JAMES MADISON UNIVERSITY®

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

40th Annual

SPRING UNDERGRADUATE RESEARCH SYMPOSIUM

THURSDAY MARCH 26, 2015

ORAL SESSION I: 1:45 – 3:30 PM (PHYS/CHEM 3216)
POSTER SESSION: 4:00 – 5:00 PM (PHYS/CHEM LOBBY)

FRIDAY MARCH 27, 2015

ORAL SESSION II: 1:15 – 3:15 PM (ISAT 259)
KEYNOTE ADDRESS: 3:30 – 4:30 PM (ISAT 159)

See back cover for image description.

Past Keynote Speakers

Each year we feature a keynote speaker for the Department's annual Spring Undergraduate Research Symposium. We are honored to have had speakers who are alumni of the department and are willing to come back and share with our students their experiences of "life after JMU". We thank each of these speakers and look forward to future alumni participation in Spring Symposium.

YEAR	JMU CLASS	SPEAKER	AFFILIATION
2015	1994	**Dr. Michael Leopold**	*University of Richmond*
2014	1996	**Dr. Dana McGraw Dattelbaum**	*Los Alamos National Laboratory*
2013	1999	**Dr. Christy Vestal Martin**	*Vorbeck Materials*
2012	1994 N/A	**Dr. Melissa C. Rhoten** **Dr. Orde Q. Monro**	*Longwood University* *University of KwaZulu-Natal*
2011	1992	**Dr. Morgan S. Sibbald**	*The Sherwin-Williams Company*
2010	1988	**Dr. Kevin Morris**	*Carthage College*
2009	1988	**Dr. Chris E. Holmes**	*The University of Vermont College of Medicine*
2008	1995	**Dr. Jonathan Dattlebaum**	*University of Richmond*
2007	1987	**Dr. Elizabeth Perry (M.D.)**	*Signature Healthcare, Inc.*
2006	1967	**Dr. Carolyn Abitbol (M.D.)**	*University of Miami (FL) School of Medicine*
2005	1975 1976	**Dr. Daniel Downey** **Dr. Gary Rice**	*James Madison University* *College of William and Mary*
2004	1987	**Dr. James (Dusty) Baber**	*National Institutes of Health*
2003	1984	**Dr. Fred King**	*West Virginia University*
2002	1977	**Dr. Roger Bertholf**	*University of Florida School of Medicine*
2001	1979	**Mrs. Katheryn Lam**	*International Business Machines*
1999	1987	**Dr. Jose Madalengoitia**	*University of Vermont*
1997	1986	**Dr. Fred R. Kinder**	*Novartis Research Institute*
1996	1976	**Dr. Terry O. Trask**	*DuPont Chemicals*
1995	1973	**Dr. Carl Lentz**	*Eastman Fine Chemicals*
1994	1990	**Dr. Michele A. Kelly**	*University of Maryland Baltimore County*
1993	1985	**Dr. Cynthia K. Fallon**	*DuPont Chemicals*
1992	1983	**Dr. Laurie Locascio**	*National Institute of Standards and Technology*
1991	1983	**Dr. Noreen Naiman**	*North Carolina School of Science and Mathematics*
1990	1982	**Dr. Matthew T. Stershic**	*Atomchem North Amercia*
1989	1982	**Dr. Michael Kinter**	*Cleveland Clinic Lerner Research Institure*
1988	N/A	**Dr. Thomas J. Meyer**	*Los Alamos National Laboratory*
1987	1980	**Dr. Steven Davis**	*Naval Research Laboratory*
1986	1980	**Dr. Steven A. Hackney**	*Michigan Technological University*
1983	1978	**Dr. Richard B. Lam**	
1982	1975	**Dr. Daniel Downey**	*West Virginia University*
1981	1959	**Mr. Ronald E. Ney**	*Environmental Protection Agency*
1980 1979	N/A 1973	**Dr. Stanley G. Sunderwirth** **Dr. Carl Lentz**	*Metropolitan State College (Denver, CO)* *Eastman Fine Chemicals*

40th Annual Department of Chemistry and Biochemistry
Spring Undergraduate Research Symposium

Keynote Speaker

Michael Leopold, PhD

(JMU Class of 1994)

