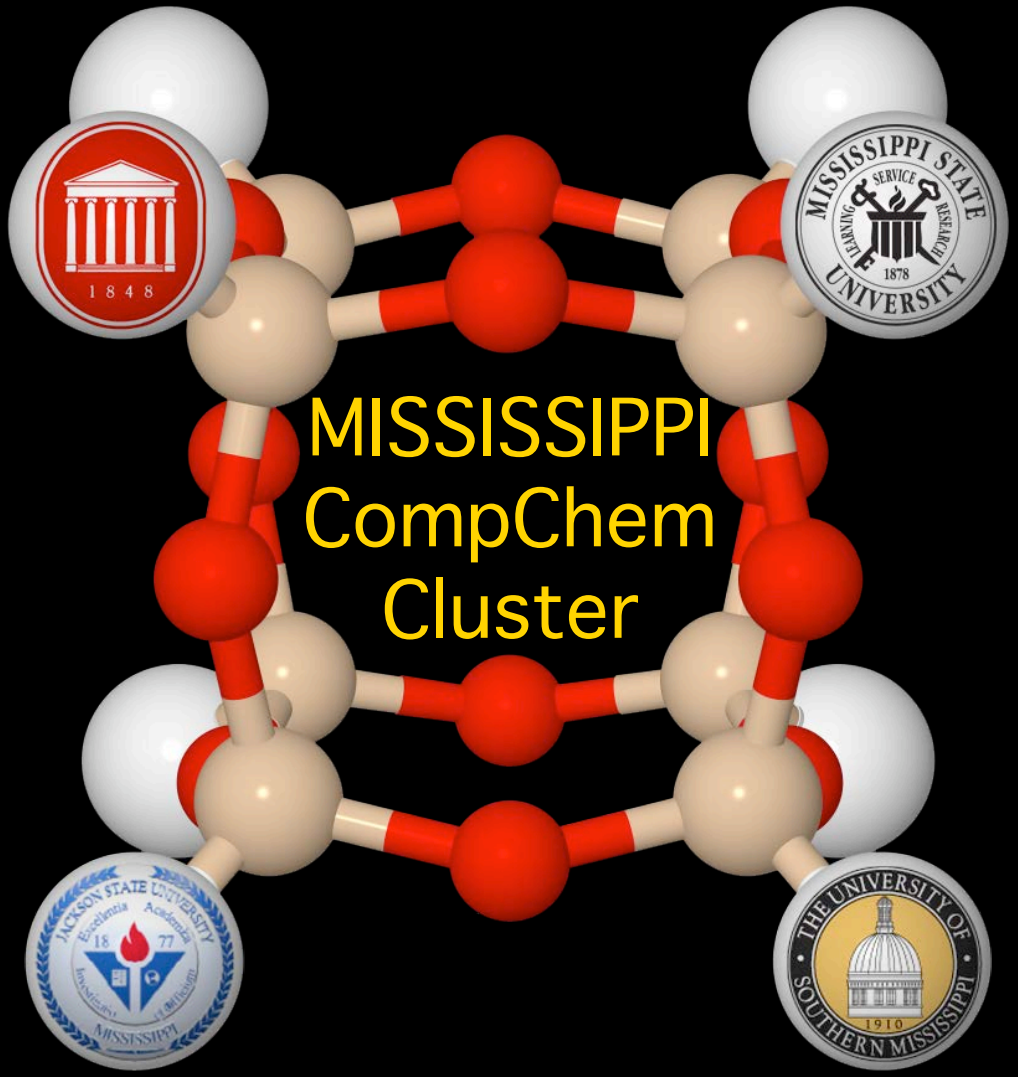
Research Area: Computational Chemistry

Modeling and Simulation of Nanoscale Chemistry



University Participants:

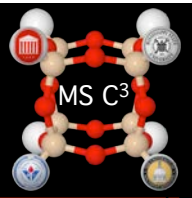
Jackson State University	*(JSU)*
Mississippi College	*(MC)*
Mississippi State University	*(MSU)*
University of Mississippi	*(UM)*
University of Southern Mississippi	*(USM)*

Mississippi EPSCoR
2010 Annual Meeting

15 April 2010

Presented by Gregory S. Tschumper

CompChem Senior Personnel

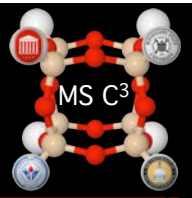


JSU:	Glake Hill		UM:	Amal Dass
	Danuta Leszczynksa			Robert Doerksen
	Jerzy Leszczynksi			Nathan Hammer
	Tigran Shahbazyan			Keith Hollis
				Greg Tschumper
MSU:	Steve Gwaltney			Randy Wadkins
MC:	David Magers	$24,578	USM:	Charles McCormick

Collaborative Seed Grant

UM:	Jason Ritchie	$38,625

CompChem Long-Term Fundamental Scientific Objective

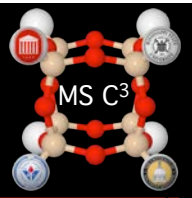


Develop a systematic understanding of the relationships between the organization and properties of matter at the atomic, molecular and supramolecular levels across the size scales from approximately 1 to 100 nm.

This understanding will dramatically improve our ability to design and synthesize controlled nanoscale objects with specific properties.

