WORKSHOP ON

GAS PHASE SPECTROSCOPY & THEORETICAL APPROACHES

2019

March 6 - 9

University of California Santa Barbara

Organizing Committee

Glake Hill	Jackson State University
Mattanjah DeVries	University of California, Santa Barbara

Staff

Shonda Allen	Jackson State University
Galina Lobodina	Jackson State University

Support

National Science Foundation (CREST Program)
NIH-RISE
NASA

Schedule of Events

JSU-UCSB Workshop on Gas Phase Spectroscopy & Theoretical Approaches 2019

MARCH 6–9, 2019

SANTA BARBARA, CA

Wednesday, March 6, 2019

1:00P–2:00P Research and Scientific Collaboration: "Near Threshold Excited State Dynamics in Nucleobases and Related Compounds"

2:00P–3:00P Educational Incubator with MROC staff
- UDRL Model Points
- Center/Industry Integration

3:00P Wrap-up

6:00P **Organizers Reception and Dinner**
- University of California, Santa Barbara Multicultural Center

Thursday, March 7, 2019 – Collaboration Research Presentations

4:00P – 4:05P Opening Remarks

4:05P – 4:30P Keynote Speaker: Dr. Glake Hill, Jackson State University

4:30P –5:10P **Miranda Sroda** "Photomechanical Material Systems—From Molecules to Devices"

Jun Hee Jang "Deoxydehydration (DODH) of Biomass-Derived Polyols with a Reusable Unsupported Rhenium Nanoparticles Catalyst"

5:10P – 5:20P **Coffee Break**

5:20P – 6:00P **Latasha M. Franklin** "A Theoretical Study of Selected Heavy Metals and Biochemical Molecules as Potential Chelation Therapy"

Emily Schueller "Developing structure-property relationships for perovskite photovoltaics"

Friday, March 8 – Collaboration Research Presentations

9:00A – 9:05A Opening

9:05A – 10:25A **Yvonne Diaz** "Probing the utility of Donor Acceptor Stenhouse Adducts as sensors"

Fredrick Allen & **Alexander Reed** "A Computational Approach to Identifying the Structure and Properties of Biochar"

Raymond Thicklin "Development of Dynamic Nuclear Polarization Hardware to Aid in DNP Research"

Micah Anderson "N-arylnaphthylamines as inhibitors of HIV integrase- LEDGF/p75 interactions: Theoretical studies"

10:25 – 10:35A **Coffee Break**

10:35A – 11:55A **Kimberly Madison** "Computational Study of Charge Carrier Mobility in Watson and Crick Deoxyribonucleic Acid (DNA) Bases Pairs for Predictions of Hole Mobility"

Gregory Gate "Extending the search for life using photostability as a metric"

Precious K. Hollins "A Full Electron Study of Metal Complexes as Antitumor Drugs"

Michael Haggmark "Mechanisms of Photostability for Indigo and Hydroxyanthraquinone dyes"

11:55A – 1:15P **Lunch**

1:15P – 2:35P **Nathan Svadlenak** "Structure and lifetime"

Lakeeta Sanders "Computational Development of an Organic Sensor and Sensor Characteristics"

Kan Tagami "Role and source of biradical J coupling in dynamic nuclear polarization"

Sadia Nowshin "Conformational Analysis of Novel Anti-microbial Alkaloid, Solenopsin"

2:35P – 2:45P **Coffee Break**

2:45P – 3:45P **Greg Campbell** "Exploring Molecular Evolution and the Many Roles of RNA"

Sabrevian Davis "A Computational Overview of Peptide Nucleic Acids"

Nate Charest "Computational Approaches to Studying Amyloid Fibril Formation"

Saturday, March 9, 2019 – Faculty Collaboration Workshops

9:00A – 12:00P Faculty Collaboration Workshop-Materials Research Laboratory

12:00P – 1:00P Lunch (on own)

1:00P – 2:00P Faculty/Staff Tour of MRL Facilities

Abstracts

JSU-UCSB Workshop on Gas Phase Spectroscopy & Theoretical Approaches 2019

MARCH 6–9, 2019

SANTA BARBARA, CA

A Computational Approach to Identifying the Structure and Properties of Biochar

Fredrick Allen, Alexander Reed, Ana Uroic Stefanko, Karina Kapusta, Danuta Leszczynska, Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