Department of Chemistry
University of Richmond
Richmond, VA

Michael Leopold is a professor of chemistry at the University of Richmond. Originally from Yorktown, VA, Mike received an ACS-certified B.S. in Chemistry from James Madison University in 1994. While at JMU, Mike performed undergraduate research with Dr. Roddy Amenta, department of geology, studying computer modeling of microstructure evolution in polycrystalline materials. He was one of the founding fathers of the Gamma Kappa Chapter of Alpha Chi Sigma. Mike attended North Carolina State University for his graduate studies and obtained a Ph.D. in Analytical Chemistry in 2000 under the direction of Professor Edmond Bowden investigating the electrochemistry of cytochrome c at modified electrodes. Dr. Leopold was a postdoctoral associate in Professor Royce Murray's group at the University of North Carolina, Chapel Hill where he researched the electronic conductivity and electrochemical properties of nanoparticle film assemblies. In 2002, Mike joined the faculty at the University of Richmond and was subsequently tenured and promoted to the rank of Associate Professor in 2008. In 2012, Dr. Leopold was named to the Floyd D. and Elisabeth S. Gottwald Endowed Chair of Chemistry and was recently promoted to the rank of full professor (2014). Dr. Leopold's research interests include the study of nanoparticle-film assemblies, amperometric biosensors, the fate and transport of nanomaterials in the environment, and quantitative analysis of heavy metals in children's toys/toy jewelry. Dr. Leopold's research efforts have been supported with over $900,000 dollars of external grant funding provided by the National Science Foundation, ACS-PRF, Jeffress Memorial Trust, and the Commonwealth Health Research Board. Dr. Leopold and his undergraduate researchers have published 22 papers with over 50 undergraduate co-authors and presented findings at over 80 local symposia or regional/national meetings of the American Chemical Society. During his time at the University of Richmond, Dr. Leopold has been recognized with several awards including the Henry Dreyfus Teacher-Scholar Award (2010), Omicron Delta Kappa Professor of the Year (2007), Distinguished Educator Award (2008), and Outstanding Research Mentor Award (2009). His research has been featured in *CUR Quarterly* (2006) as well as *Chemical & Engineering News* (2015). In 2000, Mike married fellow chemistry major and JMU alumni Tammy Kelsey who became a doctor of veterinary medicine in 1999. Together they have two children, Kelsey and Michael and reside in Glen Allen, Virginia.

Oral Session I: Thursday March 26th *Phys/Chem 3216)*		
1:45 - 2:00	Tye S. Thompson, Anthony P. Allsbrook and Dr. Yanjie Zhang	Cation Effects on Caffeine Partitioning Thermodynamics
2:00 - 2:15	Joshua E. Temple and Dr. Gina MacDonald	Probing Buffer-specific Effects on Nucleotide Binding to RecA using Difference FTIR
2:15 - 2:30	Tracy A. Caldwell, Dr. Isaiah Sumner and Dr. Nathan T.Wright	The Strength of the M-band Titin/Obscurin Interaction is Directionally Dependent
2:30 - 2:45	Taylor P. Light, Karen M. Corbett, Michael A. Metrick and Dr. Gina MacDonald	Hofmeister ion and co-solvent effects on water structure and the aggregation and solvation of RecA
2:45 - 3:00	Diana Al Husseini and Dr. Yanjie Zhang	Effects of Amino Acids on Surface Tension of Water
3:00 - 3:15	Nicholas D. Cooper and Dr. Thomas C. DeVore	Kinetics of the Decomposition of Zinc Oxalate through Traditional and Isoconversional Methods
3:15 - 3:30	Kelly E. Du Pont, Dr. Isaiah C. Sumner and Dr. Christopher E. Berndsen	The Importance of the Disulfide Bonds within BST-2 for Structure and Viral Tethering

Poster Session: Thursday March 26th 4:00 – 5:00 pm *(Phys/Chem lobby)*	
Louis M. Damiano, John Marafino, Brenna Walsh, Matt Schmachtenberg, Mark Wenzel, Kirstie Thompson, Kristin McKenna, Kou Kunneang, Tara Gallenger, Dr. Kyle Seifert and Dr. Kevin L. Caran	The Synthesis and Study of the Biological and Colloidal Properties of Bolaamphiphiles
Aaron Davis and Dr. Isaiah Sumner	Nucleotide Effects in the GroEL Subunit
Kirstie Thompson, Brenna Walsh, John N. Marafino, Kristin McKenna, Louis Damiano, Tara M. Gallagher, Matt Schmachtenberg, Kunny Kou, Mark Wenzel, Dr. Kyle Seifert and Dr. Kevin L. Caran	Synthesis and Study of Polycationic Amphiphiles as Potent Antiseptics and Novel Colloids: Exploring Structure Activity Relationships
Sarah Jamison, Sarah B. Jamison, Syndey N. Fisher, Jens P.Haraldstadt, and Dr. Daniel M. Downey	Water Chemistry of North Branch Simpson Creek Before and After a Major Forest Fire
Matthew Oehler and Dr. Nathan T. Wright	The characterization of the Ig58 domain of the giant muscle protein obscurin
Rachel Policke and Dr. Nathan T. Wright	Structural Elucidation of the Ig59 Domain of Obscurin
Michael McDougal, David J. D'Amico, Dr. Donna S. Amenta, Dr. John. W. Gilje, Cristian G. Hrib and Frank T. Edelmann	Synthesis and Supramolecular Structures of Manganese Complexes with N-Pyrazolylpropanamide-Derived Ligands
Kelsey L. Berrier and Dr. Daniel M. Downey	Analysis of Nitrate-Nitrogen and Ammonium-Nitrogen in Lake Sediment by Solid Phase Extraction and Ion
Andy Heindel and Dr. Nathan T. Wright	Structural Elucidation of AggR-activated Regulator, Aar, in Enteroaggregative Escherichia coli
Tyler Price and Dr. Barbara Reisner	Mechanisms and kinetics of solvent loss in $Na[BH(C_2H_2N_3)_3]$
Santina Cruz, Dr. John W. Gilje, Dr. Donna S. Amenta and Dr. Glenn P.A. Yap	An Evaluation of the Chemistry of $RuCl_2(PPh_3)_3$ with Nitriles

