and molecular materials

Protein Structure Refinement and Determination

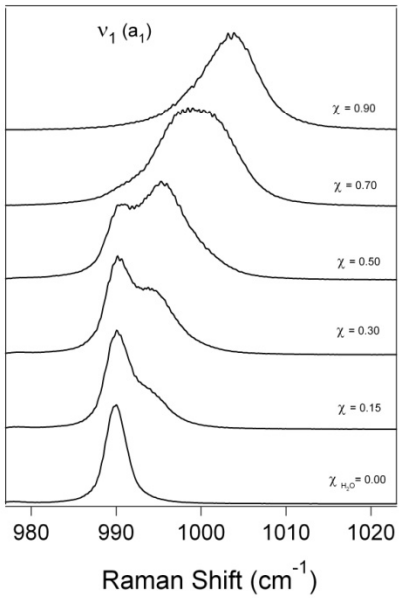
- Refinement of protein x-ray structures
- Development of high accuracy structure determination methods for use in solid and solution states, static and dynamic ways, *in vitro* and *in vivo*

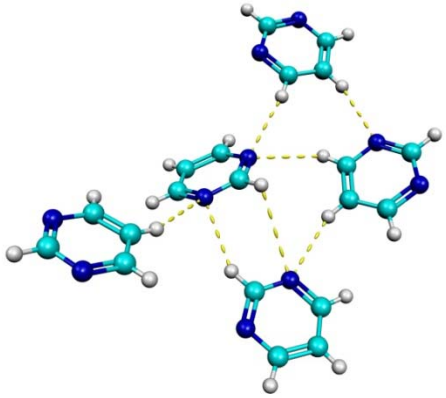
Metallobiomolecules in Cellular Regulation and Signaling and Human Diseases

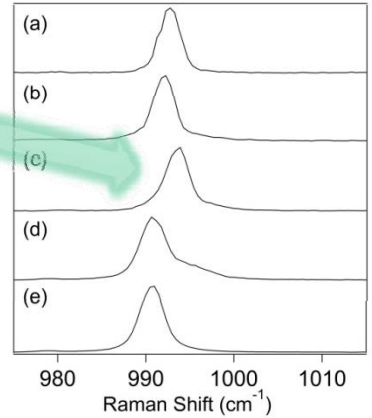
- Structure determination of metal sites
- Functional mechanism investigation of metals
- Applications to drug design

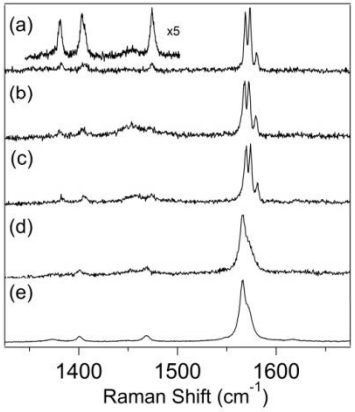
EPSCoR Start-ups at UM – Nathan Hammer, ‘06

Spectroscopic Studies of Noncovalent Interactions in Pyrimidine



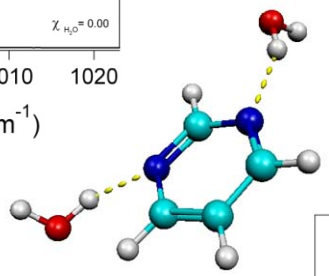




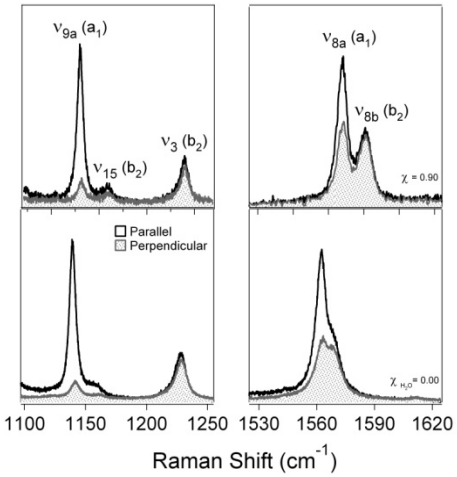


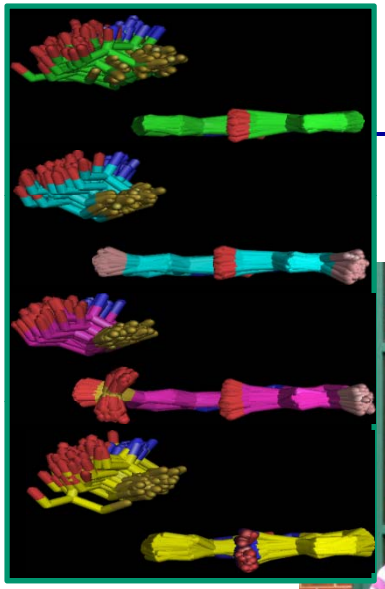
By blueshifting C-N and C-C stretching bands and probing the polarization state of the laser, we can assign ambiguous normal modes.

Compressing liquid pyrimidine induces a phase transition. The ring breathing mode experiences fluctuations due to new weak hydrogen bonds with neighboring pyrimidine molecules.



The ring breathing mode at 990 cm^{-1} blueshifts dramatically when interacting with water or other good hydrogen bond donors, indicating large fluctuations in electron density.



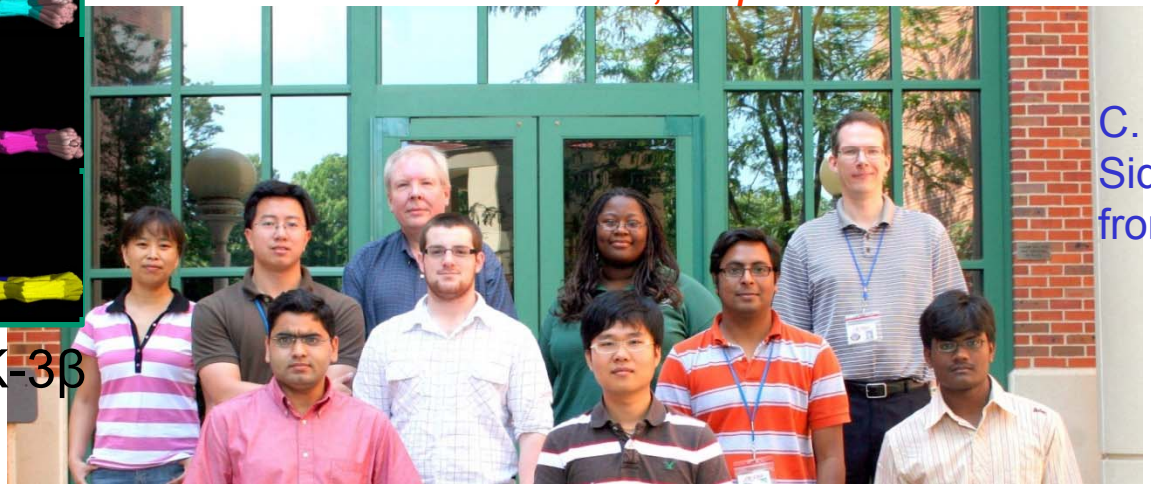


C171/GSK-3β

New Faculty Members at UM

Accurate Calculations of Protein-Ligand Interactions

Robert J. Doerksen, *Department of Medicinal Chemistry, UM*



C. Tim Rich (Instructor) & Sidney Govan (undergrad) from Rust College

- **S Prasanna**, PR Daga, A Xie and RJ Doerksen "Glycogen synthase kinase-3 inhibition by 3-anilino-4-phenylmaleimides: Insights from 3D-QSAR and docking," *Journal of Computer-Aided Molecular Design*, **23**, 113-127 (2009).
- **S Prasanna** and RJ Doerksen "Topological polar surface area: A useful QSAR descriptor. *Current Medicinal Chemistry*, **16**, 21-41 (2009).
- A Xie, **SR Clark**, **S Prasanna** and RJ Doerksen "3D quantitative structure–farnesyltransferase inhibition analysis for some diaminobenzophenones," *Journal of Enzyme Inhibition & Medicinal Chemistry*, **24**, yyy (2009).
- MA Ibrahim, AG Shilabin, **S Prasanna**, M Jacob, SI Khan, RJ Doerksen and MT Hamann "2-N-Methyl Modifications and SAR Studies of Manzamine A," *Bioorganic & Medicinal Chemistry*, **16**, 6702-6706 (2008).
- PR Daga and RJ Doerksen "Stereoelectronic Properties of Spiroquinazolinones in Differential PDE7 Inhibitory Activity," *Journal of Computational Chemistry*, **29**, 1945-1954 (2008).

- **P.R. Daga – NIH Pre-Dcotoral Fellowship recipient**
- **Blue: Supported in part by NSF EPSCoR**
- **Green: Undergraduate Researcher**

Group accomplishments for 2008-9

Books Edited	**2**
Special Journal Issues Edited	**2**
Organized Conferences	**2 (1 international co-organized)**
Book Chapters	**3**
Research Papers	**65**
Invited Talks	**18**
Conference Presentations	**Over 120**
Citations	**Over 1150**
Graduations	**4 Ph.D. (2 Afr. Am.)**

Group accomplishments for 2007-2009

Book Edited	**6**
Special Journal Issues Edited	**4**
Organized Conferences	**8 (4 international)**
Book Chapters	**6**
Research Papers	**148**
Invited Talks	**36**
Conference Presentations	**Over 250**
Citations	**Over 2300**
Graduations	**7 Ph.D. (4 Afr Am)**

High Profile Publications

April 14, 2009

D. M. Bates and G. S. Tschumper
J. Phys. Chem. A, **2009**, 113, 3555.
"CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures"

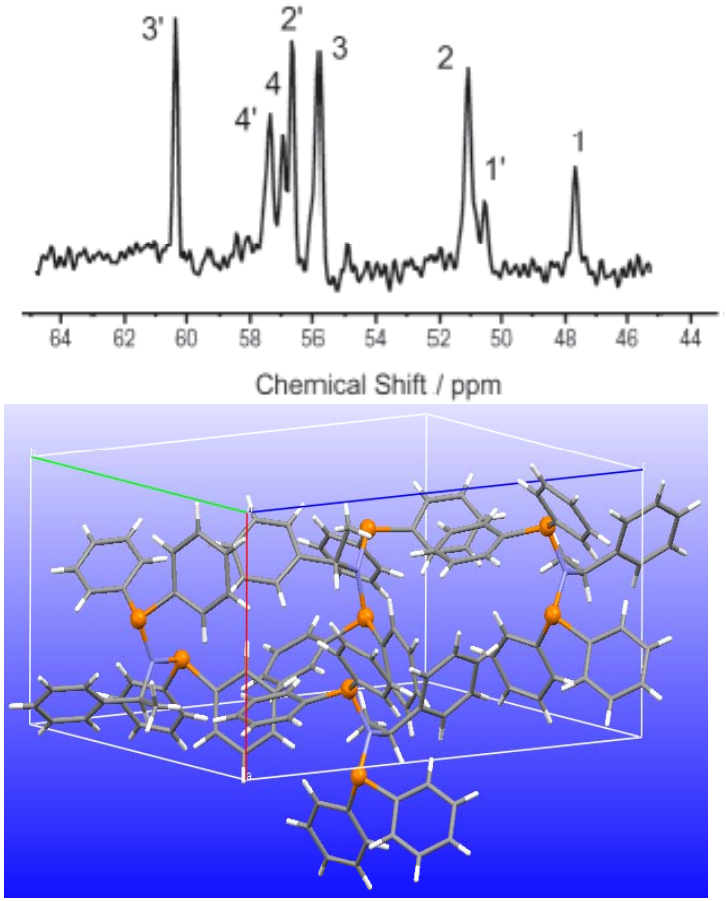
March 4, 2009

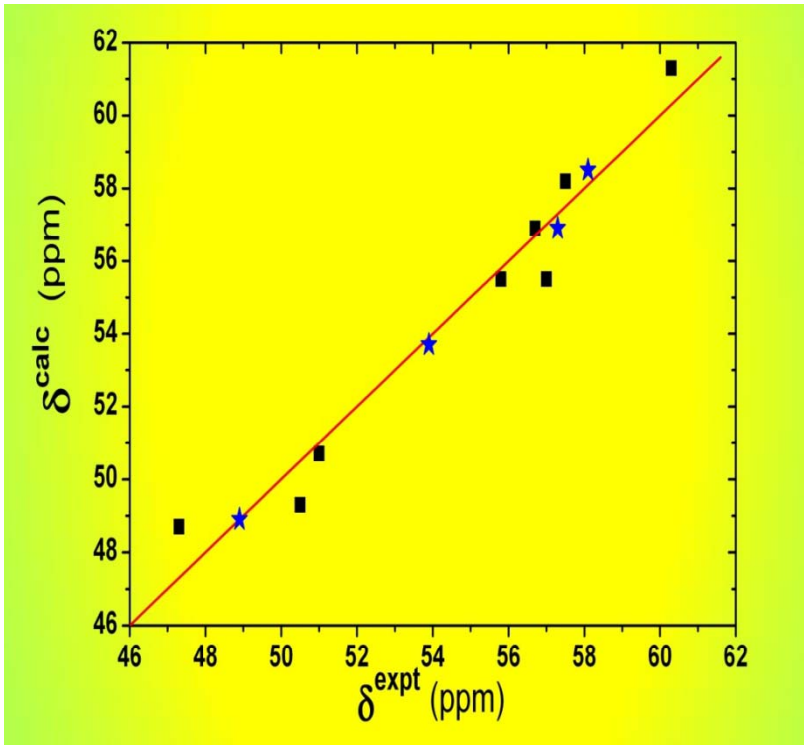
Zhang, X. and Wadkins, R.M., "DNA Hairpins Containing the Cytidine Analog Pyrrolo-dC: Structural, Thermodynamic, and Spectroscopic Studies." *Biophysical Journal 96*, 1884-1891 (**2009**).

High Profile Publications

Deciphering NMR fingerprints in a disordered solid

Cover Art in J. Phys. Chem. A





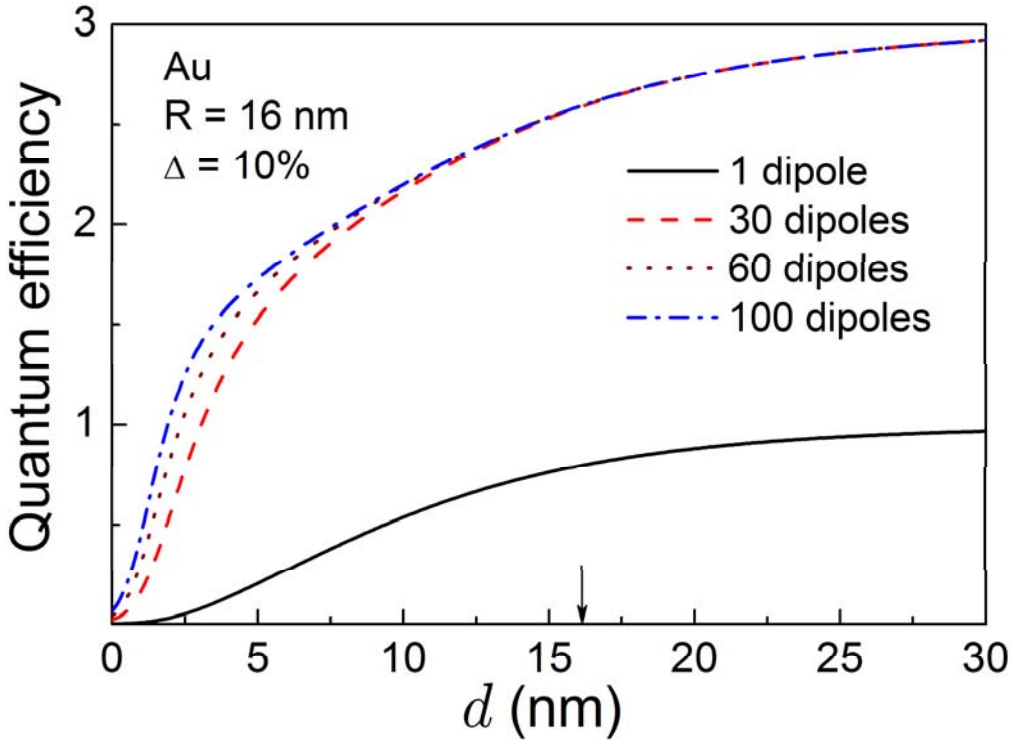
NMR shifts in disordered solid systems can now be understood