Many environmental issues such as climate change, water pollution, and soil degradation pose a danger to society. To remediate these problems, an enormous amount of research has been devoted to biochar due to its potential to adsorb harmful pollutants. Biochar's chemical and physical properties, such as, a large surface area, a cation exchange capacity, and having a high water-holding capacity, make it suitable to use in many applications. Although biochar has many possible benefits, much needs to be understood about the preparation of biochar and the structure and properties under different initial conditions. Current research at Jackson State University has shown an increased carbonization and pore formation with increased pyrolysis temperature with pine straw and corn leaves. FTIR analysis was performed to evaluate the surface changes on different experimental settings. Samples that were produced at the temperature of 300 °C showed very little or none existence of comb-like pores. Preliminary experiments for lead (Pb^{2+}) removal from aqueous solution showed high adsorption capacity of 86% for a polluted water with 150µg/l.

Some quantum-chemical studies have been done. However, it is a major challenge to visualize the proper surface of biochar for further calculations due to uneven porous surface. Computational chemistry, can become a beneficial addition to current experimental research, which will give insight into the properties of biochar. We will use a Quantitative Structure Property Relationship (QSPR) technique in order to build a model for prediction of biochar's properties, such as an adsorption of heavy metals and organic pollutants, depend on initial conditions of its production.

N-arylnaphthylamines as inhibitors of HIV integrase- LEDGF/p75 interactions: Theoretical studies

M. Anderson, J. Harris, T. Anderson, K. Kapusta, G. Hill

Interdisciplinary Nanotoxicity Center, Jackson State University, Jackson, MS, 39217, USA

Design of effective drugs is one of the most substantial goals of computational chemistry nowadays. None of the existed medication can fully treat the dangerous venereal disease AIDS. However, various drugs that could inhibit HIV activity have been discovered and studied. "LEDGINs" are the small compounds that inhibit LEDGF/p75-IN PPI. They have proven a good antiviral activity. Some of the representatives of this class of inhibitors are N-aryl-naphthylamines. Crucitti et al. [1] have analyzed the inhibitory activity of various N-aryl-naphthylamines towards HIV. The idea, that a carboxylate functional group has a positive influence on the inhibition activity has been proposed, hoverer not completely proven. Some compounds having the carboxylic and methyl-carboxylic groups have also shown low or no activity at all.

The N-aryl-naphthylamines were visualized with GaussView 15, and then Gaussian09W was applied to perform quantum chemical calculations. Structures were optimized at CAM-B3LYP/6-31G_ESKJ level of theory. Natural bond orbital (NBO) calculations have been performed in order to analyze charge distribution and active sites.

Molecular docking has been performed using Schrodinger suite. Energies obtained by docking calculations have not demonstrated a correlation with inhibition activity. It has shown that not only the process of LEGINs' binding to protein but many other factors could influence the inhibition activity. One of the assumptions is a possibility of N-arylnaphthyl-amines to bind HIV-1 IN after integration of CCD and IBD subunits. We have also performed a quantitative structure-activity relationship (QSAR) study. Three models for prediction of AlphaScreen% inhibition activity have been developed, including multiple linear regression and k-nearest neighbor methods. Developed models have shown a good prediction accuracy and have given us an idea of relationship between the structure of N-arylnaphthyl-amines and their inhibition activity against HIV.

[1] G. Cuzzucoli Crucitti, L. Pescatori, A. Messore, V.N. Madia, G. Pupo, F. Saccoliti, L. Scipione, S. Tortorella, F.S. Di Leva, S. Cosconati, E. Novellino, Z. Debyser, F. Christ, R. Costi, R. Di Santo, Discovery of N-aryl-naphthylamines as in vitro inhibitors of the interaction between HIV integrase and the cofactor LEDGF/p75, Eur. J. Med. Chem. 101 (2015) 288–294. doi:https://doi.org/10.1016/j.ejmech.2015.06.036.

A Computational Overview of Peptide Nucleic Acids

Sabrevian Davis, Latasha M. Franklin, Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

The double helix of (deoxyribose nucleic acids) DNA is the way that living organisms store, retrieve and communicate genetic information. The ability of DNA to be unwound and be placed back into the same original configuration, is a unique property that it possesses. Since DNA is specific, single strands can be synthesized. Therefore, the base genes can be further studied and manipulated. Synthetic oligonucleotides are now used by scientists in various disciplines. Originally peptide nucleic acids (PNAs) were used as ligands for the recognition of double stranded DNA. Today, however, PNAs are used for biosensors, artificial restriction enzyme systems, catalytic molecular scissors, and therapeutic intervention. In this work, we will look at several conformations of PNAs and specifically focus on their potential surface energy.