(Student presenters underlined)

Oral Session II: Friday March 27th *(ISAT 259)*		
1:15 - 1:30	Kristin McKenna, John Marafino, Brenna Walsh, Kirstie Thompson, Louis Damiano, Brenden Wimbish, Gabriel Fitzgerald, Jhosdyn Barragan, Brandi Volkers, Nick Minahan, Jason Floyd, Monica Paneru, Caroline Dilworth, Sybelle Djikeng, Suma Haji, Stephanie Masters, Tara Gallagher, Jade LaDow, Kyle Bonifer, Dr. Kyle Seifert, and Dr. Kevin Caran	Novel Triscationic Single and Double-Tailed Amphiphiles: Synthesis and Characterization of Colloidal and Antibacterial Properties
1:30 - 1:45	Daniel Corbin, Brian J. Reeves, Devon M. Shircliff, Jessi L. Shott and Dr. Brycelyn M. Boardman	Tailoring Thienyl Phosphine Ligands for Improved Charge Transfer in Hybrid Photovoltaic Systems
1:45 - 2:00	Serban Zamfir and Dr. Isaiah Sumner	Molecular Dynamics Studies of the Ubiquitin Conjugation Mechanism
2:00 - 2:15	Shelsea Ann Hurdle, Michael L. Poltash, James M. Mattilla, Melanie T. Odenkirk and Dr. Christine A. Hughey	Comparison of Negative Ion ESI Ionization Efficiencies for a Diversity of Small Acidic Molecules with Widely Varying pK_a's
2:15 - 2:30	Jessica L. Shott, Brian J. Reeves and Dr. Brycelyn M. Boardman	The Synthesis, Characterization, and Polymerization of Thienyl Phosphine Palladium(II) Complexes
2:30 - 2:45	Alexandra Iuga, Denise McKaig and Dr. Isaiah Sumner	Custom Force Field Design for Protein Folding
2:45 - 3:00	Devon M. Shircliff, Michael L. Poltash and Dr. Brycelyn M. Boardman	Synthesis and Characterization of New Low Band Gap Polymers Containing Ethyl and Phenyl Ester Fuctionalized Polythiophene Derivatives
3:00-3:15	David T. Boyle and Dr. Ashleigh Baber	Construction of an Ultrahigh Vacuum Temperature Programmed Desorption Chamber for Catalytic Studies of Metallic Model Surfaces

Special Announcements *(ISAT 159)*	
3:20pm	Announcement of Chemistry and Biochemistry Student Award Winners

Keynote Address: Friday March 27th *(ISAT 159)*		
3:30 – 4:30	Dr. Michael Leopold	Nanoparticle Networks and Xerogel Layering in Amperometric Biosensing Strategies – Adaptable Templates for Clinically Relevant Measurements

(Student presenters underlined)

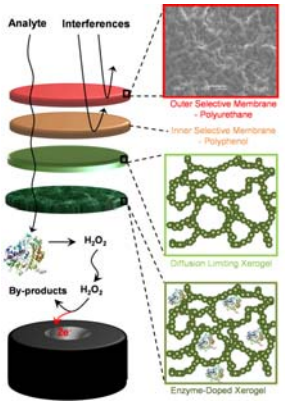
Keynote Address

Friday, March 27, 2015 at 3:30pm
ISAT Room 159

Nanoparticle Networks and Xerogel Layering in Amperometric Biosensing Strategies – Adaptable Templates for Clinically Relevant Measurements

Michael Leopold, Ph. D.
(JMU Class of 1994)
Department of Chemistry
University of Richmond
Richmond, VA