Y. Ling, Y. Zhang. *J. Phys. Chem. A,* in press (2009)

High Profile Publications

Cooperative emission of light by an ensemble of dipoles near a metal nanostucture: The plasmonic Dicke effect

V. N. Pustovit and T. V. Shahbazyan, Phys. Rev. Lett. 102, 077401 (2009)



There are *three* plasmonic super-radiant states participating in emission

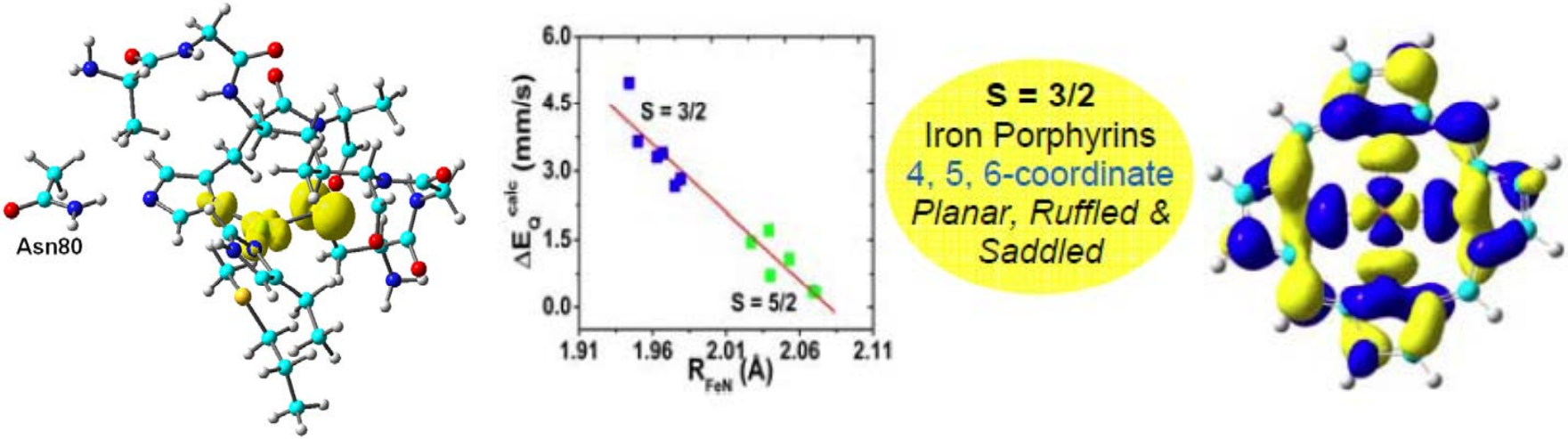
An ensemble radiates with the same power as just molecules near a NP

High Profile Publications

High accuracy protein structure determination

Y. Zhang, E. Oldfield. *J. Am. Chem. Soc.* 130, 3814-3823 (2008)

Y. Ling, Y. Zhang. *J. Am. Chem. Soc.* in press (2009)



We are currently developing the integrated quantum mechanics and spectroscopy (QMS) techniques that target an accuracy close to small molecule's x-ray structures with much broader applicability compare to x-ray crystallography. The examples show our recent work on the prototype electron transfer proteins (blue copper proteins) and heme protein models with intermediate spin states.

High Profile Award

CREST Interdisciplinary Center for Nanotoxicity (HRD-0833178)

INTERDISCIPLINARY CENTER *for* NANOTOXICITY

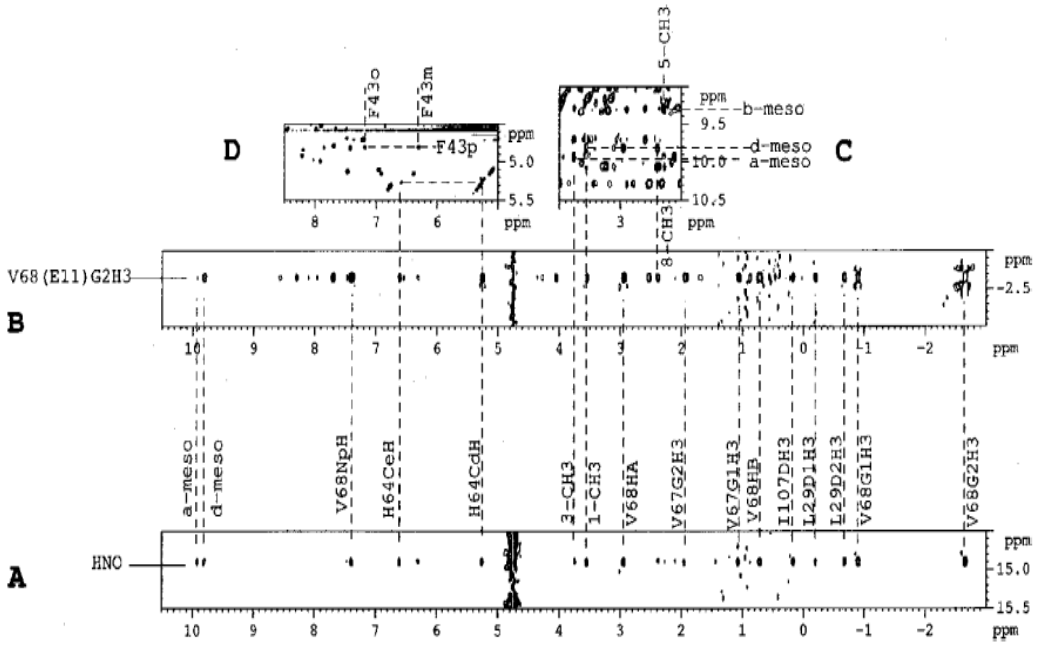
Integration of experimental and computational research

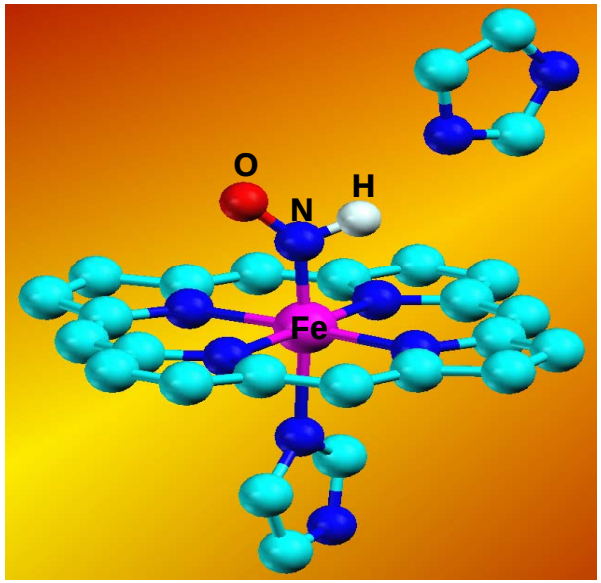
Training of minority students at both the undergraduate and graduate levels

Independent Competitive Award for New Faculty

Yong Zhang – USM
New NIH R15 grant GM-085774 (2008/7-2010/6)

HNO protein complexes and models: From spectra to structure

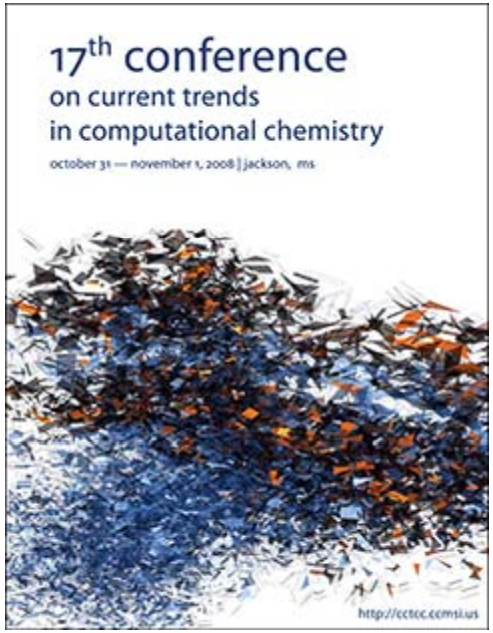




Education and Outreach

- Summer Institute in Computational Chemistry for undergraduate and graduate students
- Computational Chemistry Seminar Series
- Two series of annual conferences (regional/international)
- 1st Annual Mississippi Biophysical Consortium Meeting – co-organized
- Regional Graduate Student Recruiting from Underrepresented Groups – Prairie View and Texas Woman's University
- Chair – Region 7 Mississippi Science Fair Review Committee – 650 students

Meetings Organized




Abstracts should be formatted according to the following requirements:

- A4 paper format;
- 2 cm horizontal and vertical margins;
- single-spaced text;
- 12pt Times-family font;
- affiliation of each author should be clearly indicated using lower-case letters in superscripts (a, b, c etc.);
- presenting author name should be underlined.

Conference venue

Located in the center of the Ukraine, Kyiv has a lot to offer to visitors, and the weather in July is usually favorable for sightseeing. Kyiv is the capital of Ukraine with a population about 3 million. Convenient and good-quality accommodation is available in hotels with different prices. Kyiv has direct air, train and bus connection with a number of countries. Please participate in the brief survey at the registration page helping the Organizing Committee to form the set of excursion trips by Kyiv. At the moment, no visa is required for citizens of USA, EU and NIS countries.

Contacts

Dr. Oleg Zhikol, Conference Secretary
SSI "Institute for Single Crystals" National Academy of Sciences of Ukraine
E-mail: ualcc@xray.isc.kharkov.com
Phone: +38(057)341-02-58
Information about the Symposium http://xray.isc.kharkov.com/MACC-2

Important date

Registration and abstract submission deadline 1 May 2007


Methods and Applications of Computational Chemistry

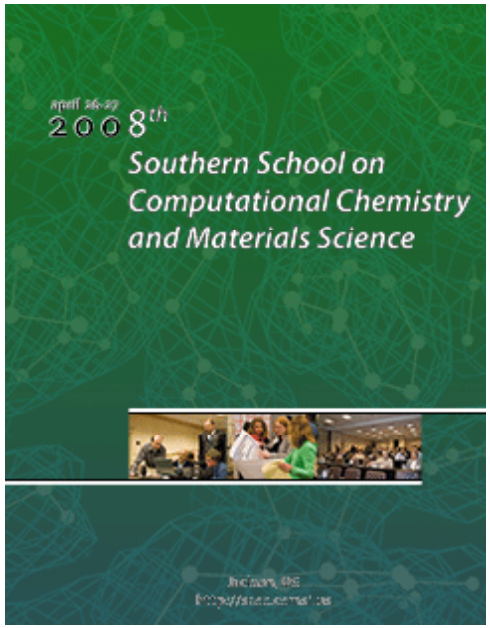
Second International Symposium

MACC-2

2 - 4 July 2007
Kyiv, Ukraine

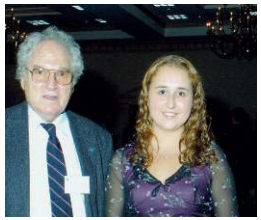
First circular and call for abstracts

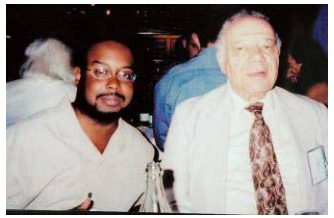
http://xray.isc.kharkov.com/MACC-2
http://ual.ccmsi.us/conference.html




Dr. W. Kohn

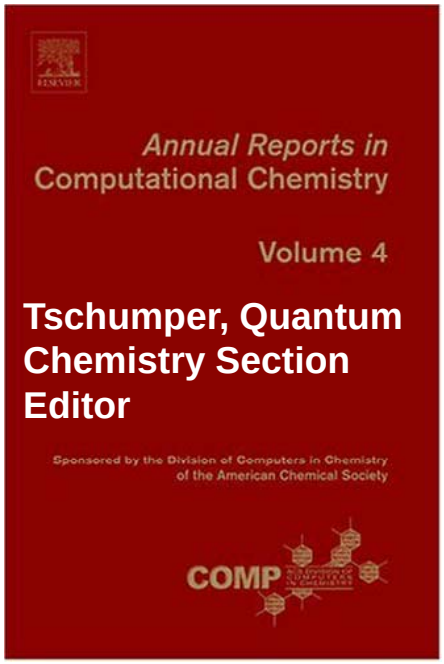

Dr. J.A. Pople


Dr. H. Hauptman

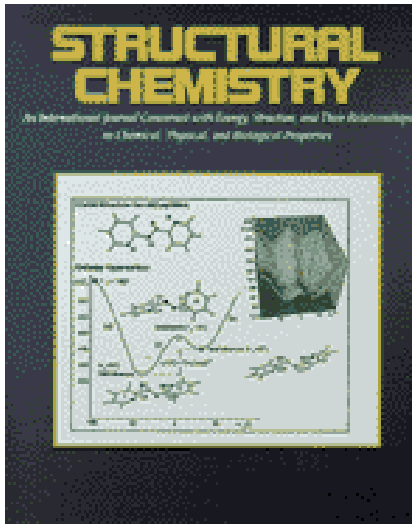

Dr. J. Karle

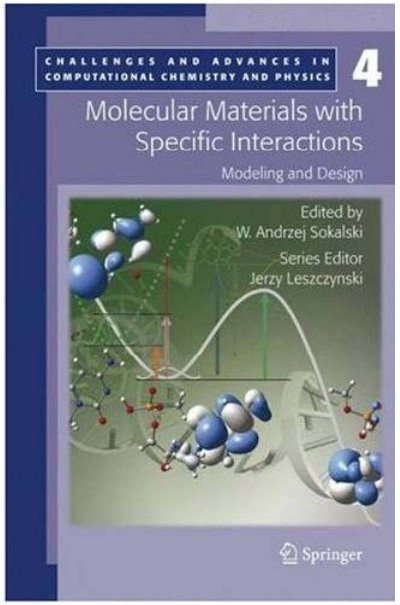

Dr. R. Curl

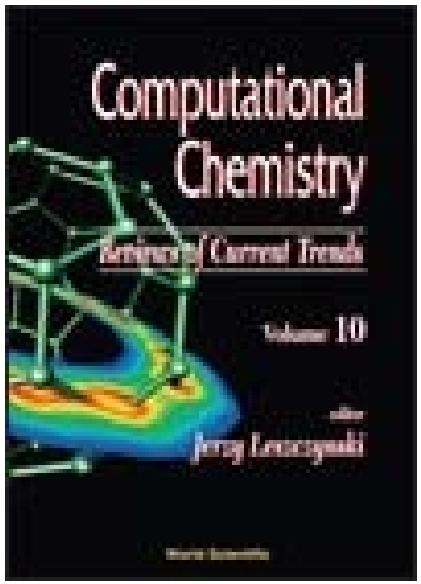
Edited Books, Journals & Special Journal Issues

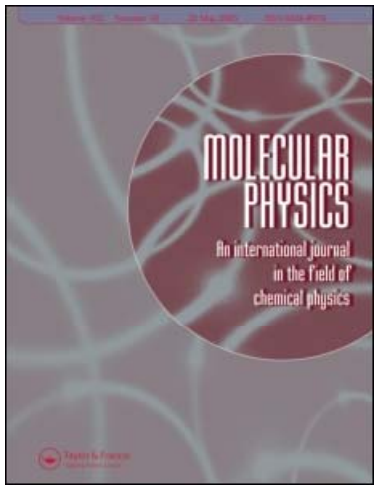


Leszczynski,Editor

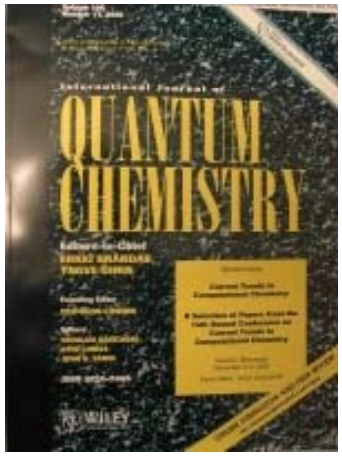








Molecular Physics, Volume 104 Issue 13 & 14 2006. A Special Issue in Honour of Professor Andrzej Sadlej



Volume 109 Issue 1 – 2009
Special Issue: 16th Annual Conference on Current Trends in Computational Chemistry

Volume 107 Issue 12 - 2007
Special Issue: 15th Annual Conference on Current Trends in Computational Chemistry

Summer Institutes

CCMSI Summer Institute

Every year CCMSI offers a summer institute (June 8-July 31 in 2009). This program is open to all graduate and undergraduate students interested in Computational Chemistry. The objective of the Institute is to teach students quantum and computational chemistry as well as general research skills. Institute's participants will also engage in research projects with the CCMSI faculty.