Position researchers in the state of Mississippi to address grand challenge issues (energy, climate, chemical/biological threats, etc.)

CompChem Cluster Long-Term Goals



1. Develop internationally recognized multi-institutional program of excellence in modeling and simulation of nanoscale chemistry that is tightly coupled to the experimental design, synthesis and characterization of nanoscale objects with specific properties

2. Recruit and retain top notch faculty in the field to assure critical mass

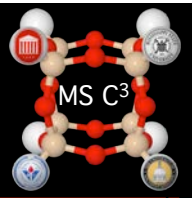
3. Ensure the availability of and access to the requisite HPC resources for increasing the scale of computational applications

4. Develop a suite of efficient computational tools for nanoscale chemistry that are thoroughly calibrated against well-characterized materials

5. Extend these computational tools for the modeling and simulation of nanoscale chemistry to new materials and biochemical phenomena, particularly those relevant to economic development in MS.

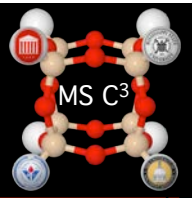
Design Principles → Grand Challenges

CompChem Objectives



1. Establish the *University and Industry Nanoscale Consortium* (*U&I-NC*)
2. Enhance collaborations within CompChem, especially inter-institutional
3. Establish cross-cutting collaborations with CompBio and BioSim
4. Develop and calibrate computational tools for nanoscale chemistry as well as their innovative application to systems relevant to economic development in Mississippi.
   - Task 1: First Principles Quantum Mechanics (QM) Methods
   - Task 2: Density Functional Theory (DFT) and Semi-Empirical (SE) Methods
   - Task 3: Molecular Mechanics (MM) Methods
   - Task 4: QSPR/QSAR Models
5. Develop, implement & disseminate a computational suite for nanomaterials

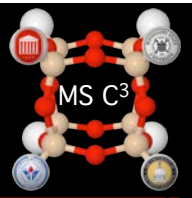
CompChem Technical Approach U&I-NC



1. Driven by and unified through real-world applications relevant to economic development in MS.
   - Nanomaterials for sensor technologies
   - Plasmonic nanostructures
   - Nanopores in organometallic and carbon nanotubes
   - Toxicity of nanomaterials
   - Polyhedral oligomeric silsesquioxanes (POSS®)
   - Bio- and synthetic-polymer hydration
   - Magic-sized gold nanoparticles
   - Carboxylesterase inspired biomimetics
2. Tightly coupled computational/experimental approach
   - Computation: development, validation, application
   - Experiment: design, synthesis, characterization

CompChem Technical Organization

U&I-NC



Computational Applications
Modeling and Simulation
JSU, MC, MSU, UM

Computational Development
New Methods for Nanoscale Chemistry
JSU, MSU, UM

Feedback

• New synthetic targets
• New experimental design

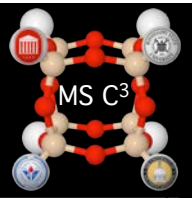
• Structure
• Properties

• Refinement
• Validation

Synthesis of Nanomaterial
UM, USM, Hybrid

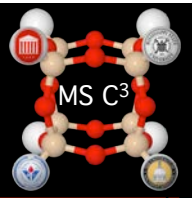
Experimental Characterization
UM, USM, Hybrid

CompChem Accomplishments: 09/01/09 - present



- 33 Peer reviewed papers published, accepted or in press
  - 7 are review articles
  - 13 acknowledge EPSCoR support
- 9 Papers submitted and currently undergoing review
  - 0 are review articles
  - 9 acknowledge EPSCoR support
- 1 Book chapter
- 16 Invited lectures at colleges and universities by senior personnel
- 12 Conference presentations by senior personnel
  - 5 were invited lectures
  - 2 were plenary or keynote lectures
- 47 Conference presentations by students
- 5 Conference presentations by research associates

CompChem Accomplishments: 09/01/09 - present



- 13 Active grants* totaling $5,251,874
- 9 Pending proposals totaling $5,969,632
- 9 Declined proposals
- 11 Graduate students supported
  - 1 Ph.D. dissertations completed
  - 2 M.S. theses completed
- 11 Undergrad researchers supported
  - 1 Undergraduate research theses completed
- 1 Provisional patent application

* Does NOT include current EPSCoR award

CompChem Student Highlights 09/01/09 - present

★ S. Stoddard (UM): Selected to attend meeting of Nobel Laureates in Lindau, Germany

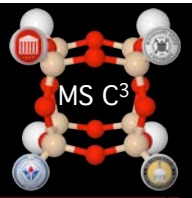
S. Stoddard (UM): Fellowship to attend the Euroscience Open Forum in Torino, Italy

★ K. Copeland (UM): 2010 Winifred Burks-Houck Graduate Student Leadership Award

K. Copeland (UM): Fellowship to attend 2010 CENTC Summer School on Organometallic Catalysis in Seattle, WA

Anna Hailey (UM): Barry M. Goldwater Scholar

CompChem Highlights 09/01/09 - present



N. Hammer (UM): NSF CAREER Award

J. Leszczynski (JSU): Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring

J. Leszczynski (JSU): Advisory Committee for NSF Directorate of Mathematical and Physical Sciences

J. Leszczynski (JSU): Editor of Computational Chemistry, Reviews of Current Trends

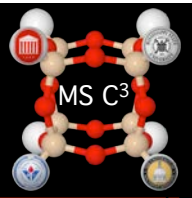
J. Leszczynski (JSU): Editor of Structural Chemistry