A Theoretical Study of Selected Heavy Metals and Biochemical Molecules as Potential Chelation Therapy

Latasha M. Franklin and Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

Frequently, we are plagued with the major environmental issue of heavy metal contamination. It is of utmost importance for this to be addressed. Even more dire is that these heavy metals from the environment progress through the ecosystem until they, eventually, enter the human body. These metals lie dormant until there is an overwhelming concentration present, thus, causing heavy metal poisoning, which leads to numerous health challenges . Because of this threat to human health, it is pertinent to examine ways to rid the body of these heavy metals upon initial contamination to prevent accumulation. To investigate the proper disposal of these toxins, heavy metal ions such as Fe+2, Cu+2, Mn+2, Co+2, and Cr+2 are bound to histidine, which is an essential amino acid found in the body. Free energy of hydration is presented, as well as, initial studies on metal interactions with histidine. The chemical properties of these complexes will be evaluated . Furthermore, this will suggest how histidine and other biochemical molecules can be remediated. Hopefully, the results will yield a more effective means of preventing heavy metal accumulation and poisoning.

A Full Electron Study of Metal Complexes as Antitumor Drugs

Precious K. Hollins, Latasha M. Franklin, Wojciech Kolodziejczyk, Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

In recent years, there has been an increase in the prevalence of metal complexes used for medicinal purposes. Particularly, vanadium, as a trace bioelement, displays a variety of biological properties. This metal exhibits potent anti-HIV effects towards infected immortalized T cells, as well as, antimicrobial, antitumor, and insulin-enhancing effects. In particular, the involvement of oxovanadium (IV) complexes in the treatment of malignant tumors will be studied, theoretically. Prior experimental studies have revealed that VO(PAHN)(phen) exemplifies behavior similar to the infamous antitumor drug, cisplatin. Both having an inhibitory concentration of 50%. It is imperative to study the interaction of this compound with relevant biomolecules and their model systems. Steric differences, electrostatic potential surfaces, DNA binding, and other chemical properties of oxovanadium(IV) complexes and cisplatin will be investigated by utilization of computational means. Potentially, an inexpensive, more effective and less toxic antitumor drug will be developed to assist in the treatment, prevention, and eradication of cancerous cells.

Computational Development of an Organic Sensor and Sensor Characteristics

Javauny Hyde, Sabrevian Davis, Lakeeta Sanders, Wojciech Kolodziejczyk, Glake Hill

Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

Water quality is important for sustaining life and for proper functioning of the ecosystem. Our ecosystems yield food and economic development for many along the Southern Coastal area. It is critical to detect and remove pollution before our ecosystems are destroyed. However, there remains very few options to detect these changes within the water system. One such change that would be important to detect are the rising carbon dioxide levels in water. When the oceans absorb CO_2, the chemical reaction that takes place produces carbonic acid (H_2CO_3), which increases the acidity (lowers the pH) of seawater. Many scientists believe that the decreasing pH in the oceans interfere with the ability of certain marine animals, such as corals and other calcifying marine organisms, to make their skeletons and shells from calcium carbonate minerals. There are several potential compounds that can be used to detect CO_2 due to the binding properties of the molecule. In this work, we will explore the absorption of carbon dioxide in water with a well-known CO_2 binding compound known as Triazabicyclodecene (TBD). TBD has been chosen to promote the insertion of CO2 because it has been proven to strongly bind CO2. Upon learning this, several experimental nitrogen base compounds were created and their pk values were calculated and compared to that of TBD.