2007	*Participants*	*Talks*	*Posters*
Southern School	120	23	85
Current Trends	225	14	161
Summer Institute	14	14	

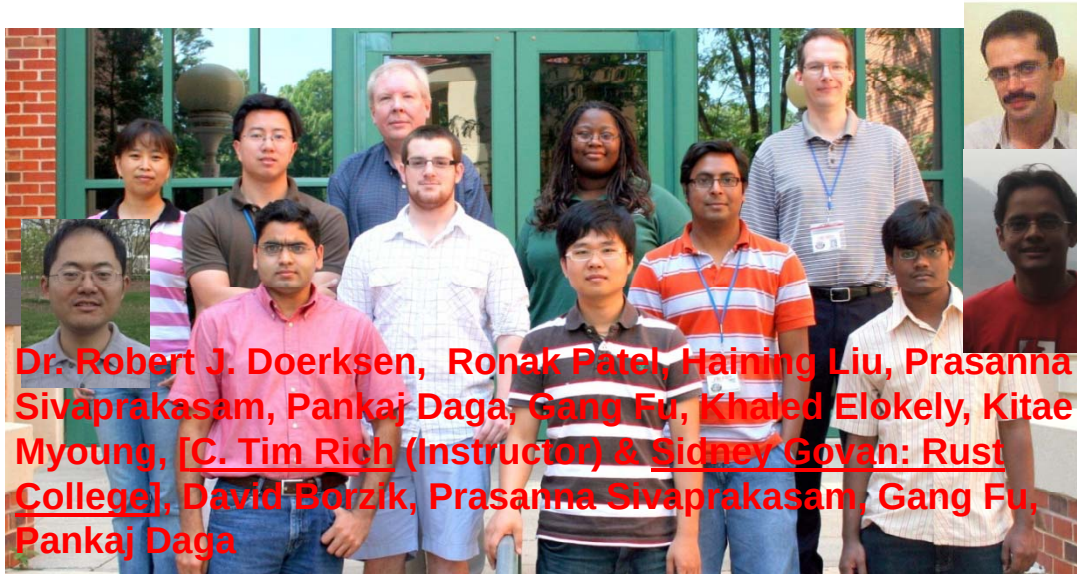
2008	*Participants*	*Talks*	*Posters*
Southern School	125	25	70
Current Trends	180	14	150
Summer Institute	15	15	

Research Groups - OUTREACH

Back Row (L to R): Coleman Howard and Ann Elizabeth Miller
Middle Row: Desiree Bates and Dr. Gregory S. Tschumper
Front Row: Kari Copeland, Bei Cao, Ginger Tipton and Brittney Smith

(L to R): **Chengjun Sun** (poster), Dr. Jason Ritchie, Larico Treadwell (@ NOBCChE conf.), Tayo Bolujon, **Ben Yancey** (poster) Brandi Ashmore

(L-R) Ashley Wright, Debra Jo Scardino, Jacob Graham, Austin Howard, Dr. Nathan Hammer



Dr. Robert J. Doerksen, Ronak Patel, Haining Liu, Prasanna Sivaprakasam, Pankaj Daga, Gang Fu, Khaled Elokely, Kitae Myoung, [C. Tim Rich (Instructor) & Sidney Govan: Rust College], David Borzik, Prasanna Sivaprakasam, Gang Fu, Pankaj Daga

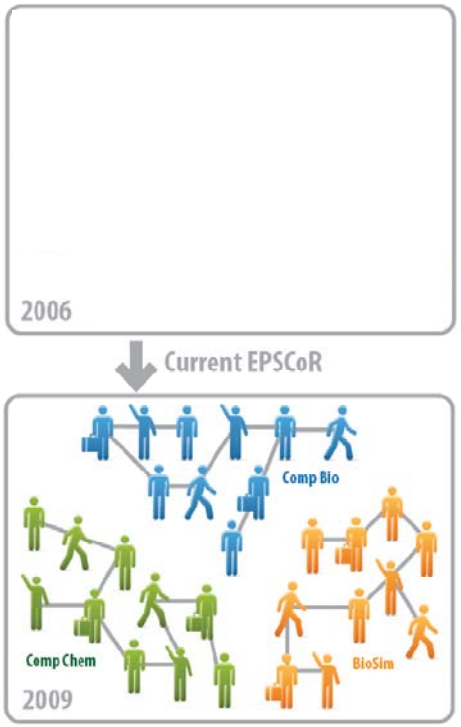
Research Groups - OUTREACH

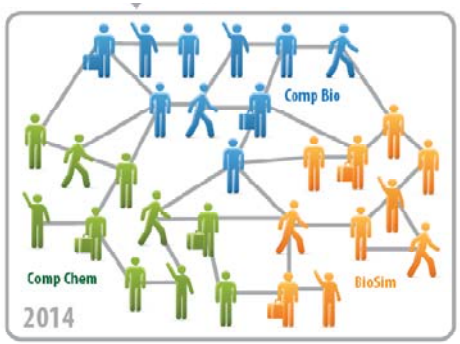
Selected Cumulative Computational Chemistry Group Highlights for 2006-2009

- Over 200 publications in peer-reviewed, high-impact journals.
- Multiple articles in high-tier journals (e.g. J. Am. Chem. Soc., Phys. Rev. Lett.).
- Several articles by group members have been selected as journal issue covers.
- Funding of new NSF CREST center: Interdisciplinary Nanotoxicity Center (4 of 5 projects involve CCG members).
- NIH support obtained by at least 2 CCG members.
- 7 Ph.D.s awarded in the area of computational chemistry (4 African American).
- New computational chemistry graduate course.

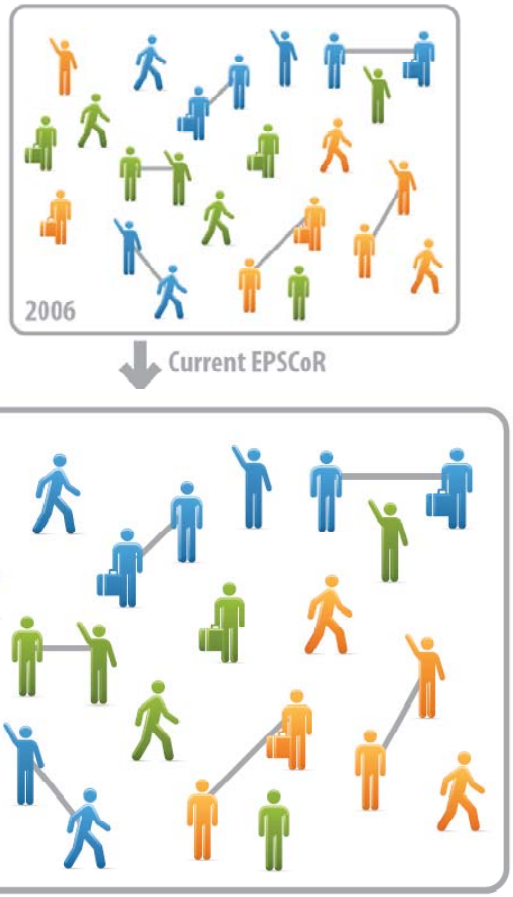
Past, Present, Future

CompBio and BioSim



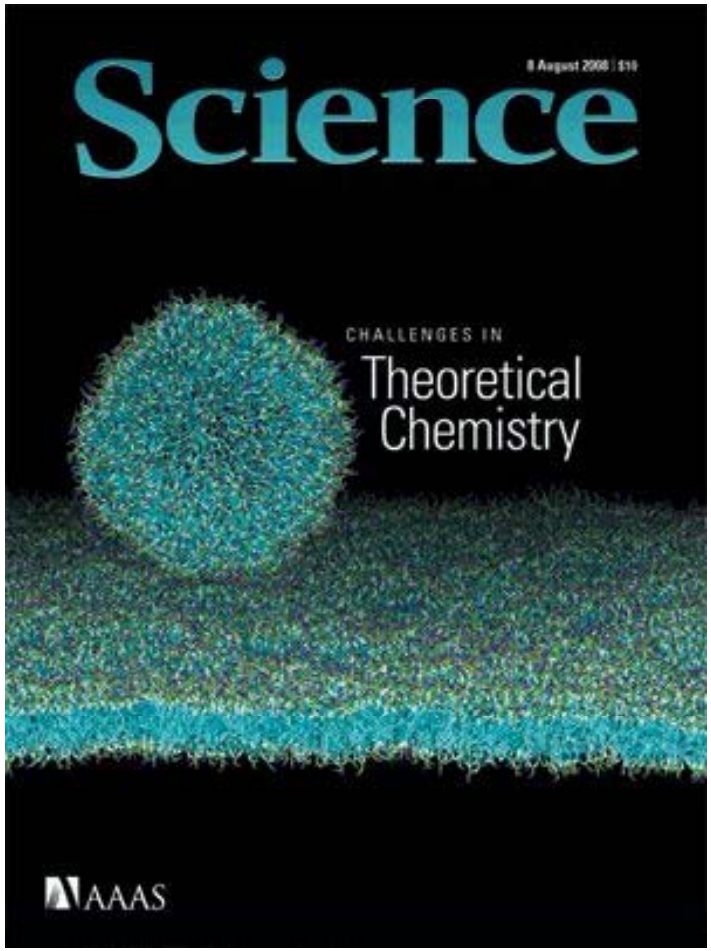


CompChem



Challenges for Computational Chemistry in Materials

A Special Issue of *Science* – "Challenges in Theoretical Chemistry"



8 August 2008 issue of *Science* (Vol. 231, pp. 800-803).

"*Discovery and design of optimal, inexpensive materials will require both experimentalists and modelers working together* …"

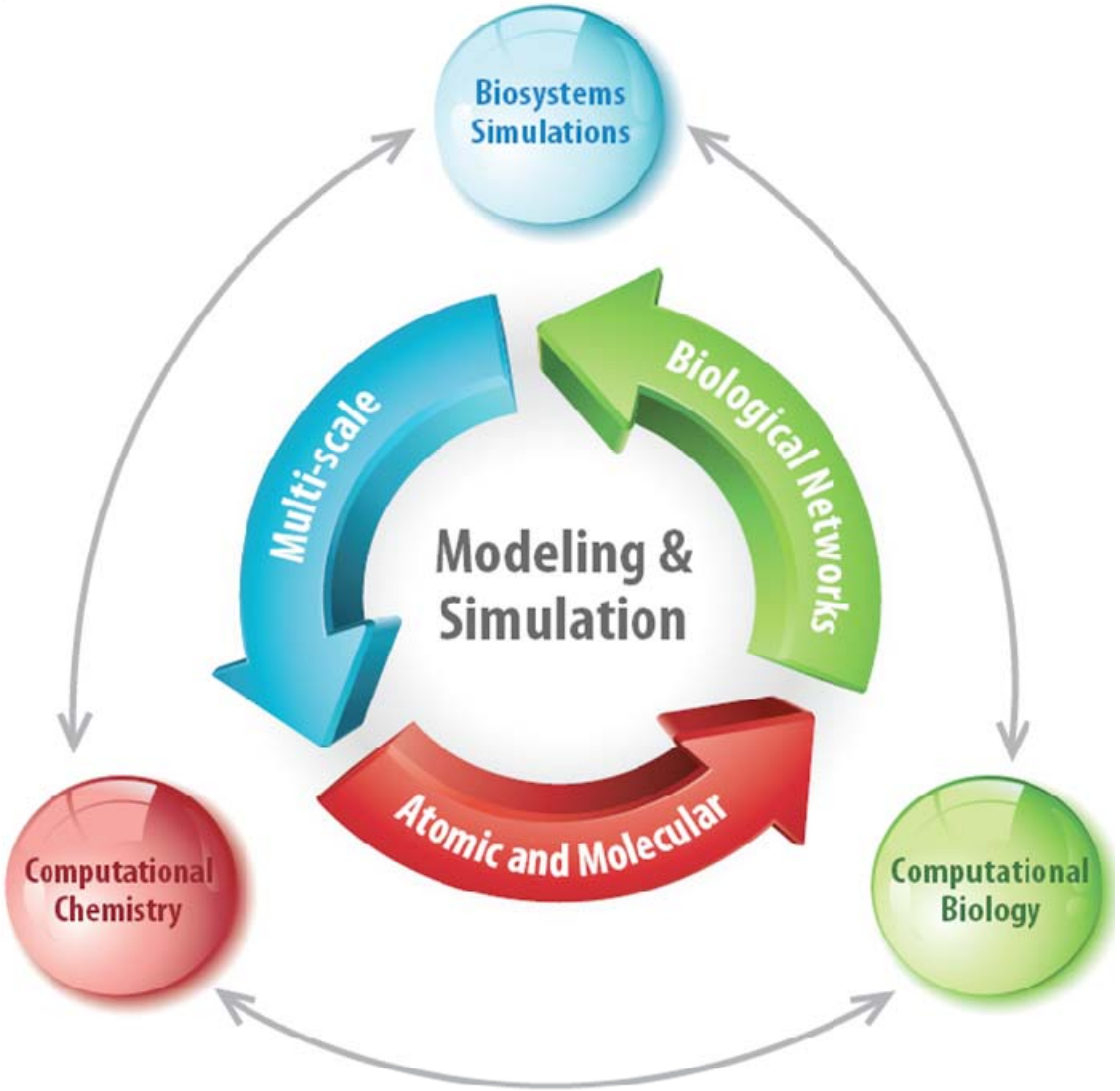
The CompChem Emphasis Area of this RII application directly addresses these challenges with proposals to provide economic stimulus to Mississippi & tools to the wider scientific community.

2008 Mississippi EPSCoR RII Application

Computational Chemistry

Emphasis Area

CompChem – Synergy of Research Projects



- Eclectic Research & Researchers with a Common Goal
- Multi-Scale Simulations spanning Atomic to Organism to Species levels

Computational Chemistry – 2008 Grant Application

Jackson State University

G. Hill
J. Leszczynski
D. Leszczynska
T. V. Shahbazyan

University of Mississippi

A. Dass
N. Hammer
G. Tschumper
R. J. Doerksen
T. K. Hollis
R. W. Wadkins

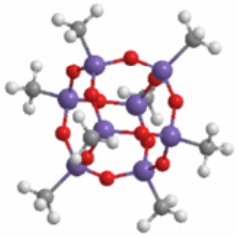
University of Southern Mississippi

C. McCormick

Mississippi State University

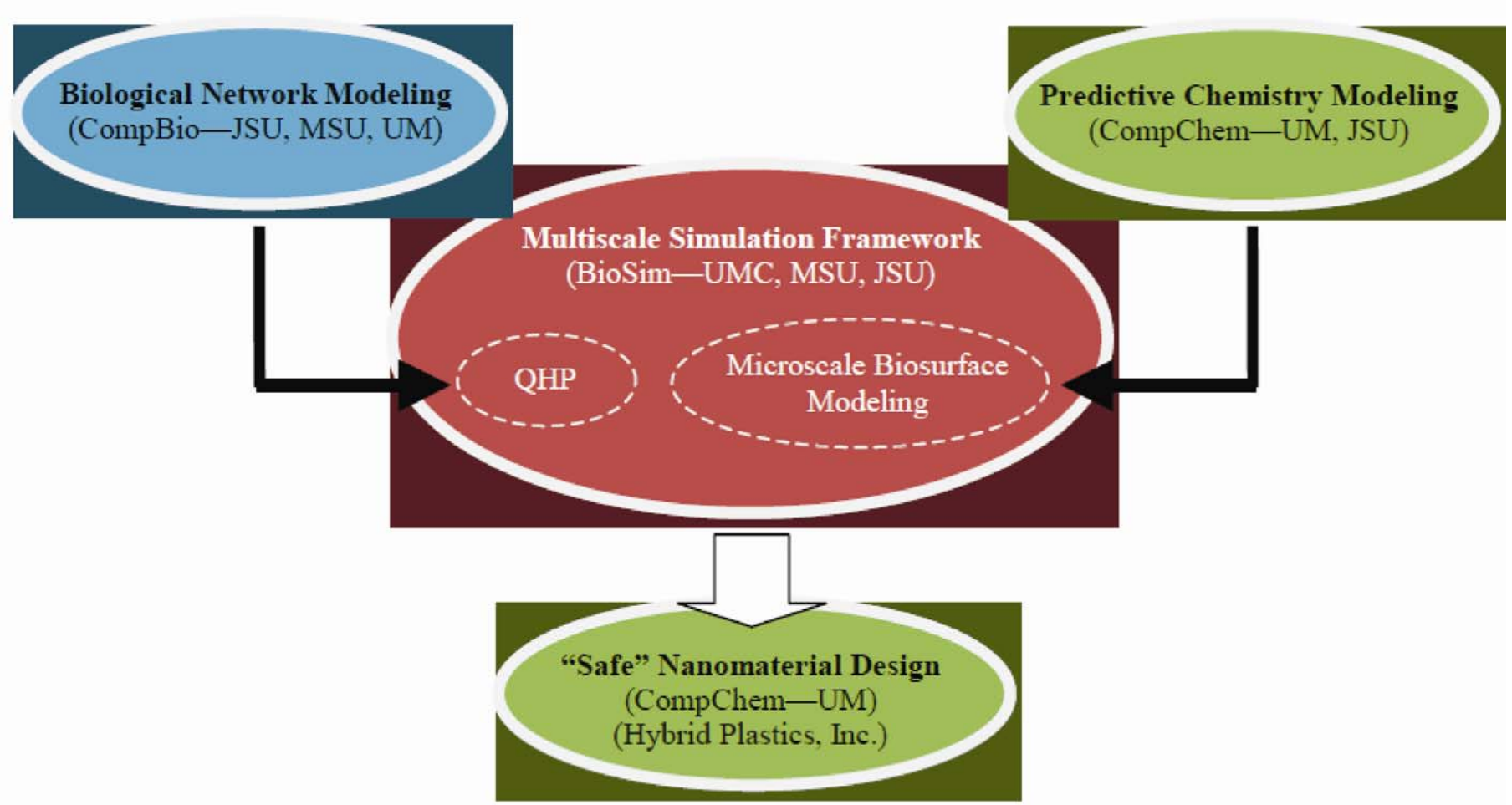
S. Gwaltney

Hybrid Plastics, Inc.