A. Dass (UM): J. Am. Chem. Soc. 2009, 131, pp 13604–13605 (and another just before reporting window 26 Aug 2009, 131, pp 11638-12020)

G. Tschumper (UM): Quantum Chemistry Section Ed., Ann. Reports in Comp. Chem.

G. Tschumper (UM): Associated Ed., Journal of Atomic and Molecular Sciences

CompChem Highlights 09/01/09 - present



T. Shahbazyan (JSU): Program Committee, 2009 SPIE Conference on Plasmonics: Metallic Nanostructures and their Optical Properties VII, Aug. 2-6, 2009, San Diego

T. Shahbazyan (JSU): Program Committee, 2009 SPIE Conference on Plasmonics: Nano-imaging, Nanofabrication and their Applications V, Aug. 2-6, 2009, San Diego, CA

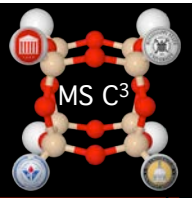
R. Doerksen (UM): Junior Investigator, NIH Centers of Biomedical Research Excellence (COBRE) Centers of Research Excellence-Natural Products Neuroscience

R. Doerksen (UM): Phi Lambda Sigma Pharmacy Leadership Society

R. Doerksen (UM): Rho Chi Academic Honors Society in Pharmacy

R. Doerksen (UM): Session Chair, "Quantum Chemistry. The Quantum and Physical Worlds Meet." 237th ACS National Meeting, Division of Computers in Chemistry, Salt Lake City, UT, March 2009

Cyber Infrastructure Upgrades at MCSR

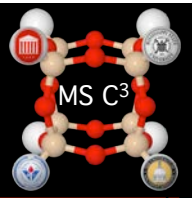


CompChem dedicated $88,713 for a hardware upgrade to “sequoia”, an SGI Altix XE Xeon cluster housed at the MCSR on the UM campus.

- 50% increase in computing power of sequoia (from 2.4 to 3.6 Tflops)
- 20% increase in overall computing power at MCSR

MCSR resources (hardware and comp chem software) are freely available to ALL senior personnel as well as their students and staff.

Reasearch Activities and Highlights



Synthesis and Characterization of Gold-Nanoparticles

QSAR/QSPR Models for Nanoparticles

Modeling of Defects in Carbon Nanotubes with QM Methods

Modeling of Plasmonic Nanostructures

Systematic Computational Analysis of Human Protein Kinases

Synthesis & Characterization of Highly Stable Blue-Emitting Molecular Crystals

Efficient and Accurate QM Methods for Clusters: Fragmentation + ONIOM

Synthesis and Characterization of Gold-Nanoparticles

Key Senior Personnel:

A. Dass, UM

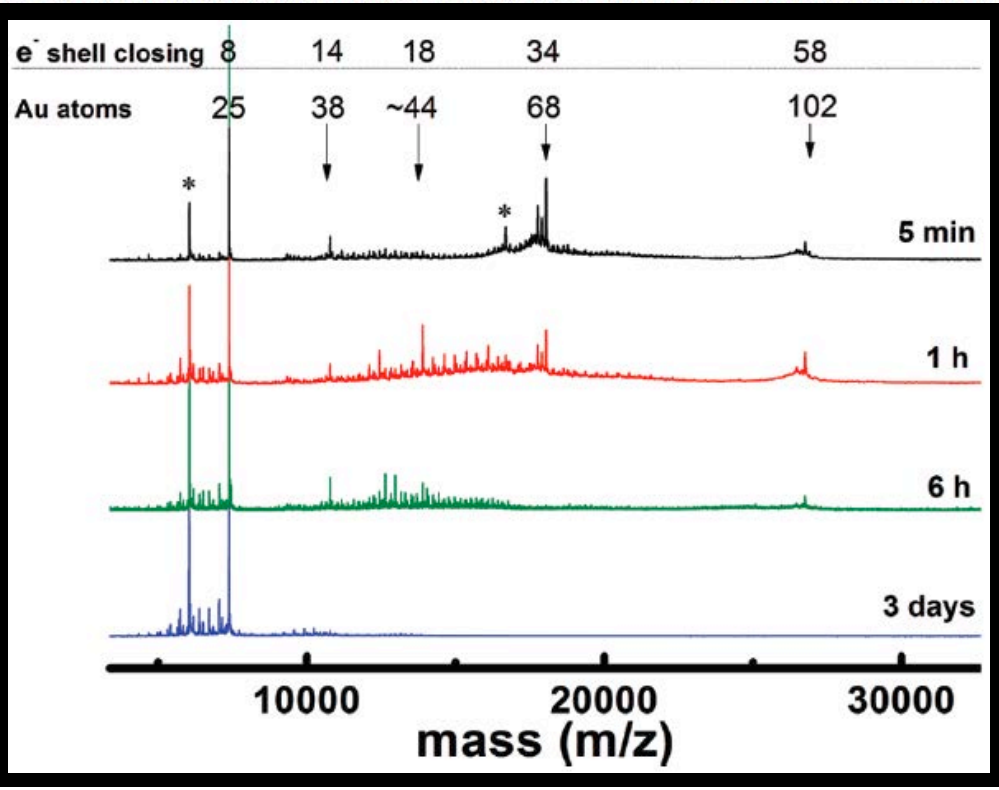
J|A|C|S COMMUNICATIONS

Published on Web 09/02/2009

Nanocluster Size Evolution Studied by Mass Spectrometry in Room Temperature $Au_{25}(SR)_{18}$ Synthesis