First generation amperometric biosensors for glucose have been investigated as model systems with potential *in vitro* or *in vivo* application in clinical settings. The strategies being employed in developing these biosensors stem from fundamental protein monolayer electrochemistry studies of redox protein adsorption and electron transfer at unique electrode interfaces, including interfaces of assembled films of gold nanoparticles known as monolayer protected clusters (MPCs). Specific layering of xerogel materials or the incorporation of networked MPCs within xerogels has yielded glucose sensing schemes with significantly enhanced performance attributes including greater sensitivity, faster response time, and extended linear/dynamic ranges for glucose detection, for examples. Results suggest that sensing enhancements are directly related to the structure-function relationships within the composite films. The understanding these relationships and how they affect the sensing mechanism within these schemes is a critical step for these strategies to be deliberately and easily adapted toward the detection and real-time monitoring of other clinically relevant targets, such as uric acid, used as a diagnostic in the risk assessment for women with pregnancy-induced hypertension (PIH) and preeclampsia.



STUDENT ABSTRACTS

(Student presenters underlined)

Effects of Amino Acids on Surface Tension of Water

Diana Al Husseini and Dr. Yanjie Zhang
Department of Chemistry and Biochemistry, James Madison University

Ionization state of amino acids is dependent on the pH of the solution and the pK_a of the amine, carboxyl and side groups. Amino acids with varied side groups affect the surface tension differently. Herein, we use optical tensiometry by a pendant drop method to study the amino acids effects on the surface tension of water at different pH. Depending on the species present at a particular pH, whether its anion, cation or zwitterion, the surface tension of water varies. It has been observed so far that the ionic species contribute more to the increase of surface tension comparing to the neutral species in glycine and serine, and the hydrophobic methyl group in alanine contributes to the decrease of surface tension. This type of study will provide us with some valuable data that would help further the understanding of the behaviors of amino acids at the air/water interface.

Analysis of Nitrate-Nitrogen and Ammonium-Nitrogen in Lake Sediment by Solid Phase Extraction and Ion Chromatography

Kelsey L. Berrier and Dr. Daniel M. Downey
Department of Chemistry and Biochemistry, James Madison University

Measurements of ammonium-nitrogen and nitrate-nitrogen nutrients in lakes and reservoirs can provide information for management decisions concerning health and biological productivity. Traditional methods of nutrient determination in soil and sediment samples require a preliminary extraction step essential for freeing anionic and cationic species from the exchange sites on soil particles. Following extraction, nutrient determination generally requires time and labor consuming colorimetric quantification. Ion chromatography (IC) has become the method of choice for anion and cation analyses in aqueous samples due to its simplicity, automated system and convenience. However, the high salt concentration required for the extraction step has excluded IC as a technique for sediment nutrient determination due to column and detector saturation. Recently solid phase extraction cartridges for salt removal have been marketed, including silver, barium, hydronium and mixed bed cartridges. The purpose of this study is to develop methods to use these cartridges post-extraction in sediment analysis, followed by IC for nutrient determination. It has been found that at least 99.9% of chloride in the solution can be removed using silver cartridges. Nitrate and ammonium standards were assayed in a similar way with no loss of nitrate ($p<0.001$). However, in the process of extraction salt removal, ammonium is lost. Currently an alternative extraction method with strontium chloride is being investigated to avoid loss of ammonium. Field collected sediment samples from Strasberg Reservoir, Lake Shenandoah and Slate Lick Reservoir as well as test samples have been assayed by both colorimetric and IC methods for statistical evaluation.

Construction of an Ultrahigh Vacuum Temperature Programmed Desorption Chamber for Catalytic Studies of Metallic Model Surfaces

David T. Boyle, Cameron Stopak, Dylan Boeckmann and Dr. Ashleigh Baber
Department of Chemistry and Biochemistry, James Madison University

As the world's energy requirements increase, there is a demand for more fuel to power our lives in an environmentally conscious way. Finding a material that efficiently reduces carbon dioxide, a harmful greenhouse gas, into useable fuels will help to remove CO_2 byproducts from industrial reactions. The fundamental investigation of the structure/activity relationship of model catalysts will enhance the design of more efficient materials for energetically useful reactions. The interface of gold supported titania (TiO_2) nanoparticles has shown promising catalytic activity for the water gas shift reaction ($CO+H_2O \rightarrow CO_2+H_2$) and for CO_2 hydrogenation. In order to study the catalytic properties of Titania nanoparticles supported on Au(111), an ultrahigh vacuum (UHV) temperature programmed desorption (TPD) chamber was built. TPD and temperature programmed reaction (TPR) studies will be used to acquire information on the kinetic and thermodynamic properties of chemical reactions occurring on the model catalyst surface. Details regarding the UHV-TPD chamber and preliminary data on the chemisorption of reactant molecules on the model surface will be discussed, as well as future plans for the project.