J. Lichtenhan
C. Hagstrom

CompChem – Cross-Cutting Research



CompChem Emphasis Area – Synergy of Research Projects

The University & Industry Nanoscale Consortium

Integration of experimental and computational research in academia & industry

NanoMaterials Computational Suite

CompChem – Cross-Cutting Research Tasks

- Task 1: *Collaborative Methodologies for Predicting Biological Impact of Newly Developed Nanomaterials*. The specific goal of this effort is to combine multiple predictive tools and techniques from each of the three focus areas to develop the initial version of a framework that allows for the prediction of biological impacts of nanomaterials on humans. *Researchers: Tschumper, Leszczynska, K.B. Walters, Lichtenhan*
- *Will combine*
  1. the *multi-scale simulation framework for biological systems* developed by the BioSim group;
  2. the techniques for *modeling and reconstruction of biological networks* developed by the CompBio group;
  3. the *next generation predictive computational models/methods for new materials* developed by the CompChem group.

- Task 2: Seed Grants for Collaborative Projects between Disciplines. 6 per year @ $36,250. *Researchers: to be determined*

CompChem - Research Tasks

- Task 1: *Development and Application of First Principles QM Methods.* Well-established first principles techniques for modeling small molecules are difficult to apply to nanoparticles because of their exorbitant computational requirements. We have demonstrated that it is possible to overcome this limitation for weakly interacting molecular clusters by coupling recently developed multi-centered (MC) approaches to integrated QM computations. *Researchers: Theory: Tschumper, Leszczynska, Shahbazyan; Experimental: Dass, Lichtenhan, Hammer*

- Task 2:*Development and Application of Density Functional Theory and Semi-Empirical Methods*. CompChem researchers will use electronic structure techniques based on density functional theory (DFT) and semi-empirical (SE) Hamiltonians to characterize a wide variety of nanomaterials including those with potential for sensor and electronic applications. *Researchers: Theory: Leszczynski, Hill; Experimental: Hollis, Lichtenhan, Dass, Hammer*

- Task 3: *Development and Application of Molecular Mechanics Methods.* This third research component will use computation and simulation to study complex nanoscale processes in nature such as biopolymer hydration, large-scale enzyme motion, and molecular recognition in order to elucidate design principles for biomimetic nanoscale materials. *Researchers: Theory: Leszczynska, Hill, Gwaltney, Doerksen; Experimental: Wadkins, McCormick*

- Task 4: *Development and Application of QSPR/QSAR Models.* QSAR methods have been efficiently used for the last twenty-five years by the pharmaceutical industry, but have not been applied to nanomaterials. We have demonstrated the applicability of these approaches to prediction of physical and chemical properties for a limited test set of nanoparticles. *Researchers: Theory: Leszczynska, Esperimental: Dass, Lichtenhan*

CompChem - Outcomes

Our collaborative research efforts will

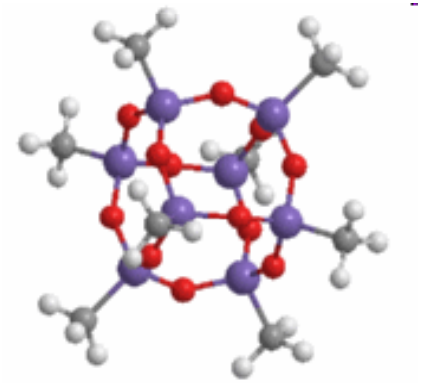
1) produce next generation predictive computational models/methods
   – that are validated through computationally-guided design, synthesis and characterization of novel nanomaterials.

2) extend these methods, models and design principles to biochemical phenomena at the nanoscale.

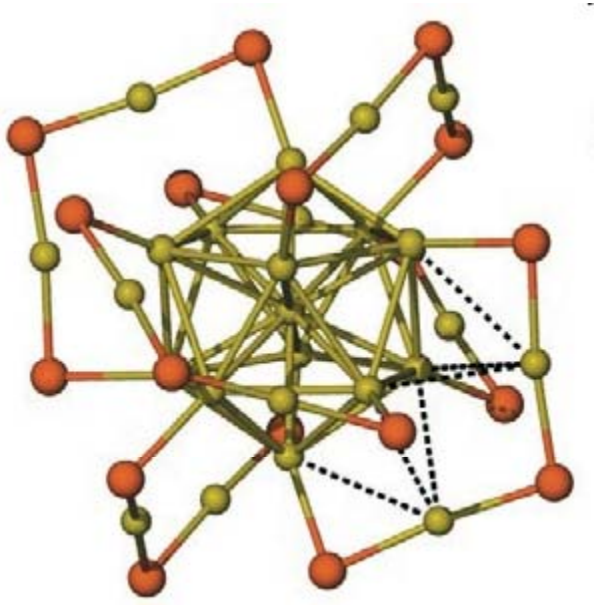
3) lead to the development, implementation & publication of a NanoMaterials Computational Suite.

Task 1

- Extend Current Computational Methods and Develop Improved Methods – Multi-Center Methods



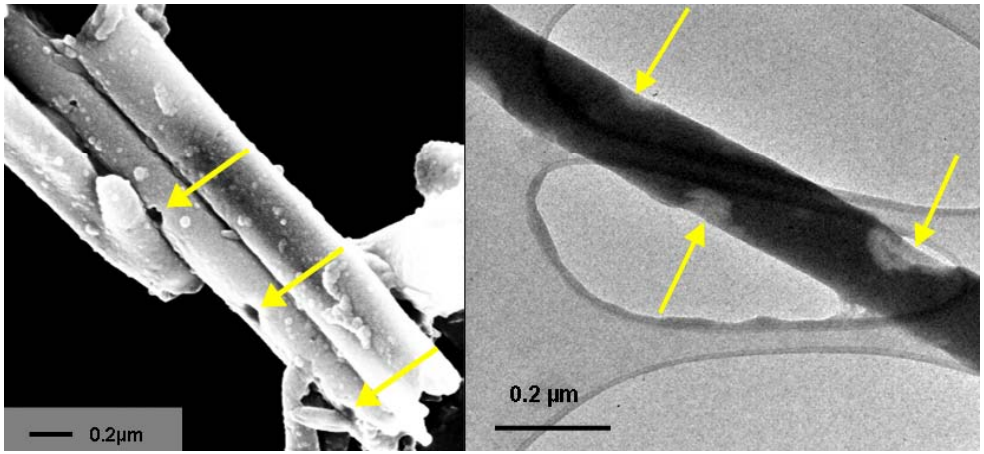
POSS® Nano-Chemicals



Au – 25 nanoparticle

Task 2

- Extend Current Computational Methods and Develop Improved Methods – Molecular Mechanics



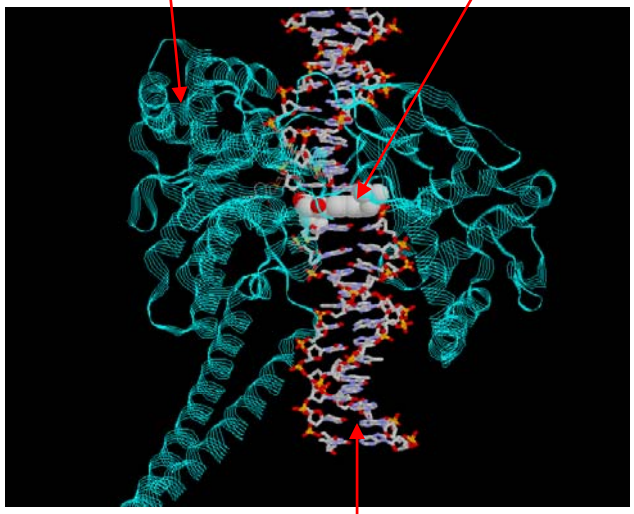
Perforated Organometallic nanotubes

Task 3

- Biopolymer solvation

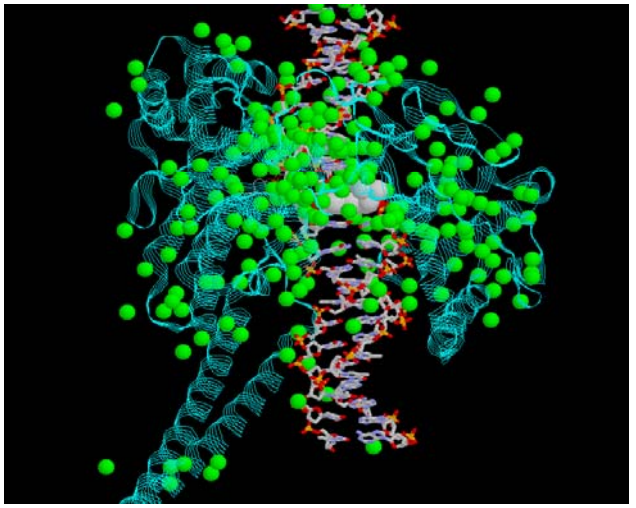
Topoisomerase

Anti-Cancer Drug



DNA

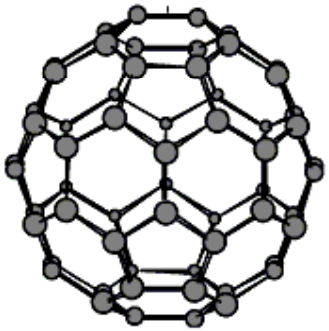
Water everywhere!



- *Design new drugs to take advantage of water layers around topoisomerase I.*
- *Model with polymer hydration study*

Task 4

- *QSPR/QSAR Models for Nanomaterials*



POSS® Nano-Chemicals

Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C-60 solubility in organic solvents

Toropov AA, Rasulev BF, Leszczynska D, et al., *Chem Phys. Lett.* **457**,332-336 (2008).

Thank You

Computational Chemistry:
Research Highlights

- Structures and Properties of Biologically Important Species
- New Materials with Designed Properties
- Bonding and Structures of Model Systems

Structures and Properties of Biologically Important Species

R. J. Doerksen, UM

G. Hill, JSU

J. Leszczynski, JSU

R. W. Wadkins, UM

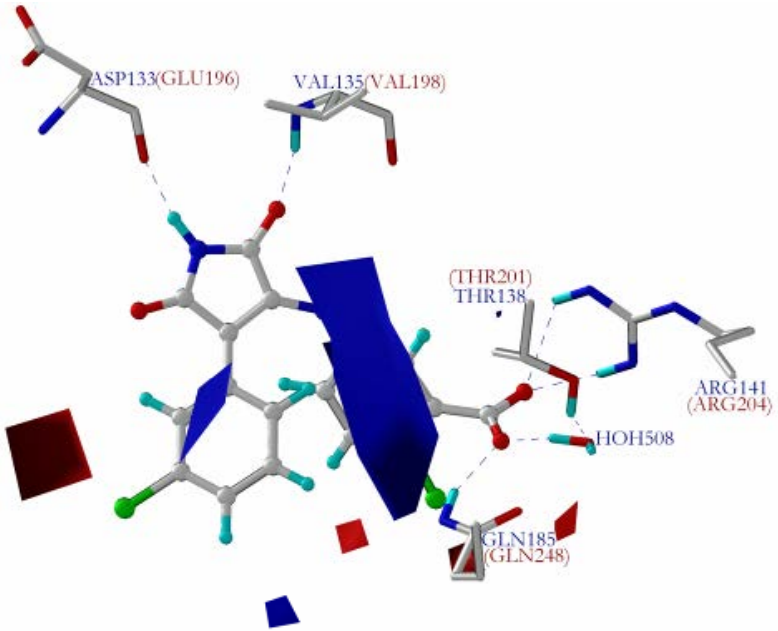
Y. Zhang, USM

Robert Doerksen, University of Mississippi

Protein-Ligand Interactions: Glycogen Synthase Kinase 3

- Docking and molecular dynamics for

- Collaboration with natural products chemist to study binding to the kinase activation loop



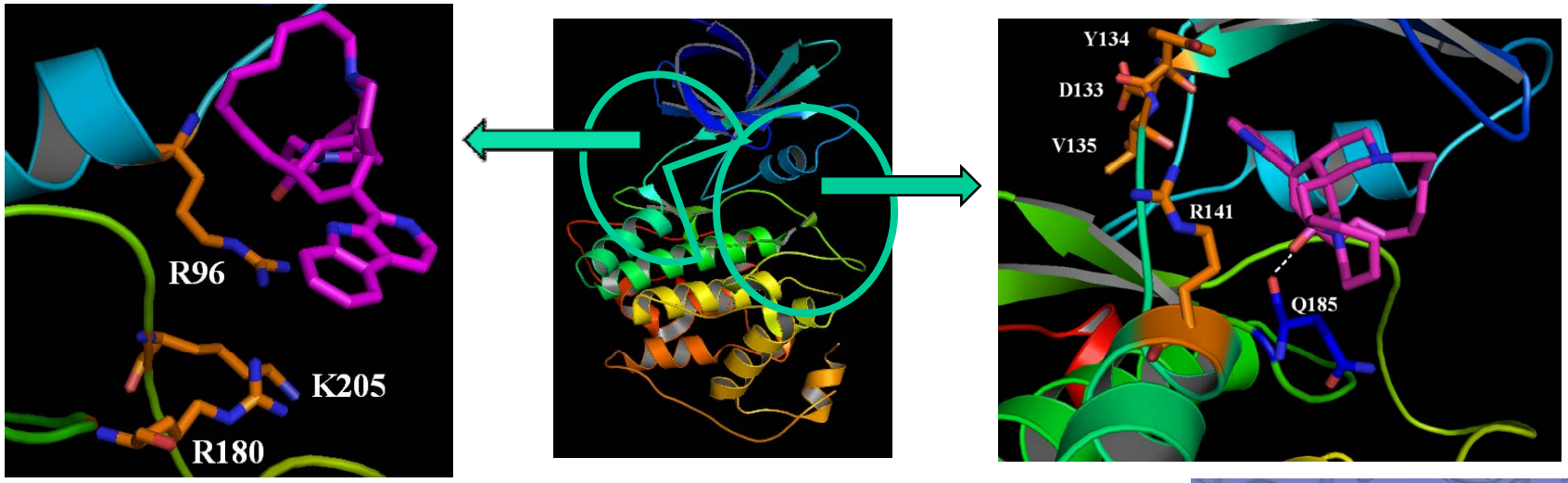
• J Peng, S Kudrimoti, S Prasanna, S Odde, RJ Doerksen, HK Pennaka, Y-M Choo, KV Rao, BL Tekwani, AG Shilabin, AMS Mayer, MR Jacob, LC Tu, J Gertsch and MT Hamann "Structure Activity Relationship and Mechanism of Action Studies of Manzamine Analogues for the Control of Malaria and Neuroinflammation," in preparation for submission to *Journal of Medicinal Chemistry*, 2008.