Asantha C. Dharmaratne,† Thomas Krick,‡ and Amala Dass*,†

Department of Chemistry and Biochemistry, University of Mississippi, University, Mississippi 38677, and Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, St. Paul, Minnesota



Other Collaborators:

Laurence Angel (Texas A&M-Commerce)

Bernedette Quinn (Finland)

Sang-Kee Eah (Renesselaer)

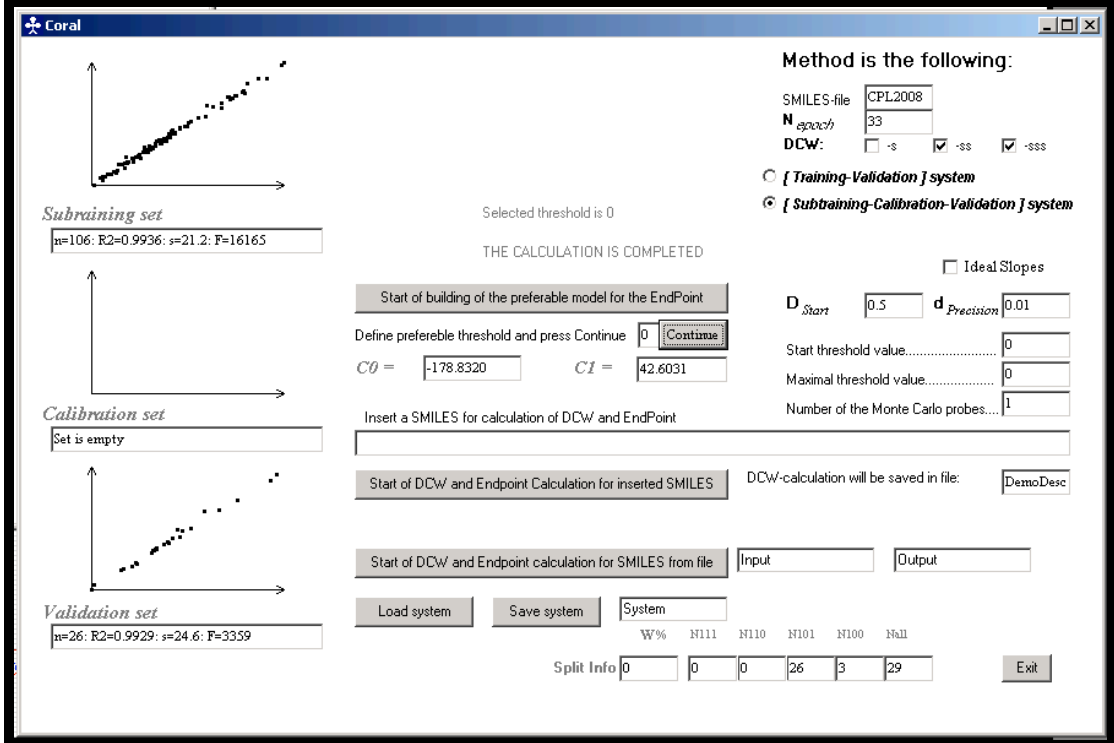
Thomas Burgi (U. of Heidelberg)

CORAL (CORelations And Logic) Freeware

Key Senior Personnel: *D. Leszczynska, JSU* *J. Leszczynski, JSU*

CORAL – a new QSAR program for predicting the properties of nanoparticles

Looking for Quantitative Structure – Property Relationships (QSPRs) between the molecular structure of [C60] and [C70] fullerene derivatives and their solubility



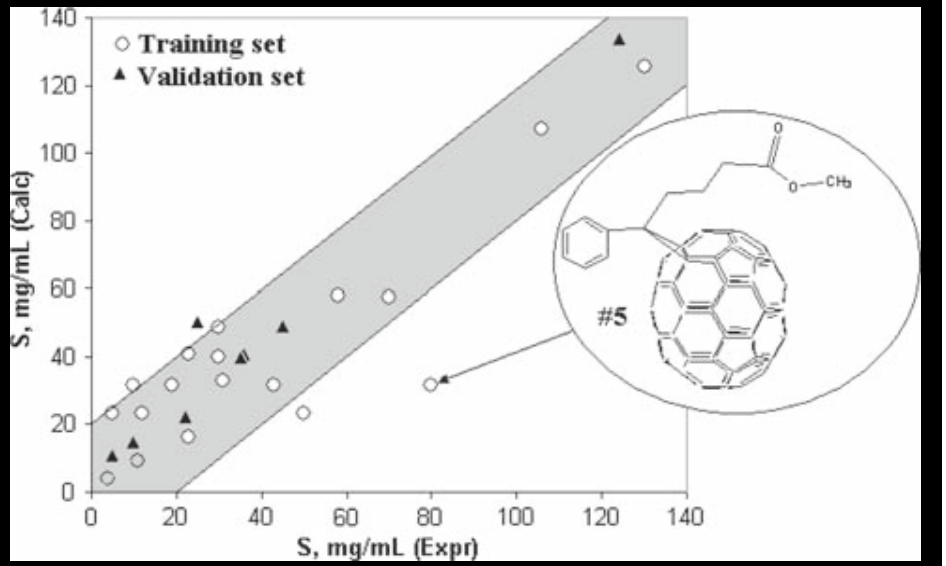
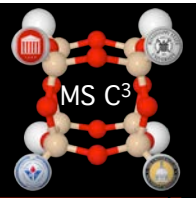