The Strength of the M-band Titin/Obscurin Interaction is Directionally Dependent

Tracy A. Caldwell, Dr. Isaiah Sumner and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University

Obscurin (800-900 kDa) is a giant muscle protein vital to muscle cell maintenance and organization. It is the only known connection between the contractile apparatus and the sarcoplasmic reticulum and also binds to specific cytoskeletal, signaling, or membrane-associated proteins. Obscurin domains Ig58/59 bind to titin ZIg9/10, which is hypothesized to stabilize the sarcomeric cytoskeleton. Mutations in this obscurin region lead to malformed muscle architecture and, eventually, to hypertrophic cardiomyopathy (HCM). For obscurin/titin binding to occur, all four of these domains must be present. In order to fully characterize this physiologically important region of obscurin, and by extension determine the molecular factors that drive HCM, here we present the Ig58 and Ig59 structure using both X-ray crystallography and heteronuclear multidimensional NMR spectra. Low-resolution structure and dynamics of these tandem domains, along with how these domains react to physical stress, are also discussed.

Kinetics of the Decomposition of Zinc Oxalate through Traditional and Isoconversional Methods

Nicholas D. Cooper and Dr. Thomas C. DeVore
Department of Chemistry and Biochemistry, James Madison University

The decomposition of zinc oxalate has long been thought to follow a one-step mechanism, but newer isoconversional methods indicate this assumption may not be correct. Investigations using TGA, EGA-IR and DSC indicate that the gaseous products from the decomposition, CO and CO_2, are produced at different rates and follow different rate equations. The rates and activation energies were studied using tradition Arrhenius equation, model fitting methods and the newer isoconversional or "model-biased free" methods. The traditional methods indicate that CO is formed initially and follows the Avrami–Erofe'ev equation with $n\approx3$ while CO_2 forms later and follows the Avrami–Erofe'ev equation with $n\approx2$. The activation energy found for CO was ≈245 kJ/mol while the EA for CO_2 was ≈257 kJ/mol. Isoconversional methods have been applied to these decompositions and activation energies were found through the Starink method. The activation energies range from 189 kJ/mol to 229 kJ/mol and show a clear dependence on both sample mass and extent of reaction which points towards a multi-step reaction.

Tailoring Thienyl Phosphine Ligands for Improved Charge Transfer in Hybrid Photovoltaic Systems

Daniel A. Corbin, Brian J. Reeves, Devon M. Shircliff, Jessi L. Shott and Dr. Brycelyn M. Boardman
Department of Chemistry and Biochemistry, James Madison University

Cobalt selenide clusters with 2-bromo-5-diethylphosphinothiophene (1), 2-bromo-5-diphenylphosphinothiophene (2), and 5-diphenylphosphino-2,2'-bithiophene (3) ligands are described. Ligands 1 and 2 are obtained via lithium halogen exchange of 2,5-dibromothiophene followed by addition of chlorodiethylphosphine and chlorodiphenylphosphine, respectively. Ligand 3 is obtained via lithium halogen exchange of 2,2-bithiophene followed by the addition of chlorodiphenylphosphine. The prepared phosphine ligands are then sequentially reacted with elemental selenium followed by dicobalt octacarbonyl to yield $Co_6Se_8(P(Et)_2(ThBr))_6$ (4) (Th = C_4H_2S), $Co_6Se_8(P(Ph)_2(ThBr))_6$ (5), and $Co_6Se_8(P(Ph)_2(Th\text{-}ThH))_6$ (6), respectively. The three new cobalt selenide clusters were characterized by UV-visible spectroscopy and ^{31}P Nuclear Magnetic Resonance spectroscopy. Emission spectra were recorded for the addition of $Co_6Se_8(PEt_3)_6$ (7), 4, 5, and 6 to a 0.004 wt% solution of poly-3-hexyl thiophene (P_3HT) in toluene to investigate the charge transport of the system. The quenching of the polymer's emission follows first-order like decay for each cluster. Clusters containing thienyl moieties exhibit better quenching of P_3HT than 7, with 6 being the most efficient and 5 being better than 4. This suggests ligands can be structurally tailored to maximize charge transfer between the polymers and inorganic clusters.