• MA Ibrahim, AG Shilabin, S Prasanna, M Jacob, SI Khan, RJ Doerksen and MT Hamann "2-N-Methyl Modifications and SAR Studies of Manzamine A," *Bioorganic & Medicinal Chemistry*, submitted 2008.

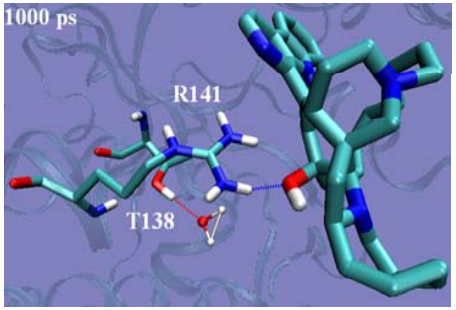
• S Prasanna, PR Daga, A Xie and RJ Doerksen "Glycogen synthase kinase-3 inhibition by 3-anilino-4-phenylmaleimides: Insights from 3D-QSAR and docking," *Journal of Molecular Graphics & Modelling*, submitted 2007.

• P. Sivaprakasam, A. Xie and R. J. Doerksen "Probing the physicochemical and structural requirements for glycogen synthase kinase-3alpha inhibition: 2D-QSAR for 3-anilino-4-phenylmaleimides," *Bioorganic & Medicinal Chemistry*, **14**, 8210-8218 (2006).

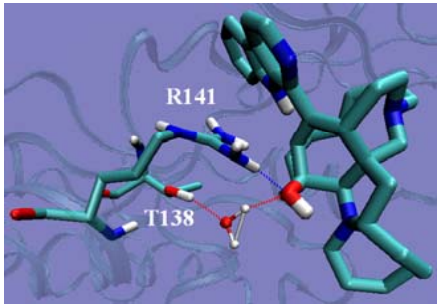
Glycogen Synthase Kinase 3



Above: Docking results. Middle: GSK-3β (PDB: 1I09) showing two possible binding sites for manzamine A: Left: Close view of MA bound to the ATP-noncompetitive binding site. Right: Close view of MA bound to the ATP binding site. The top ranked binding pose of MA for ATP-noncompetitive and ATP binding sites showed Glide G-scores of −4.77 and −6.86, respectively.



At Right: A snapshot from a 1000 ps molecular dynamics simulation showing the 12-hydroxyl of MA interacting with R141 and T138 (right, upper). A less stable water-mediated hydrogen bonding between 12-hydroxyl of MA and T138 is also shown (right, lower).



Doerksen, 2

Glake Hill, JSU

Experimental and Computational Study of Xanthine Tautomers

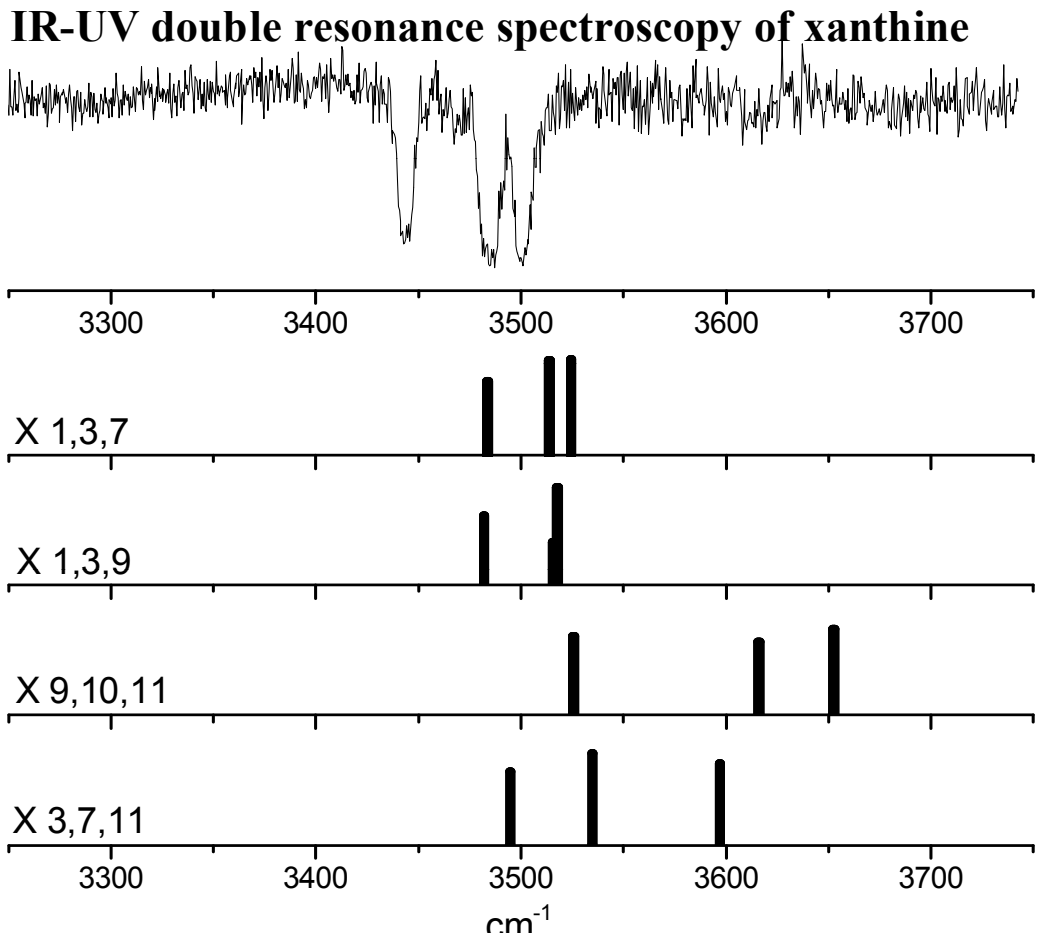


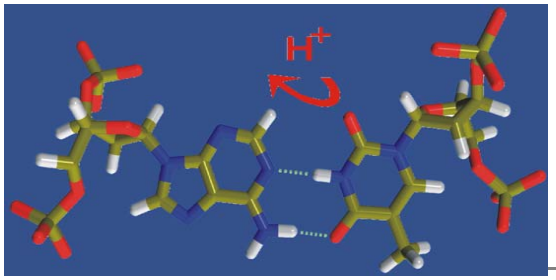
Figure: The IR-UV double resonance (top trace) spectrum of xanthine with the R2PI laser set to 36741 cm-1. The bands at 3444, 3485, 3501 cm-1 are all assigned as N-H stretching vibrations. The calculated frequencies of the 4 most stable tautomers taken at the B3LYP/6-31G** level are shown below.

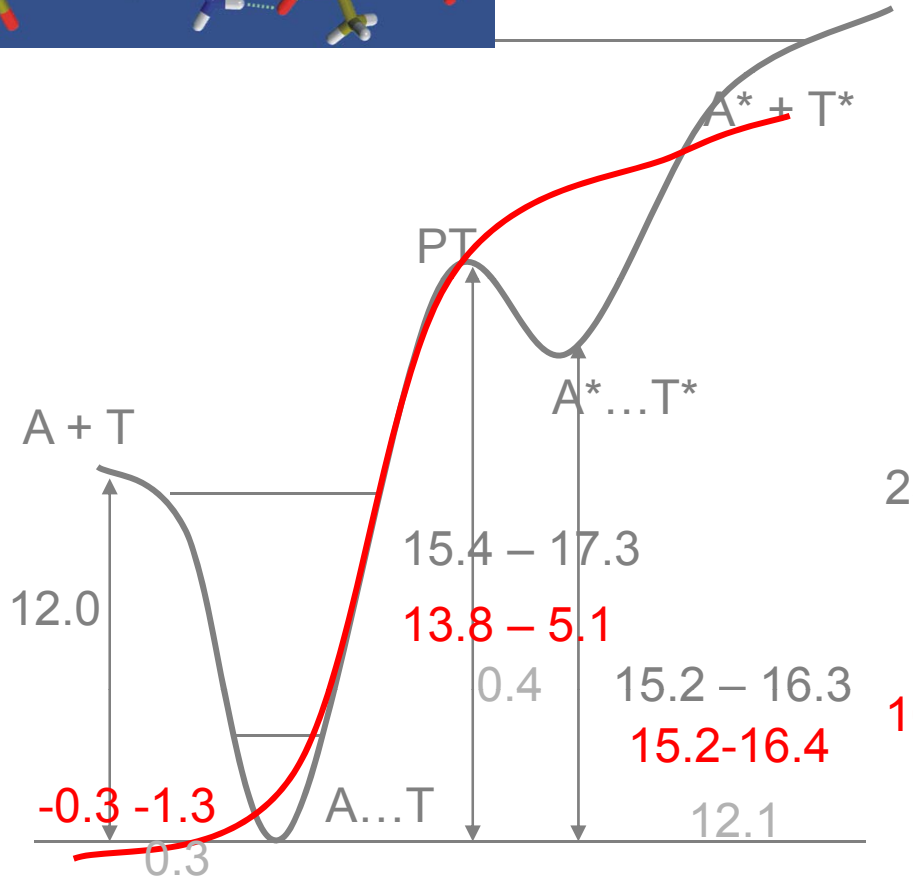
Phys. Chem. Chem. Phys., 2007, **9**, 4587 - 4591

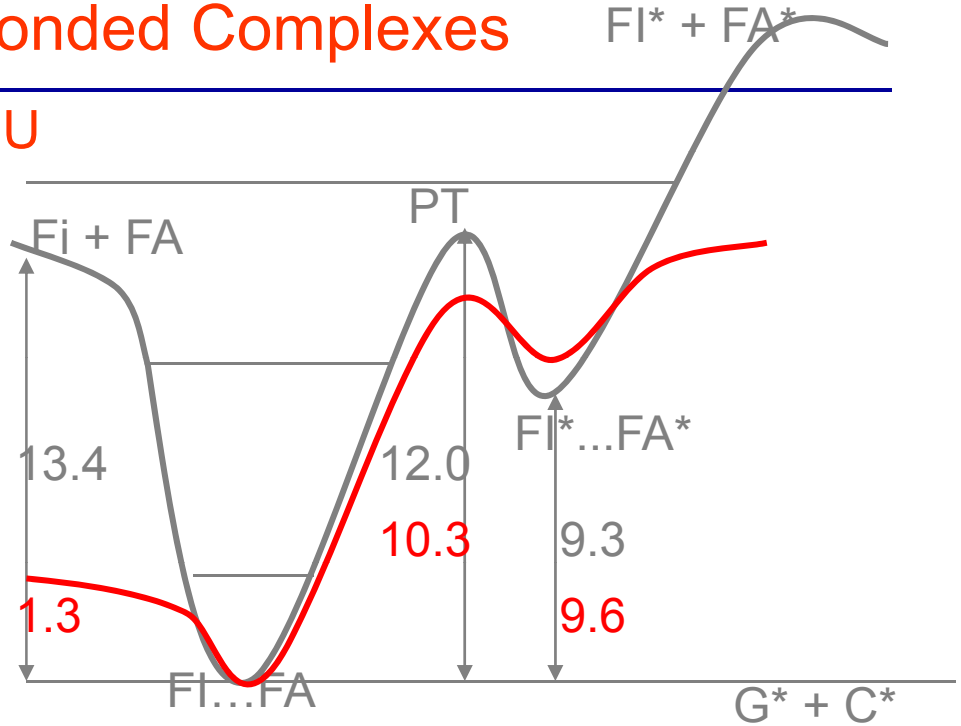
We present resonant two-photon ionization (R2PI), UV-UV, and IR-UV double resonance spectra of xanthine seeded in a supersonic jet. We show that there is only one tautomer of xanthine which absorbs in the wavelength range of 36700 to 37700 cm^{-1}. The IR-UV double resonance spectrum shows three strong bands at 3444, 3485, and 3501 cm^{-1}, which are all assigned as N-H stretching vibrations. By comparing the IR-UV double resonance spectrum to frequencies and intensities obtained from density functional theory (DFT) calculations, the observed xanthine is most likely the diketo N(7)H tautomer.

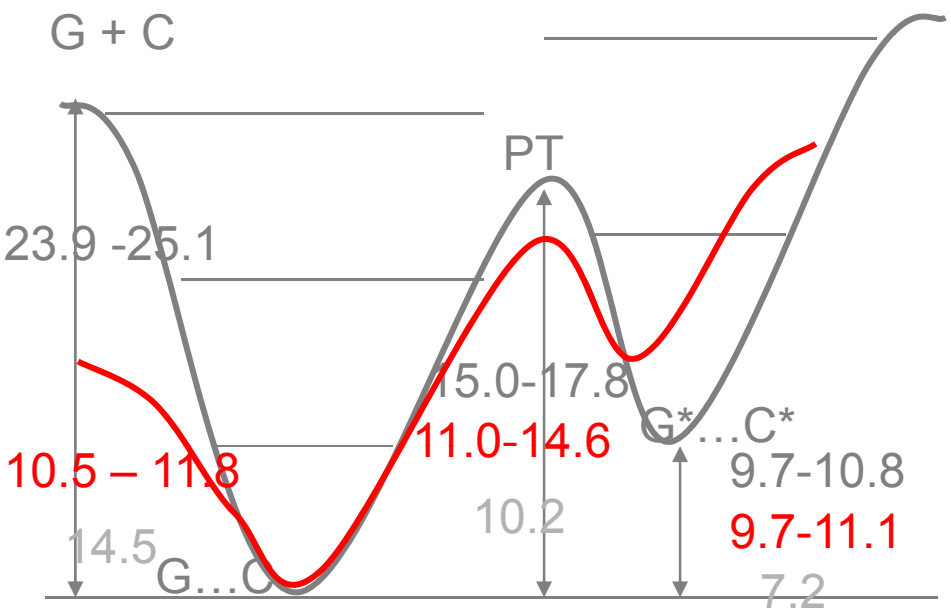
GIBBS FREE ENERGY OF H-bonded Complexes

J. Leszczynski, JSU









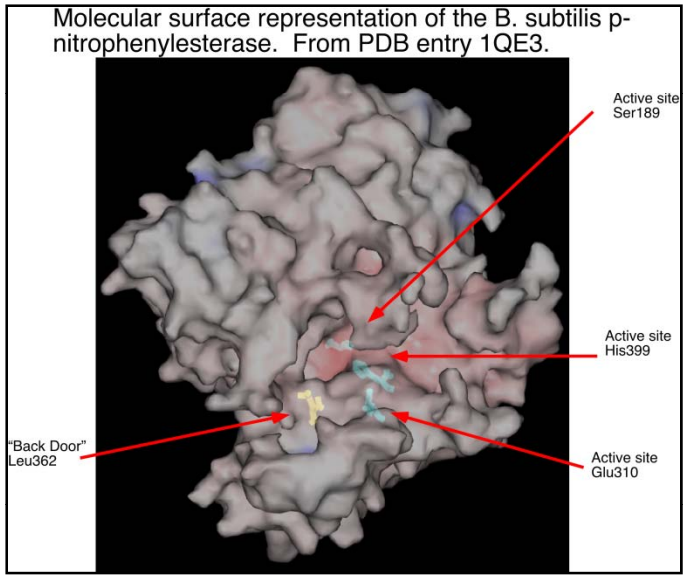
Molecular Dynamics of Carboxylesterases

Their Implications in Substrate Selectivity

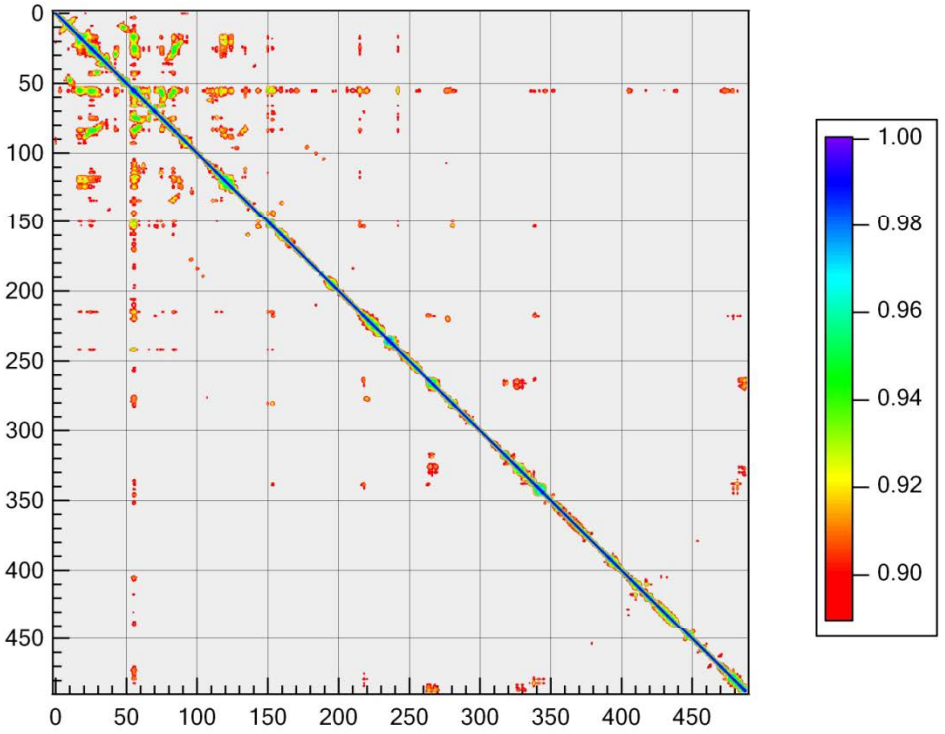
Xiaozhen Yu[1], Monika Wierdl[2], Philip M. Potter[2],
and Randy M. Wadkins[1]