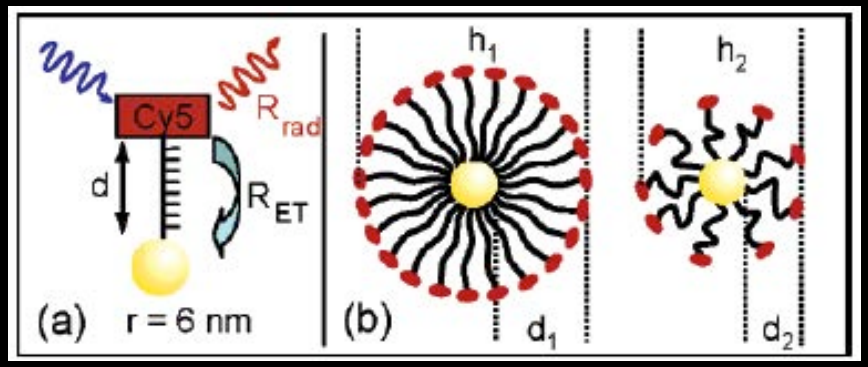
Figure. Experimental and calculated values of [C60] and [C70] fullerene derivatives solubility in chlorobenzene. Structure #5 is an outlier.

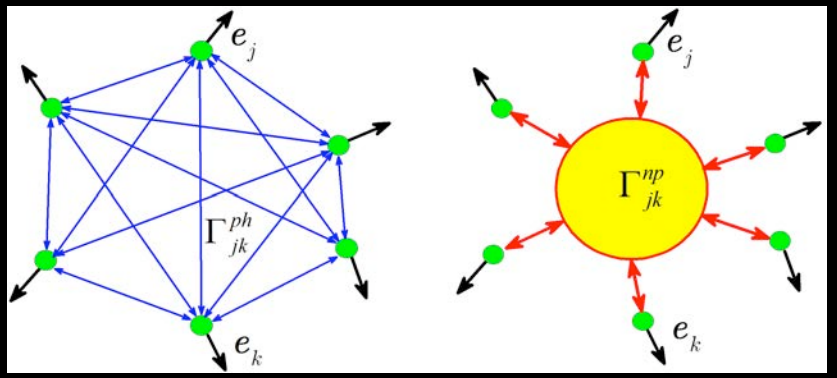
Modeling Plasmonic Nanostructures

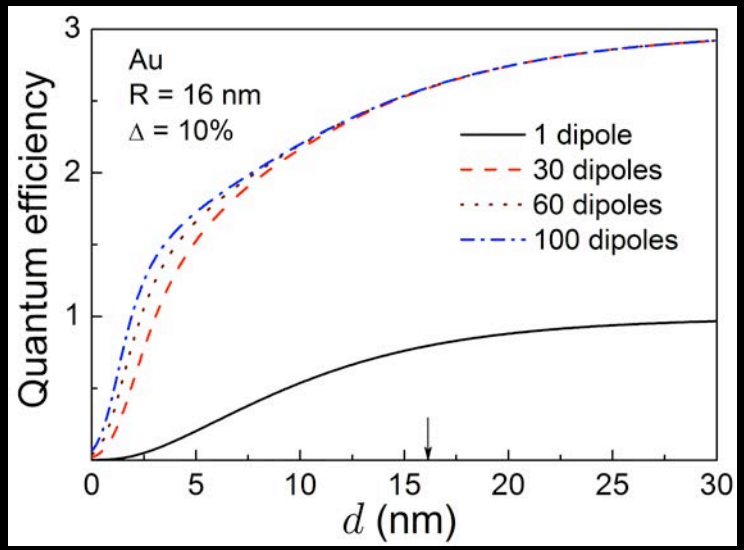


Key Senior Personnel: *T. Shahbazyan, JSU*

Plasmonic Dicke Effect: A new mechanism for cooperative emission of light by an ensemble of fluorescing molecules located near a metal nanostructure – via exchange of surface plasmons. The radiated energy of an ensemble is just thrice that of a single molecule near a nanostructure.







V. N. Pustovit and T. V. Shahbazyan, Phys. Rev. Lett. 102, 077401 (2009); Submitted to PRB; arXiv:1001.0422

Systematic Computational Analysis of Human Protein Kinases

Key Senior Personnel: *Robert Doerksen, UM*

Multiscale modeling used to combine detailed QM calculations on important residue-residue interactions; protein binding site prediction routines; approximate protein-protein docking; and force-field calculations to refine the predicted structure and dynamics of the kinase-protein interactions.