Computational Study of Charge Carrier Mobility in Watson and Crick Deoxyribonucleic Acid (DNA) Bases Pairs for Predictions of Hole Mobility

Kimberly Madison, Wojciech Kolodziejczyk, Glake Hill

[1]Interdisciplinary Center for Nanotoxicity, Jackson State University, Department of Chemistry, Physics, and Atmospheric Sciences

Deoxyribonucleic acid (DNA) is the genetic make-up that carries instructions for the development and function of all living organisms. While DNA synthesis have repair mechanisms to correct for mismatch base pairs, however, there are chances in which a genetic mutation can occur. These mutations are the cause of diseases such as, sickle cell disease, Huntington's disease, cancer, and many other diseases in which some of these diseases can be fatal. DNA could possibly be used in high performance devices such as organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and biosensors as the organic semiconductor (OSC) active layer. Using DNA as the OSC layer could have a profound affect in the medical technology field due to allowing early detection for the treatment and prevention of diseases we face in todays' world. In this work, we aim to calculate and increase the charge carrier mobility of these DNA bases.

Conformational Analysis of Novel Anti-microbial Alkaloid, Solenopsin

Sadia Nowshin, Glake Hill

Interdisciplinary Center for Nanotoxicity,Department of Chemistry, Physics, and Atmospheric Sciences, Jackson State University

Solenopsin is anti-microbial and anti-inflammatory alkaloid collected from Solenopsin invicta, commonly known as fire ants. The venom can provide defence against microbial pathogens and communication and serve as a novel source of bio-insecticide. In this study, the structure of the Solenopsin compound is being studied via m062x method and 6-31+g(d,p) basis set to find the lowest energy conformations, as they are considered more accurate methods for conformational analysis. The mechanism of bacterial membrane perturbation is studied using these lower energy conformations.

List of Participants

JSU-UCSB Workshop on Gas Phase Spectroscopy & Theoretical Approaches 2019

MARCH 6–9, 2019

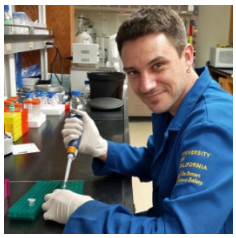
SANTA BARBARA, CA

Shonda Allen
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1325 Lynch St.
Jackson, MS 39217 U.S.A.
Tel: 6019793723
Fax: 6019797823
E-mail: shonda@icnanotox.org

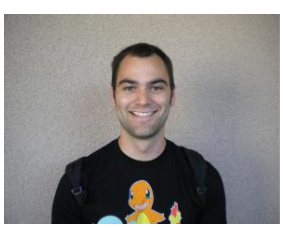
Fredrick Allen
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J.R. Lynch Street
Jackson, MS 39217

Micah Anderson
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J.R. Lynch Street
Jackson, MS 39217

Terica Anderson
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J.R. Lynch Street
Jackson, MS 39217



Greg Campbell
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

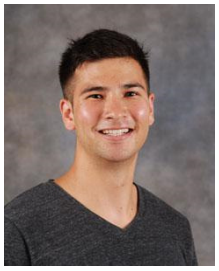


Nate Charest
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Sabrevian Davis
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
Jackson, MS 39217

Yvonne Diaz
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Latasha Franklin
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J. R. Lynch Street
P.O. Box 17910
Jackson, MS 39217-0510



Gregory Gate
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Michael Haggmark
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Precious K. Hollins
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J. R. Lynch Street
Jackson, MS 39217

Jun Hee Jang
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Sadia Nowshin
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
Jackson, MS 39217

Glake Hill Jr.
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1325 Lynch St.
P.O. Box 17910
Jackson, MS 39217 U.S.A.
E-mail: glakeh@icnanotox.org

Alexander Reed
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
Jackson, MS 39217

Karina Kapusta
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J.R. Lynch Street
Jackson, MS 39217

Lakeeta Sanders
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
1400 J.R. Lynch Street

Wojciech Kolodziejczyk
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J.R. Lynch Street
Jackson, MS 39217

Emily Schueller
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Galina Lobodina
Jackson State University
Department of Chemistry, Physics and Atmospheric Sciences
1400 J. R. Lynch Street
Jackson, MS 39217 U.S.A.
E-mail: galina@icnanotox.org

Takia Smith
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
Jackson, MS 39217

Kimberly Madison
Jackson State University
Department of Chemistry, Physics, and Atmospheric Science
1400 J.R. Lynch Street
Jackson, MS 39217 U.S.A.

Miranda Sroda
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Nathan Svadlenak
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Raymond Thicklin
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Kan Tagami
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106

Mattanjah S. de Vries
University of California Santa Barbara
Department of Chemistry and Biochemistry
Santa Barbara, CA 93106-9510, USA
E-mail: devries@chem.ucsb.edu