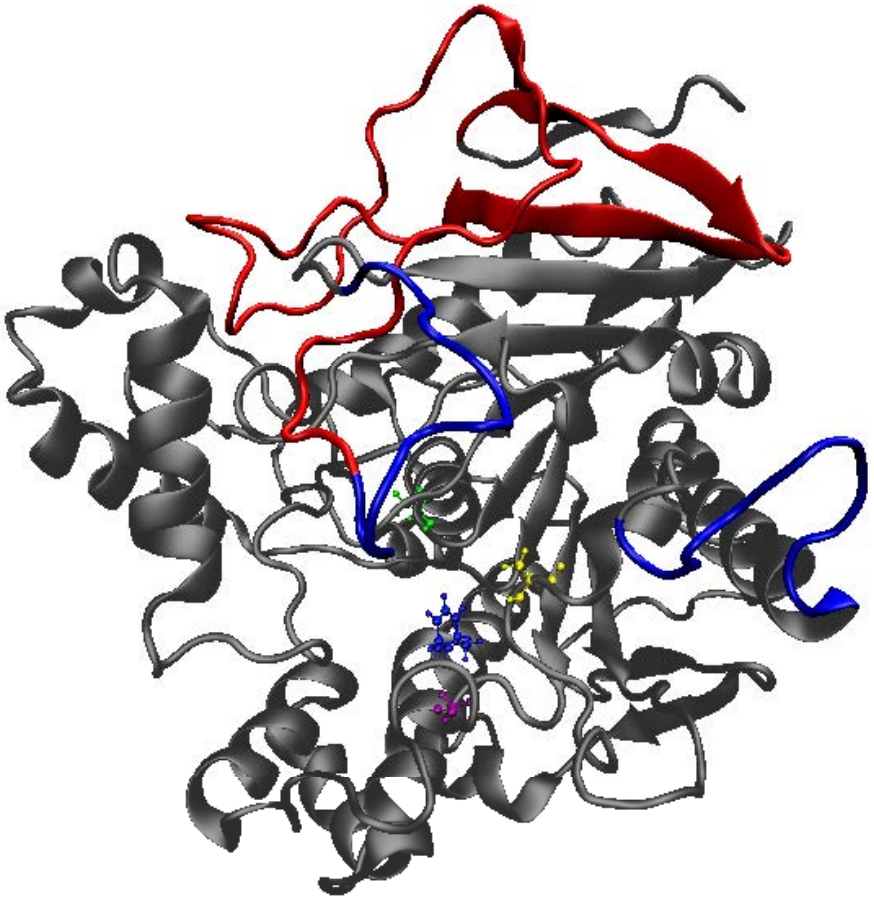
[1]Dept of Chemistry & Biochemistry, University of Mississippi
[2]Dept. of Mol. Pharmacol., St. Jude Children's Res. Hospital

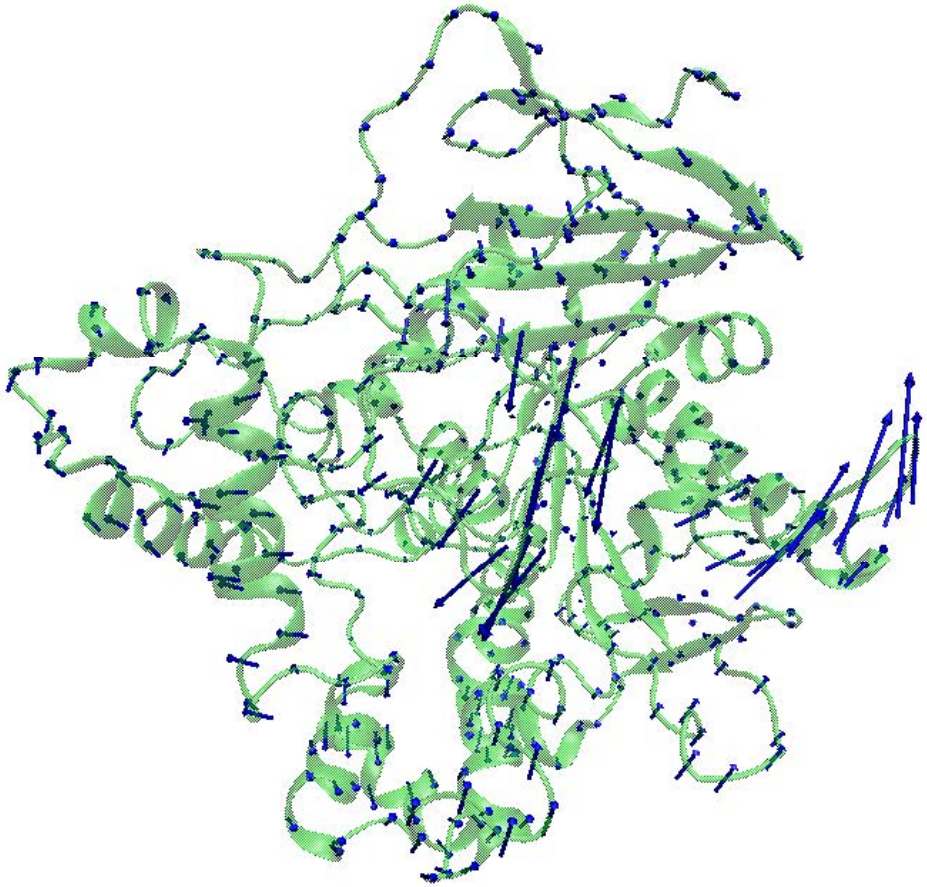
- The dynamic cross-correlation (DCC) map from a 10 ns MD calculation.



Molecular dynamic simulation – DCCM
(Dynamical Cross-Correlation Map)





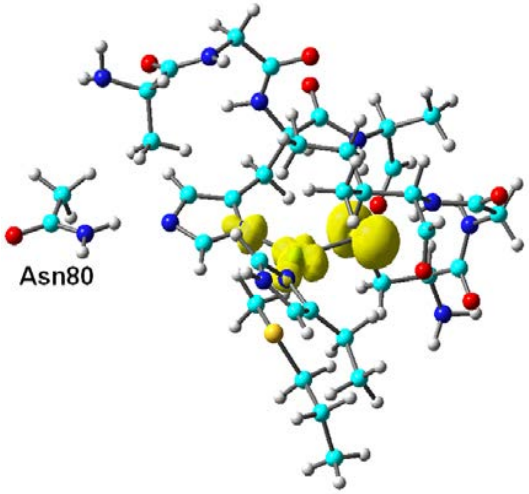


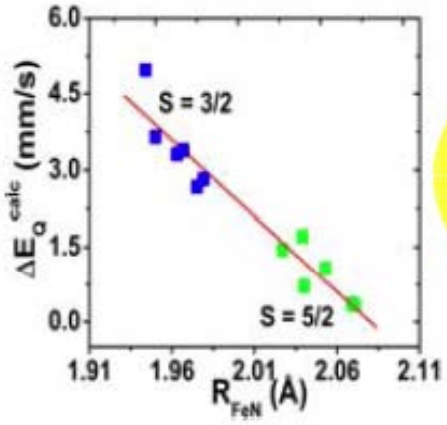
MD: According to our 10-ns MD calculation, The region showing the highest correlated motion are residues 10-90, indicated by the red regions.

NM: The largest displacements of residues were calculated via normal modes. Blue arrows on the green transparent backbone indicate the displacements of the alpha carbon atoms of the enzyme.

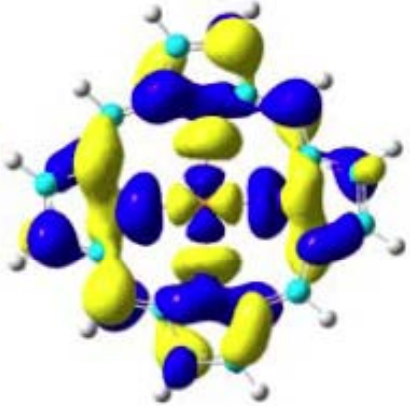
USM – Yong Zhang Group

High accuracy protein structure determination





S = 3/2
Iron Porphyrins
4, 5, 6-coordinate
Planar, Ruffled & Saddled



We are currently developing the integrated quantum mechanics and spectroscopy (QMS) techniques that target an accuracy close to small molecule's x-ray structures with much broader applicability compare to x-ray crystallography. The examples show our recent work on the prototype electron transfer proteins (blue copper proteins) and heme protein models with intermediate spin states.

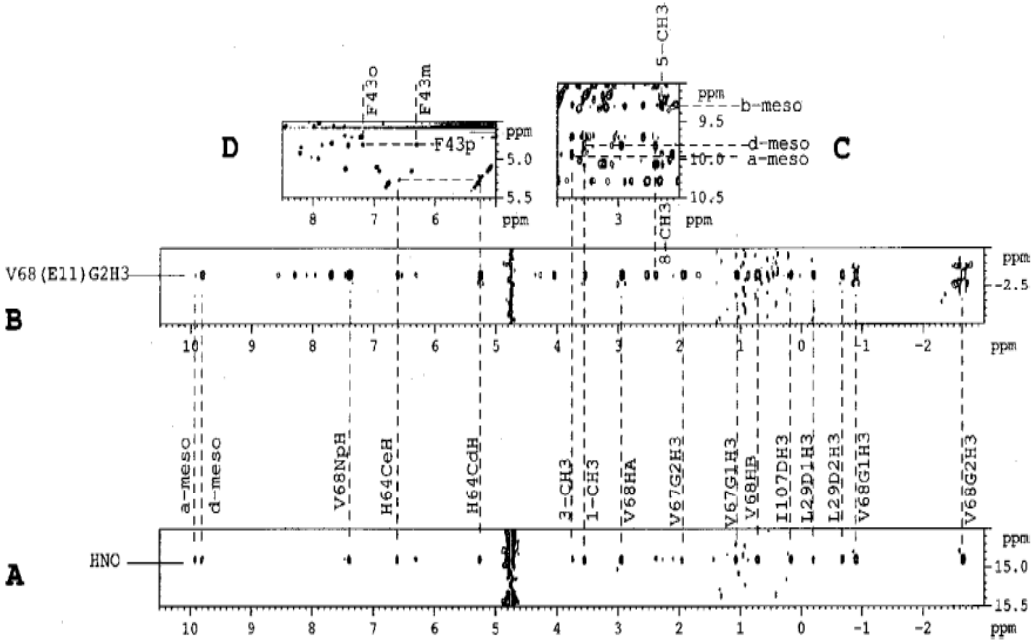
Y. Zhang, E. Oldfield. *J. Am. Chem. Soc.* 130, 3814-3823 (2008)

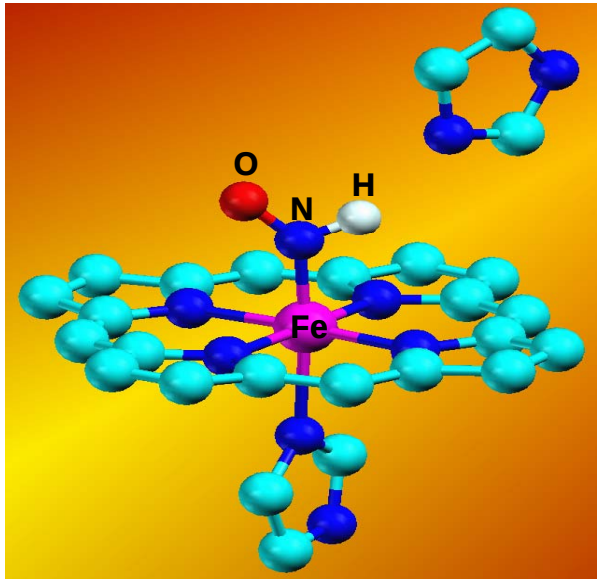
Y. Ling, Y. Zhang. *J. Am. Chem. Soc.* in press (2009)

USM – Yong Zhang Group

New NIH R15 grant GM-085774 (2008/7-2010/6)

HNO protein complexes and models: from spectra to structure





New Materials with Designed Properties

S. Davis, UM

G. Hill, JSU

M.-J. Huang, JSU

J. Leszczynski, JSU

J. Ritchie, UM

T. V. Shahbazyan

Steven Davis, University of Mississippi

Energy Storage through Bond Strain

We are studying ways to store potential energy through molecular geometries.

1) We have shown that small carbon and heteroatom rings can accommodate trans double bonds. This isomeric geometry imports substantial bond strain into the molecule to maintain its cyclic structure.

2) This bond strain can be used as a way to store energy.

3) The stored energy can be released by thermal isomerization via rotation of the trans double bond to the cis isomeric geometry.

4) Computational chemistry techniques are used to determine the geometries, relative energies, activation barriers, and potential energy surfaces for the potential energy-storing structures.