Proteomic information on clustering of the whole kinome according to similarity is used to select target kinases for detailed study from each cluster.

The ever-growing databases of experimental kinase structural and interaction data will be used to test/validate the methods.

External Collaborators:
Dr. Mark Hamann of Dept. of Pharmacognosy, UM
Dr. Alejandro Mayer, Midwestern U. (Illinois)
Dr. Douglas Walker, Sun Health Research Institute (Arizona)

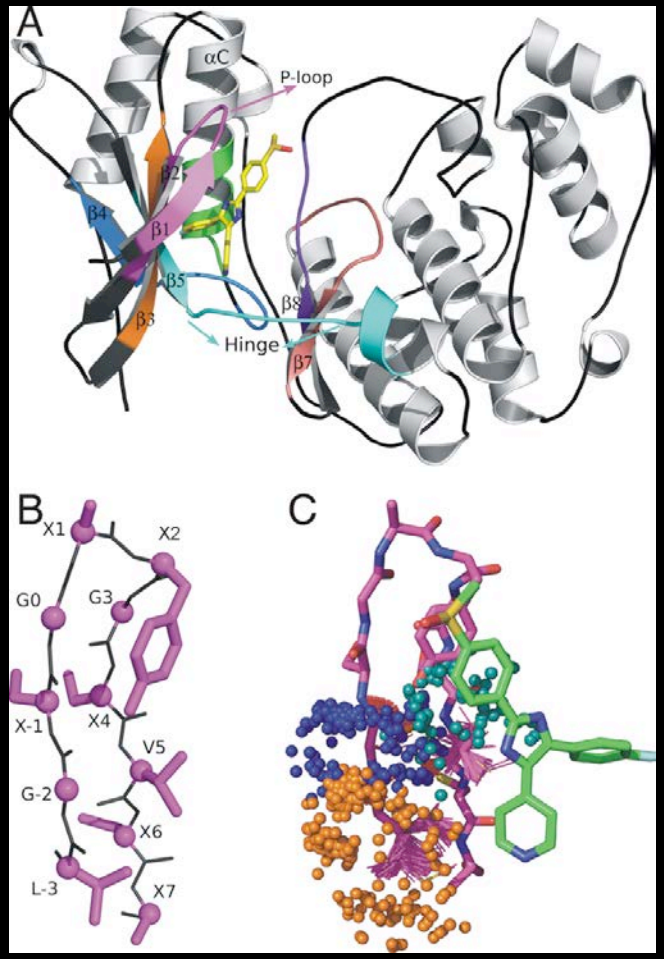
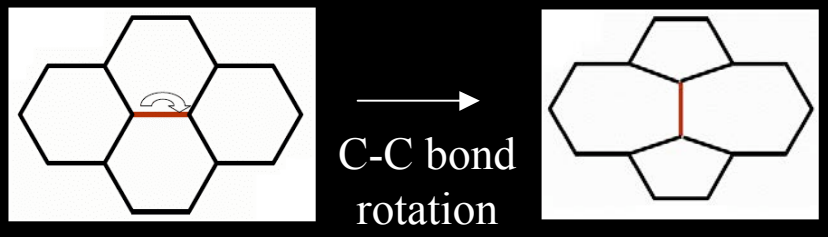


Figure taken from: RY Patel; RJ Doerksen "Protein kinases-inhibitor database: Analysis of structure variability and protein-inhibitor interactions within the P-loop," Journal of Proteome Research, submitted (2010).

Modeling Carbon Nanotube Defects

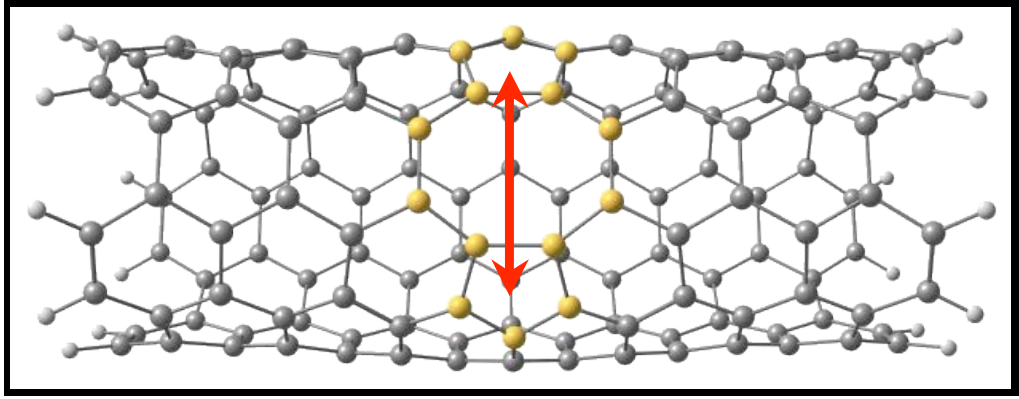
Key Senior Personnel: *J. Leszczynski, JSU*