An Evaluation of the Chemistry of $RuCl_2(PPh_3)_3$ with Nitriles

Santina Cruz[1], Dr. John W. Gilje[1], Dr. Donna S. Amenta[1] and Dr. Glenn P.A. Yap[2]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Chemistry and Biochemistry, University of Delaware

Due in part to our interest in the metal catalyzed hydrolysis of nitriles, we are investigating the coordination chemistry of nitriles with ruthenium. A number of years ago Wilkinson[1] characterized by IR cis- and trans-$RuCl_2(PPh_3)_2(NCR)_2$ from the reaction of $RuCl_2(PPh_3)_3$ with excess RCN. We have restudied this reaction with benzonitrile in several solvents and have characterized the complex cis-$RuCl_2(PPh_3)_2(NCPh)_2$ by IR and NMR spectroscopy, and x-ray crystallography. However, we have been unable to detect an isomer containing trans- nitrile ligands. This is analogous to acetonitrile, where the cis rather than the trans complex is obtained[2]. With excess $RuCl_2(PPh_3)_3$ quite a different product forms with benzonitrile. In this case the diruthenium, triply chloro-bridged $(Ph_3P)_2(Cl)Ru(\mu\text{-}Cl)_3Ru(PPh_3)_2(NCPh)$ forms in good yield and has been spectroscopically and structurally characterized. In solution, the ^{31}P NMR spectrum consists of two sets of doublets. This is consistent with the solid state structure and indicated that the molecule is not fluxional and does not undergo isomerization or ligand exchange in solution. Similar reactions with acetonitrile, acetamide, and N-pyrazolylpropanamide appears to produce analogous diruthenium products as indicated by ^{31}P NMR spectroscopy.

1. Gilbert, J.D.; Wilkinson, G. J. Chem. Soc.(A), 1969, 1749-1753.
2. Al-Far, Acta Cryst. E64, 2008, m184.

The Synthesis and Study of the Biological and Colloidal Properties of Bolaamphiphiles

Louis Damiano[1], John Marafino[1], Brenna Walsh[1], Matt Schmachtenberg[1], Mark Wenzel[1], Kirstie Thompson[1], Kristin McKenna[1], Kou Kunneang[1], Tara Gallenger[2], Dr. Kyle Seifert[2] and Dr. Kevin L. Caran[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Biology, James Madison University

Over the past decade, antibiotic resistant bacteria have caused infections in patients throughout the world. The rise in antibiotic resistance is primarily due to the misuse and overuse of antibiotics. To counter the increase in antibiotic resistance, infection control mechanisms have been aggressively researched in recent years. In particular, drug delivery has become a focal point to fight antibiotic resistant infections. Amphiphiles have a wide range of applications in the clinical setting, including the ability to inhibit bacterial transference because of their bactericidal activity. Bolaamphiphiles are a subclass of amphiphiles that possess two or more hydrophilic heads on either side of hydrophobic linker (typically a hydrocarbon chain). Altering the length of the hydrophobic linker or structure of hydrophilic heads can change their biological and colloidal properties. This study includes the synthesis as well as the colloidal and biological study of a novel series of hexacationic bolaamphiphiles with three cationic groups on each end of an intervening tail. The critical micelle concentration (CMC) and minimum inhibitory concentration (MIC) have been determined. In addition preliminary studies on interactions between hexacationic bolaamphiphiles and a hexaanionic salt will be presented.

Nucleotide Effects in the GroEL Subunit

Aaron Davis and Dr. Isaiah Sumner
Department of Chemistry and Biochemistry, James Madison University

GroEL is a molecular chaperonin protein that looks like a molecular beaker. The interior of GroEL catalyzes the folding of substrate proteins in E. coli. GroEL is made up of two heptameric rings that open up from the T state to R state when ATP is present in the binding pockets of the subunits. When GroEL is in the R state, the substrate protein enters the cavity and a second chaperonin, GroES, binds to the top of GroEL, causing it to open up even further into R´´ state. This also causes ATP to hydrolyze into ADP. The exact mechanism for this allosteric change is an active area of research. We are focusing our efforts on a single GroEL subunit. The subunit has three domains: apical, intermediate, and equatorial. When ATP is present, the majority of any movement is found in the apical domain and the area between the apical and intermediate domain, which acts as a hinge for this molecule. We have studied this mechanism in two ways. First, we performed unbiased molecular dynamics simulations on individual subunits with ATP or ADP in the binding pocket and with an empty biding pocket (apo). At least 20 ns of simulation were performed on each subunit and the angle between the apical, intermediate, and equatorial domain was monitored. Second, we are using umbrella sampling to calculate the potential of mean force for opening/closing the ADP, ATP and apo subunits. Preliminary results are presented and discussed.