Consider Dihydropyridine as a Potential Energy Storage Structure

Scheme 1 - trans double bond at 2 position, cis double bond at 4 position

Scheme 2 - trans double bond at 4 position, cis double bond at 2 position

Scheme 3 - trans double bond at 2 position, cis double bond at 5 position

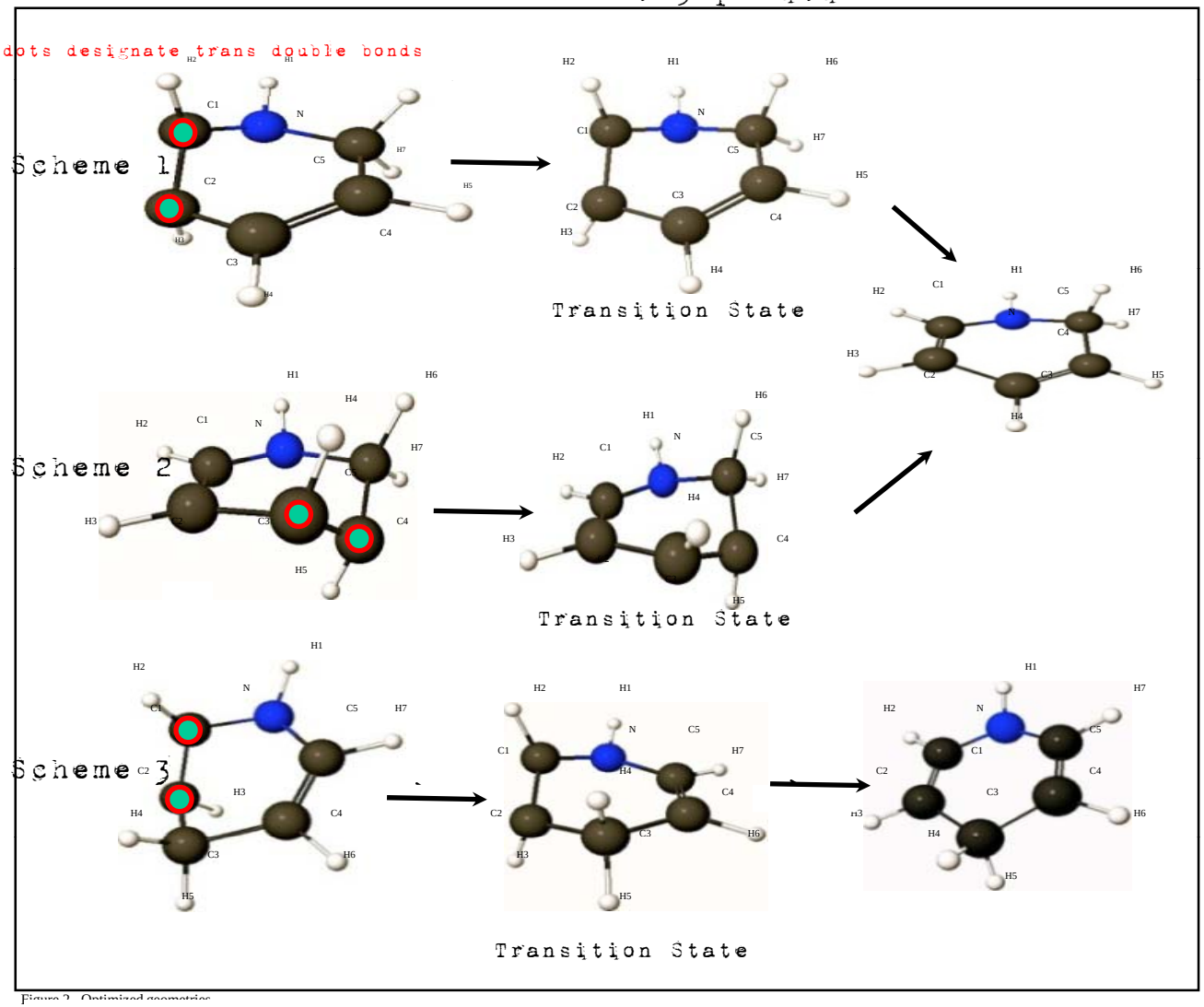


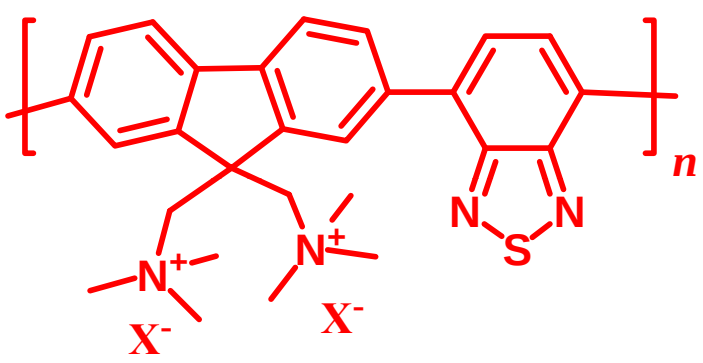
Figure 2. Optimized geometries

The three Schemes show that about 54-61 kcal/mol of energy can be stored in a single trans double bond.

The activation barriers show that the structures in Schemes 1 and 2 are too unstable with barrier of only 3-4 kcal/mol.

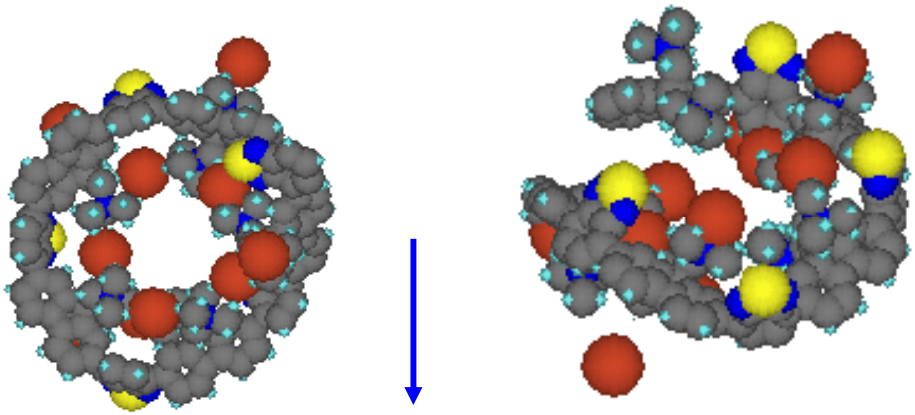
Moving the cis double bond to the 5 position raises the barrier to 10 kcal/mol, greatly increasing the stability.

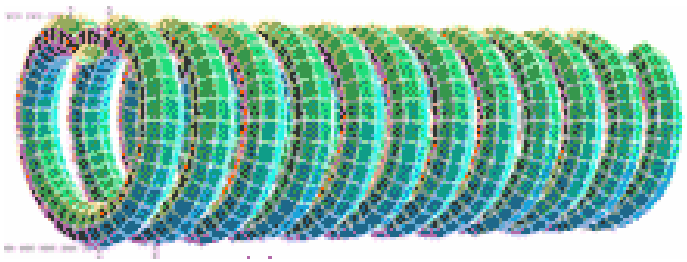
Cationic Conjugated Polyelectrolytes G. Hill, J. Leszczynski, JSU

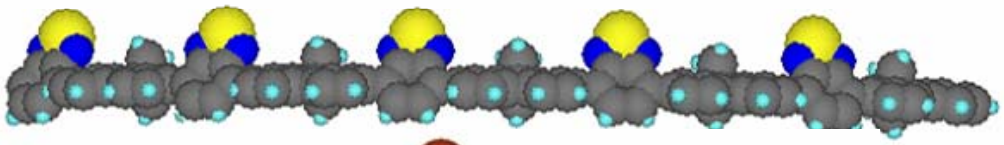


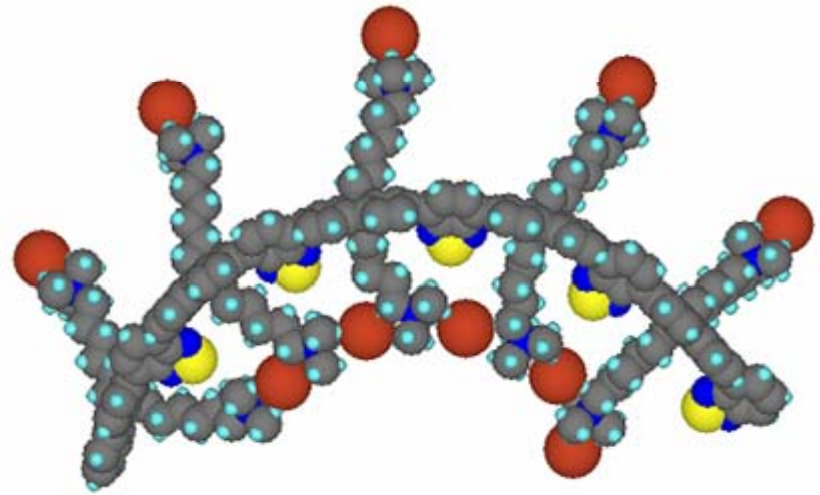
X= Br, BF_4, CF_3SO_3, PF_6, ...

Ionic polyelectrolytic conjugated polymers









- Dipole moment
- HOMO and LUMO levels
- Electron distribution: HOMO, LUMO
- Oxidation and Reduction potential

Ming-Ju Huang, JSU
Theoretical Modeling of Interactions of THC with Cyclodextrins

Δ^1-THC

Potential anticancer agents
Prevent nausea, vomiting and pain
Stimulate appetite
Inhibit tumor growth
Well tolerated and not toxic as conventional chemotherapies

has a very low aqueous solubility (restricts its use)

Cyclodextrins (CDs)

form inclusion complexes with poorly water soluble compounds
increase the aqueous solubility, stability, and bioavailability of lipophilic drugs
have potential for extraction in other areas
hydroxypropyl-β-cyclodextrin (HP-β-CD) is less toxic than β-cyclodextrin

demonstrates that THC forms a drug-HP-β-CD complex that increases the THC solubility a thousand-fold (Pekka Jarho et al. (1998)).

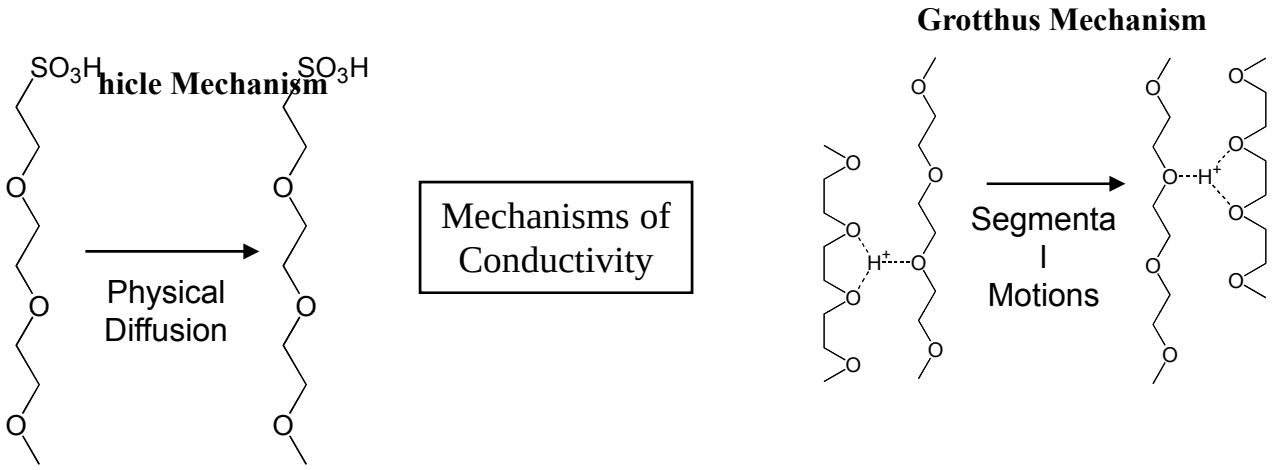
The mechanism of complex formation is not fully understood

Jason Ritchie, University of Mississippi

Effects of Structure on Ionic and Molecular Transport in an Anhydrous Proton Conducting Polymer Electrolyte

Goal: the overall goal of this project is to gain a fundamental understanding of how the structure of our "MePEG polymer" affects ionic and molecular transport in this material.

Problem: We need to develop proton conducting membranes that are capable of operating at high temperatures and low relative humidities.



Conductivity & Rearrangement

We have found that proton conductivity is dependant on polymer rearrangement and that our system displays **Grotthus type proton conductivity** through this polymer rearrangement. However, we have recently found that at higher temperatures, this behavior reverses, and is dominated by the vehicle mechanism of conductivity. The cross-over on the figure indicates that the acid vehicles are diffusing as fast as the H^+ ions, indicating a vehicle mechanism.

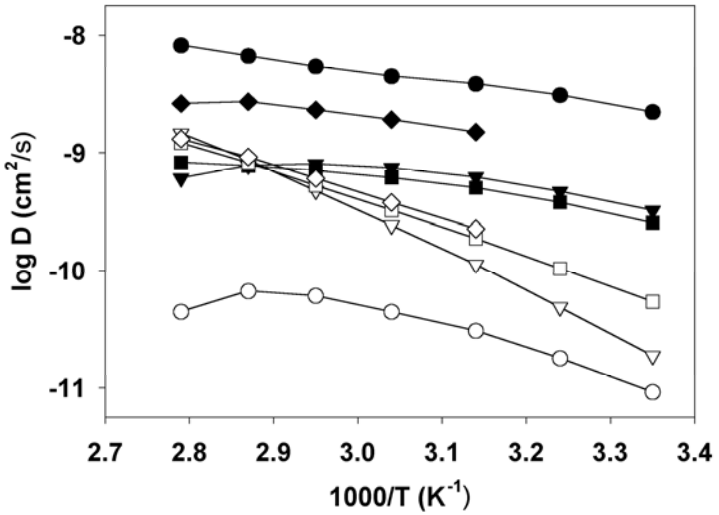
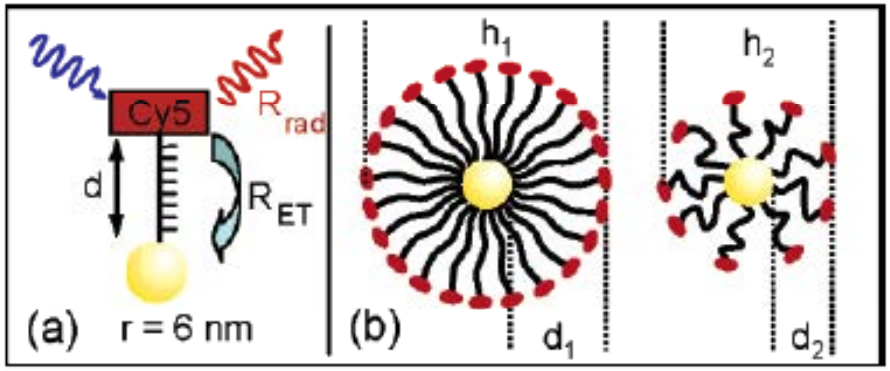


Figure: Activation of diffusion for H^+ cations (solid markers: ●◆■◆) and $MePEG_nSO_3$ anions (open markers: ❍▽□◇) in anhydrous mixtures of 1.32M $MePEG_nSO_3H$ in the $MePEG_7$ polymer.

Modeling of Hybrid Nanomaterials for Sensing Applications

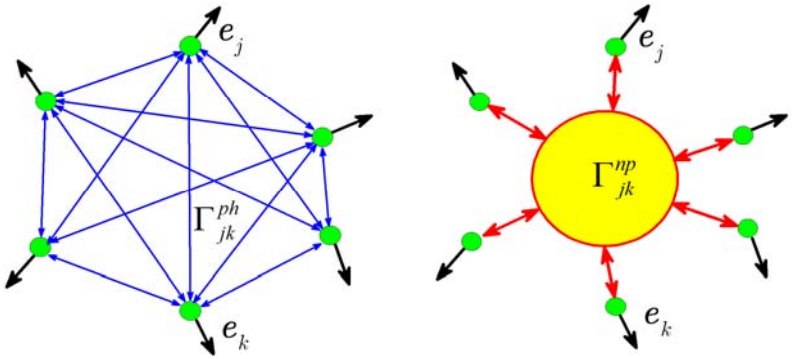
Tigran Shahbazyan, *Department of Physics, JSU*

Fluorescence of an ensemble of molecules near a metal nanoparticle (NP)



A large number of fluorescing molecules are attached to NP via ssDNA linkers

Plasmon exchange – a new mechanism of *cooperative emission*



Hybridization of molecules via surface plasmon in a NP leads to the formation of plasmonic super-radiant states