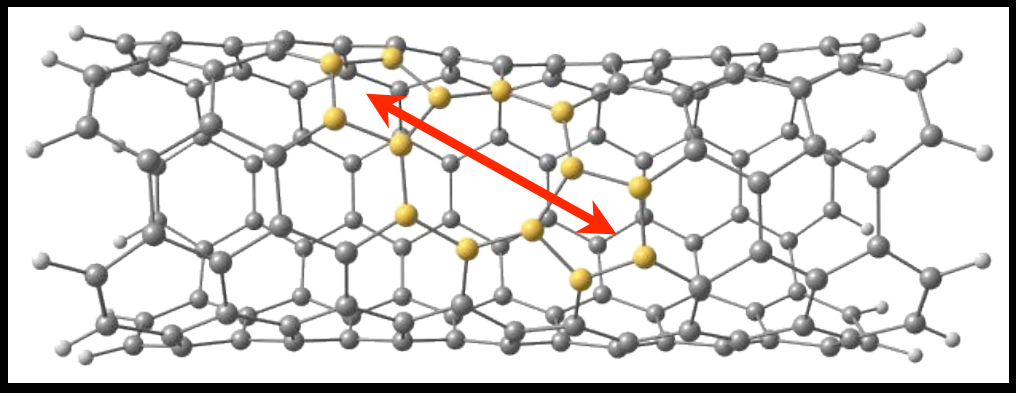
Stone-Wales (SW) defect is one of the most important defects in the nanotubes. A single C-C bond rotation by 90° generates two pentagon-heptagon pairs.



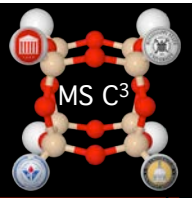
Vacancy defects (single, double, etc.)

DFT computations reveal significant energetic dependencies on the alignment of the defect with the the main axis as well as on the curvature of the nanotube





Ongoing and Planned Research Activities



Regular (annual or semiannual) CompChem meetings (supporting SSCC-MS)

Monthly CompChem meetings via webinar software

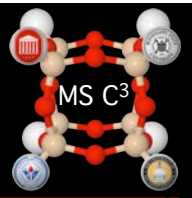
Wadkins (UM) and Gwaltney (MSU) are collaborating with researcher at Univ. of Notre Dame (Dr. Izaguirre) to couple normal mode and molecular dynamics calculations in order to better describe the low frequency motions of enzymes

Hill (JSU) and Magers (MC) collaborating on ring strain projects and are co-directing a female Ph.D. student at JSU (Shelley Huskey)

Hollis (UM) is in discussion with Hybrid Plastics to prepare a joint grant proposal

Dass (UM) is establishing international collaborations for his work on nanoparticles

Ongoing and Planned Research Activities



Spectroscopic Studies of Nanoparticles

- Single Molecule Spectroscopy of Molecules with Nonlinear Optical Properties
- Single Molecule Spectroscopy of Molecular Rectifiers
- Tracking Quantum Dots in Skin for Future Drug Delivery Applications
- Spectroscopy of Stable Blue-Emitting Molecular Crystals

Potential overlap between the organometallic nanotubes with nanopores synthesized by Hollis (UM) and the CNT defects studied by Leszczynksi (JSU)

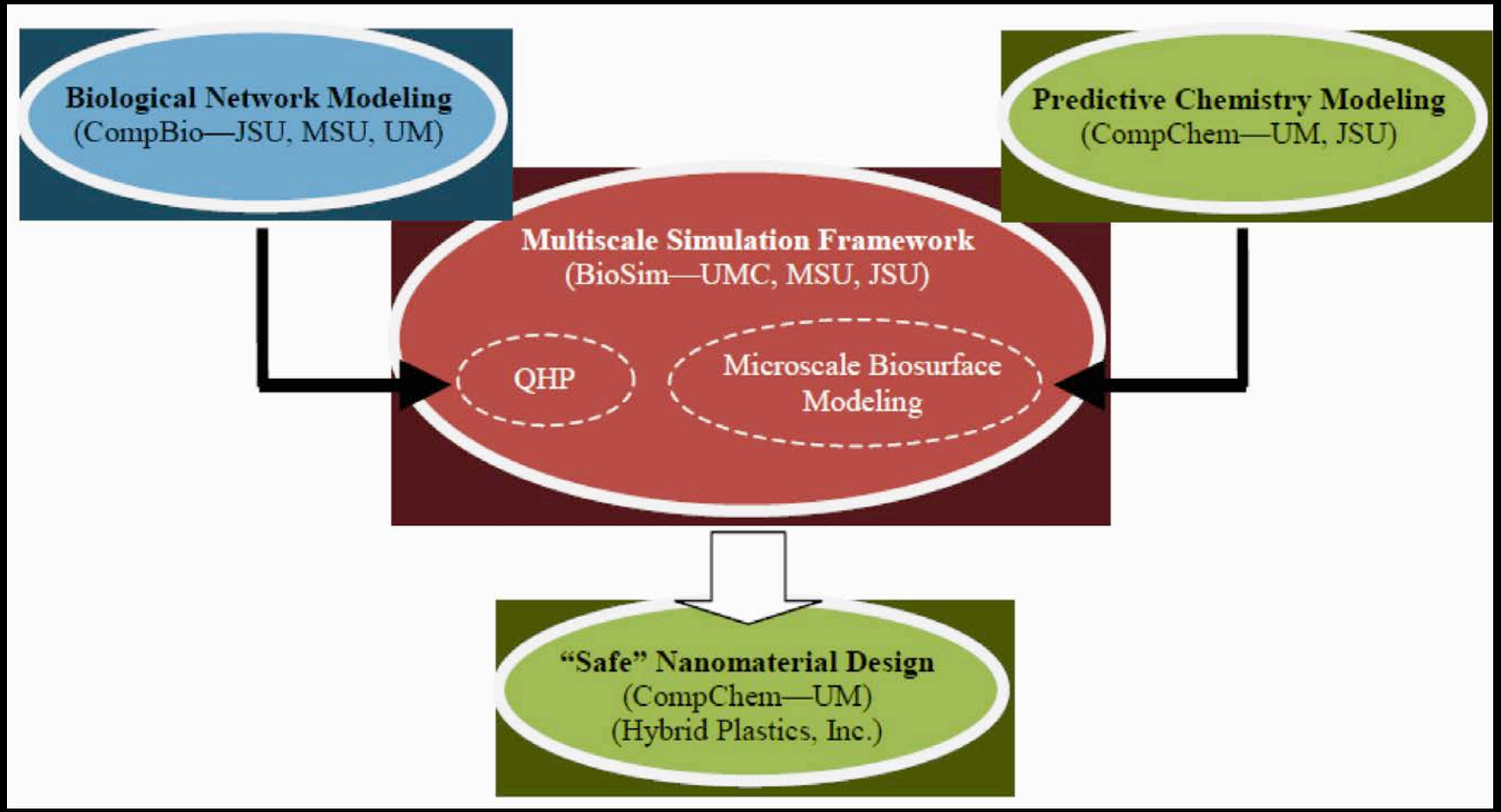
Magers (MC) and Ritchie (UM) performing a joint computational and experimental investigation of the mechanism of proton conductivity in an anhydrous proton conducting electrolyte