The Importance of the Disulfide Bonds within BST-2 for Structure and Viral Tethering

Kelly E. Du Pont, Dr. Isaiah C. Sumner and Dr. Christopher E. Berndsen
Department of Chemistry and Biochemistry, James Madison University

Human BST-2/tetherin is a host factor that inhibits release of HIV-1, HIV-2, and SIV from the cell surface by tethering viruses to the host cell membrane. Viruses can evade this inhibition through antagonistic viral protein interactions with BST-2. Structurally, full-length BST-2 consists of an N-terminal cytoplasmic domain, a transmembrane domain, an ectodomain, and a C-terminal membrane anchor. BST-2 forms dimers in cells with the ectodomains of each monomer intertwining to form a coiled-coil. The N-terminal half of the ectodomain contains three cysteine residues; each can contribute to the formation of cysteine-linked dimers between BST-2 monomers. During viral tethering, one of the transmembrane domains is taken up into the cell wall of the budding virus. After the virus detaches from the host cell, BST-2 acts as a tether between the two. To further understand the role the disulfide bonds play in viral tethering, we mimicked the purposed mechanism of BST-2 under oxidized, reduced and monomeric conditions through steered molecular dynamics. We find that the disulfides increase the strength of the coiled coil during viral tethering. These data are contrary to the belief in the field that the disulfide bonds are required for maintaining the dimer conformation. Our data provide insight into the structural mechanism of viral tethering of HIV-1 to the cell.

Structural Elucidation of AggR-activated Regulator, Aar, in Enteroaggregative *Escherichia coli*

Andy Heindel and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University

Travelers' Diarrhea is the number one cause of childhood death in the world. Enteroaggregative *Escherichia coli* (EAEC) is one of the main causes of this disease. EAEC adhere to the surface of the intestine and stack in a brick-like pattern. Via an unstudied quorum-sensing mechanism, these bacteria express a variety of virulence factors that lead to diarrhea. The long-term goal of this research is to elucidate the mechanism by which EAEC changes from benign to virulent. A previously-unstudied open-reading frame in EAEC, AggR activated repressor (Aar), has recently been hypothesized to act as one of the major transcription factors influencing virulence. Here, we describe initial attempts to structurally characterize this polypeptide. Aar appears to be stable in solution. However, mechanisms to separate Aar from its fusion partner are still unclear. Circular dichroism (CD) data suggests a partially α-helical structure. Further tests, including multi-dimensional NMR and X-ray crystallography, are currently being conducted to determine the tertiary structure of the protein.

Comparison of Negative Ion ESI Ionization Efficiencies for a Diversity of Small Acidic Molecules with Widely Varying pK_a's

Shelsea A. Hurdle, Michael L. Poltash, James M. Mattilla, Melanie T. Odenkirk and Dr. Christine A. Hughey
Department of Chemistry and Biochemistry, James Madison University

Negative ion electrospray (ESI), an ionization technique that selectively ionizes acidic molecules by deprotonation, has not been studied as extensively as positive ion ESI. As a result, our long-term goals are to elucidate the mechanisms of ionization and to develop a model that predicts ESI response for a diversity of small acidic molecules with a wide range of acidities (NSF CHE-1307226). To date, negative ion ESI studies have largely focused on two compound classes: phenols and benzoic acids (Anal. Chem. 2014, 84, 4822-4830). Here we measure the ionization efficiencies of ~100 compounds by triple quadrupole mass spectrometry. The compounds were systematically selected among n-carboxylic acids, benzoic acids, phenols, thiophenols, acetanilides, indoles and steroids. The pKa's for compounds studied ranged from -0.78 to 20. Within each class, compounds substituted with electron-withdrawing groups (EWGs), such as CF_3, NO_2, CN and Cl exhibited much higher responses than compounds with electron donating groups (EDGs), such as $-OCH_3$, NH_2 and CH_3. We observed this trend previously among substituted phenols and benzoic acids (Anal. Chem. 2012. 84. 9942-9950). This larger data set further supports our hypothesis that EWGs withdraw electrons from the benzene ring through induction and/or resonance stabilization and, thereby, makes it easier to remove the proton during ionization. Induction stabilization also explains the increased response of indoles compared to other compound classes, as indoles have a benzene ring fused to a pyrrole ring.

Custom Force Field Design for Protein Folding

Alexandra Iuga[1], Denise McKaig[2] and Dr. Isaiah Sumner[1]
[1]Department of Chemistry and Biochemistry, James Madison University
[2]Department of Physics, College of William and Mary

Force field-based molecular dynamics (MD) is a powerful tool that has produced many key insights into the mechanisms of protein folding. However, MD is not without its flaws. One well-documented problem with MD is that some force fields have unphysical biases towards certain secondary structures. We propose a method wherein we add corrections to existing force fields based on DFT calculations. Namely, the force-matching algorithm will be used to change the force field so that it reproduces DFT energies and forces. However, density functionals need to be benchmarked to ensure that they give accurate results for proteins. Therefore, we also present a comparison of several functionals with and without empirical dispersion corrections benchmarked against several protein databases. Since the initial target for this approach is force field bias seen in folding of pin1WW with the CHARMM27 force field, we also compare density functional and force field calculations of several folded and misfolded pin1WW states.