Bonding and Structures of Model Systems

S. Davis, UM

G. Hill, JSU

J. Leszczynski, JSU

G. Tschumper, UM

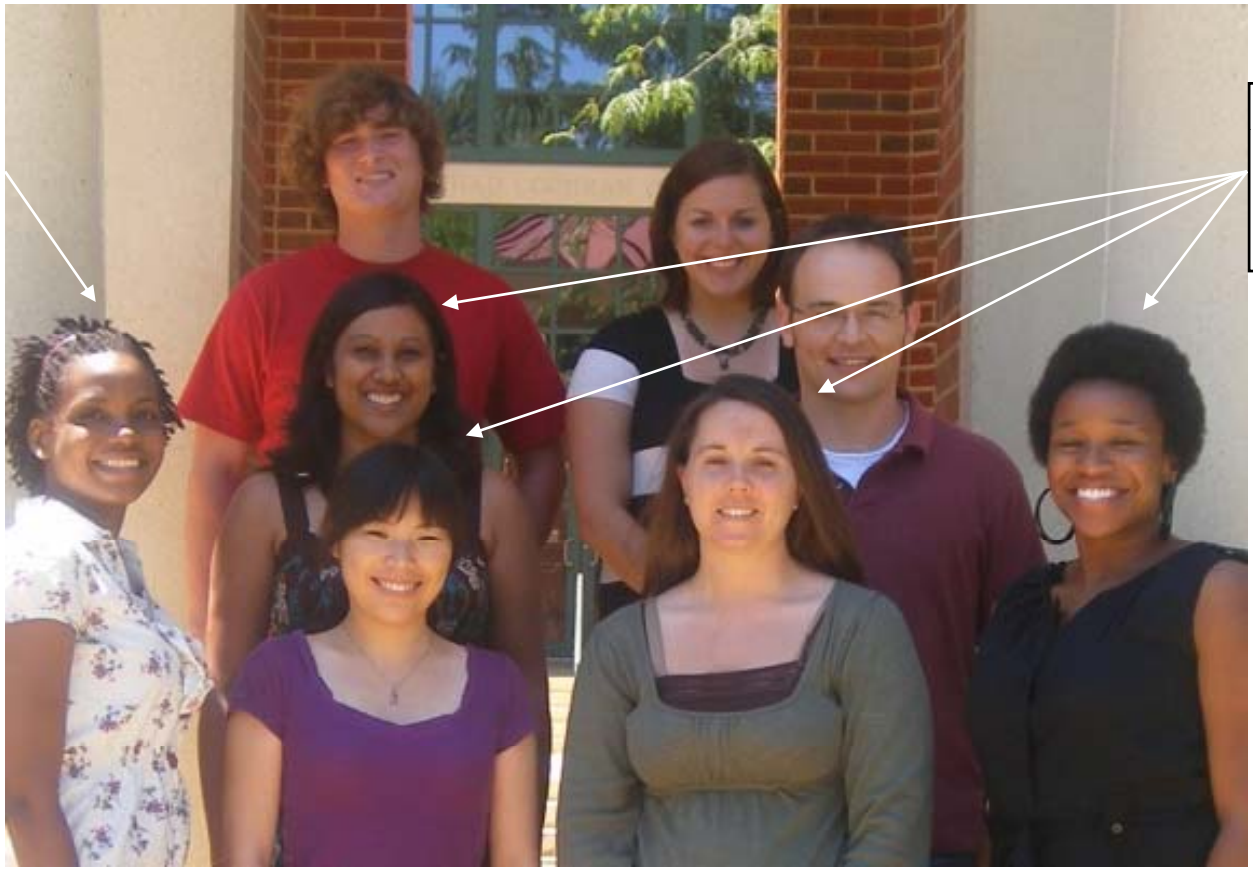
J. D. Watts, JSU

Characterization of Non-Covalent Interactions

Gregory S. Tschumper, *Department of Chemistry and Biochemistry, UM*

Tschumper Research Group Summer 2008

Presenting at annual NOBCChE conference



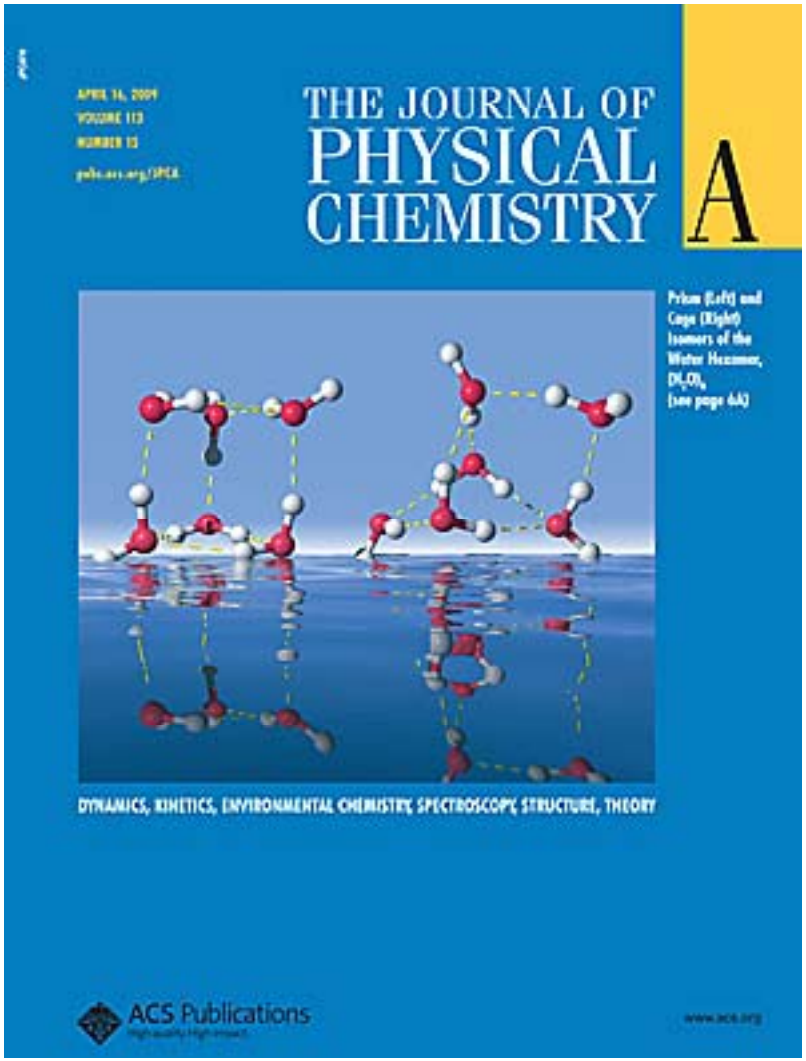
Presenting at this meeting

Back Row (L to R): Coleman Howard and Ann Elizabeth Miller
Middle Row: **Desiree Bates** and Dr. Gregory S. Tschumper
Front Row: Kari Copeland, **Bei Cao**, **Ginger Tipton** and **Brittney Smith**

Characterization of Non-Covalent Interactions

Gregory S. Tschumper, *Department of Chemistry and Biochemistry, UM*

April 14th cover of *The Journal of Physical Chemistry A*



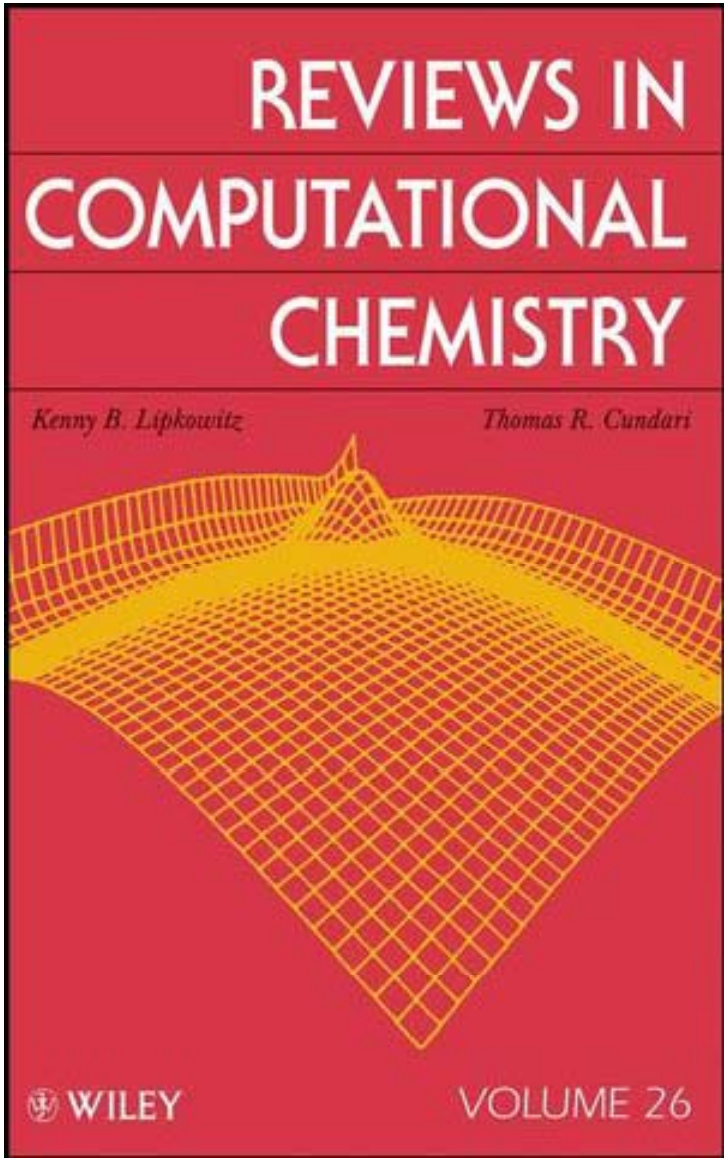
D. M. Bates and G. S. Tschumper
J. Phys. Chem. A, **2009**, 113, 3555.

"CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures"

Characterization of Non-Covalent Interactions

Gregory S. Tschumper, *Department of Chemistry and Biochemistry, UM*

Chapter in Volume 26 of *Reviews in Computational Chemistry*



G. S. Tschumper in *Reviews in Computational Chemistry*, K.B. Lipkowitz and T.R. Cundari, Eds., VCH, New York, 26, 39-90 (2009)

"Reliable Electronic Structure Computations for Weak Noncovalent Interactions"

Publications and Presentations

Publications

- A.M. ElSohly, B. W. Hopkins, K.L. Copeland and G.S. Tschumper, ***Anchoring the Potential Energy Surfaces of the Diacetylene Dimer***, Molecular Physics, accepted (2009).
- D. M. Bates and G. S. Tschumper, ***CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures***, J. Phys. Chem A, 113, 3555-3559 (2009)
- G.S. Tschumper and T.R. Cundari, ***Reliable Electronic Structure Computations for Weak Non-Covalent Interactionsin Clusters***, Reviews in Computational Chemistry, K.B. Lipkowitz, Eds., Wiley-VCH, Inc., Hoboken, NJ, Vol. 26, 39-90 (2009).
- D.M. Bates, J.A. Anderson, P. Oloyede and G.S. Tschumper, ***Probing the effects of heterogeneity on delocalized pi...pi interaction energies***, Phys. Chem. Chem. Phys., 10, 2775-2779 (2008).
- A.M. ElSohly and G.S. Tschumper, ***Comparison of polarization consistent and correlation consistent basis sets for noncovalent interactions***, Int. J. Quantum. Chem., 109, 91-96 (2009).
- K.L. Copeland, J.A. Anderson, A.R. Farley, J.R. Cox and G.S. Tschumper, ***Probing Phenylalanine/Adenine Pi-Stacking Interactions in Protein Complexes with Explicitly Correlated and CCSD(T) Computations***, J. Phys. Chem. B, 112 , 14291-14295 (2008).

Publications and Presentations

Invited Talks

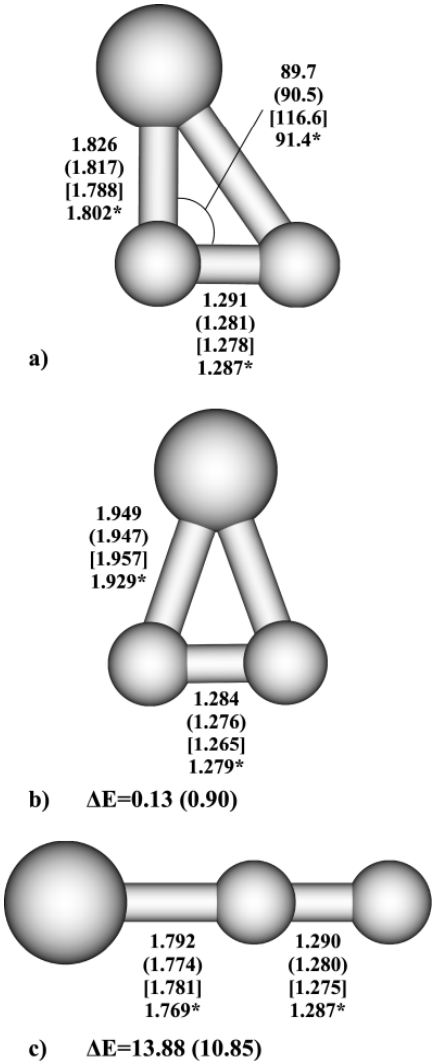
- *Latsis-Symposium "Intramolecular Dynamics, Symmetry and Spectroscopy"*, September 6-10, 2008, ETH Zurich, Switzerland
- *49th Sanibel Symposium*, Feb 26 - March 3, 2009, St. Simons Island, GA

Contributed Talks and Posters

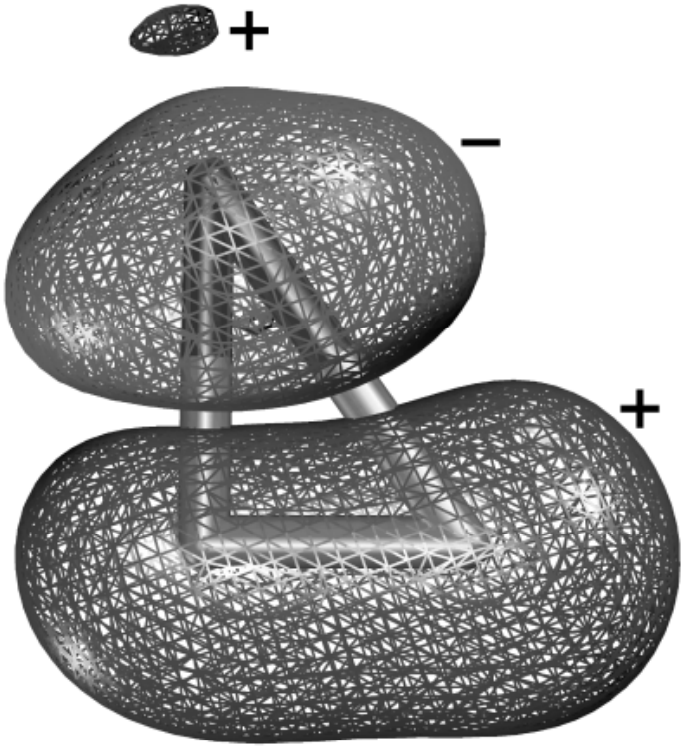
- *235th National Meeting of the ACS*, April 6-10, 2008, New Orleans, LA
- *236th National Meeting of the ACS*, August 17-21, 2008, Philadelphia, PA
- *8th International Congress of the World Association of Theoretical and Computational Chemist(WATOC 2008)*, Sept 14-19, 2008, Sydney, Australia

Conference	Student Presentations
235th National Meeting of ACS	4
236th National Meeting of ACS	1
WATOC 2008	1
17th CCTCC	2
49th Sanibel Symposium	2

Properties of Ge/C Nanomaterials J.Leszczynski, G. Hill, JSU



Ge/C Microclusters (GeC2)

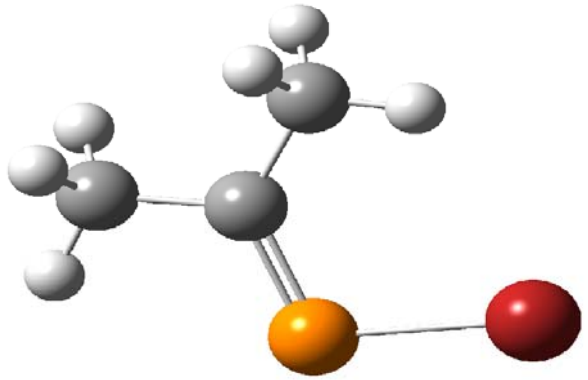


John D. Watts, JSU:
Applications of High-Level Coupled-Cluster Methods

Substituent Effects for Phosphaalkenes

Species containing C=P
Potential ligands in TM-catalyzed reactions
Sources for new inorganic polymers

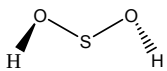
Address formation from vinylphosphines
Assess substituent effects on tautomerism and deprotonation
Coupled-cluster benchmarks for DFT



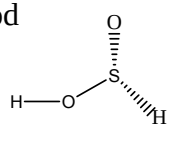
J. D. Watts, D. J. Watts, and M.-J. Huang, J. Phys. Chem. A 113, 1886-1891 (2009).

Transient/Rare Sulfur-Oxygen Species

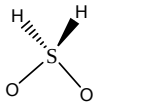
Atmospheric/combustion chemistry of sulfur compounds
Example: CC calculations on isomers of H_2SO_2
Kinetics and mechanism of reaction of H_2S and O_2 not well understood



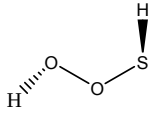
Sulfoxylic acid (C_2)



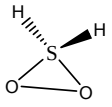
Sulfinic Acid (C_1)



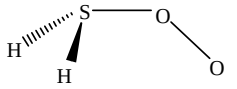
Dihydrogen Sulfone (C_{2v})



Sulfhydryl hydroperoxide (C_1)



Thiadioxirane (C_s)



Dihydrogen persulfoxide (C_s)

B. Napolion, M.-J. Huang, and J. D. Watts, J. Phys. Chem. A 112, 4158-4164 (2008).
B. Napolion, Ph.D. thesis (2008).