Magers (MC) and Hammer (UM) collaborating to study the fundamental solvation shells of the important osmolyte Trimethylamine N-oxide (TMAO) spectroscopically and computationally

Technical Organization of Proposed RII

Cross-Cutting Research Activities

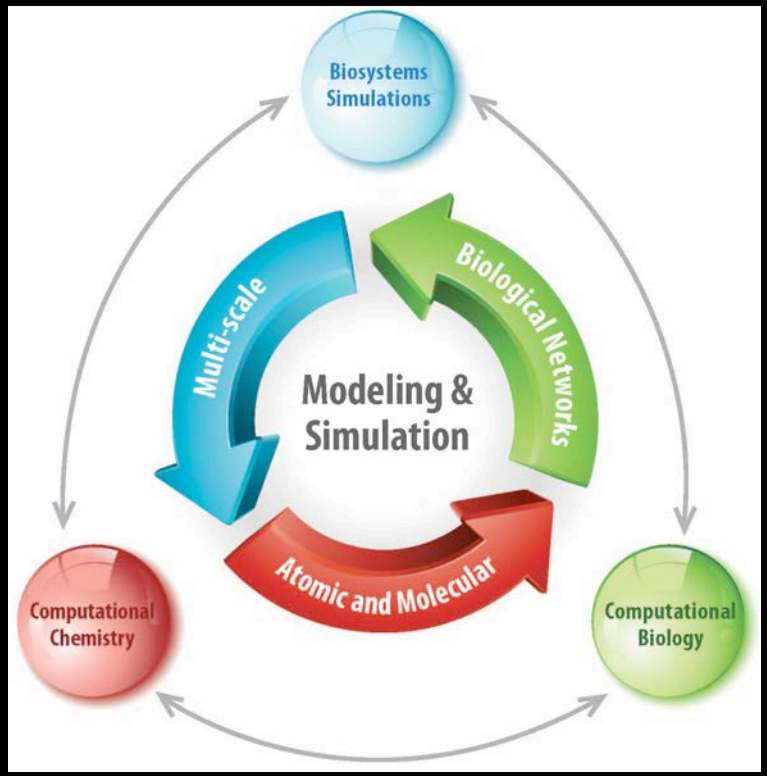
Predicting Biological Impact of Newly Developed Nanomaterials



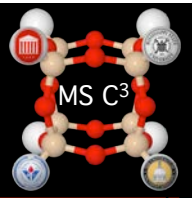
Other Cross-Cutting Activities

An IGERT proposal is being prepared at UM with PIs from CompChem (Wadkins) and CompBio (Wilkins). "IGERT: Knowledge from Data" The central theme of the project is the handling and analysis of large data sets, whether from genomics or a molecular dynamics simulation. This project could potentially unify all three areas.

A potential collaboration between R. Doerksen (UM), A. Wysocki (UMMC) and Hybrid Plastics has been identified. Wysocki has received a Seed Grant to engineer and test POSS-modified biomaterials for cartilage replacement/regeneration in joints.



Summary



Current Progress (09/01/09 - present)

- Significant upgrade to computational facilities at MCSR
- Several inter-institutional collaborations within CompChem established
- CORAL freeware available

Future Plans

- Continue to identify cross-cutting applications
- Collaborations with Hybrid Plastics
- Method and software development for computational nanoscale chemistry

Questions?