Water Chemistry of North Branch Simpson Creek Before and After a Major Forest Fire

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In April 2012, a major forest fire occurred in Virginia that consumed the entire 6000 acre Rich Hole Wilderness Area (RWHA) including 100% of the watershed of North Branch of Simpson Creek (NBSC). Although the fire completely burnt the understory of the forest, it occurred before leaf out and the major timber stands have survived. This fire has provided a unique opportunity to study the effects of forest fires on streams in the Appalachian Mountains that are already degraded by acid deposition. In other locations damaged by forest fires there have been changes in soil composition, water chemistry, and surface run-off, so studies were directed to assess similar effects in this location. Since the most dramatic effects of forest fires on streams have been the result of episodic discharge, sampling was conducted May-September 2012 for precipitation run-off events. In addition synoptic samples were taken periodically in 2012-2014 throughout the stream reach. Chemical parameters including pH, acid neutralizing capacity, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, NO_3^-, SO_4^{2-} , Al, turbidity and conductivity were measured for comparison to previous data sets. A second stream, Bob Downy Branch, was not affected by the forest fire and served as a “control” with samples collected coincidentally with those from NBSC. Soil samples revealed that the char layer was superficial and that bicarbonate was elevated. However the stream was already so acidic that the added alkalinity was insufficient to raise pH enough to support trout in the headwater reach.

Hofmeister ion and co-solvent effects on water structure and the aggregation and solvation of RecA

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RecA is an Escherichia coli protein that catalyzes the strand exchange reaction utilized in DNA repair. Previous studies have shown that the presence of salts influence RecA activity, aggregation, and stability. Here we utilized attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy and circular dichroism (CD) to further investigate how various Hofmeister salts and co-solvents alter RecA structure, aggregation, and solvation. Spectroscopic studies performed in water and deuterium oxide suggest that salts alter amide I (or I') and amide II (or II') vibrations arising from the protein backbone. Specific infrared vibrations that may arise from protein-solvent interactions were identified. Infrared vibrations that correlate with protein desolvation were observed in the presence of strongly hydrated SO_4^{2-} anions. The vibrations that correlate with protein solvation were observed in the presence of weakly hydrated Cl^- and ClO_4^- anions. Additional experiments were performed under solution conditions known to influence protein-solvent and protein-water interactions. An increase in the infrared frequency of amide I (or I’) correlated with increasing concentrations of trifluoroethanol (TFE) and sucrose. This result suggetmts an increase in desolvation of the amide backbone with an increase in the concentration of co-solvents. Additionally, increasing concentrations of TFE resulted in an increase in RecA aggregation. These results show that salts and co-solvents alter the solvation water surrounding proteins and influences overall structure and aggregation.

Synthesis and Supramolecular Structures of Manganese Complexes with N-Pyrazolylpropanamide-Derived Ligands

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The syntheses and single crystal X-ray structures of the multifunctional acrylamide-derived ligands N-pyrazolyl-2-methylpropanamide (1 = N-ppaMe) and a mixture of 3- and 5-methyl-pyrazolylpropanamide (2a and 2b = N-3Meppa/N-5Meppa), and their Mn^{2+} complexes are reported. Compounds 1 was prepared by the reaction of 2-methylacrylamide with pyrazole. A mixture of 2a and 2b was obtained from the reaction of acrylamide with 3-methylpyrazole. In the latter reaction, the first step involves the deprotonation of 3-methylpyrazole, followed by tautomerization that ultimately results in the formation of both the 3- and 5-methyl isomers of 2. The general synthesis of the Mn2+ complexes involves treatment of $MnCl_2{\cdot}4H_2O$ with the appropriate ligand in ethanolic solution in the presence of triethylorthoformate as dehydrating agent. This way $Mn_2Cl_4(N\text{-}ppaMe)_2(EtOH)_2$ (3), and $[Mn(N\text{-}3Meppa)_2(N\text{-}5Meppa)][MnCl_4]$ (4). In 3 the N-ppaMe ligand acts as N,O-chelating ligand whose oxygens bridge the two Mn^{2+} ions. The ligands are also chelating in 4. Very recently we prepared 3,5-dimethylpyrazolyl-N’-isopropylpropanamide (5). The molecular and crystal structures of 1, 2a, 3, 4, and 5 have been determined by X-ray diffraction. The hydrogen bonding that occurs in these compounds is discussed.

Novel Triscationic Single and Double-Tailed Amphiphiles: Synthesis and Characterization of Colloidal and Antibacterial Properties

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Three novel series of triscationic, triple-headed amphiphiles were synthesized. Each compound has a benzene core, three benzylic ammonium bromide groups, and either one or two alkyl chains, varying in length from 8 to 22 carbons. The impact of the variable number and length of the hydrocarbon tails on antibacterial and colloidal properties was determined through the determination of the critical micelle concentration (CMC), heat of micellization (ΔHmicelle), and minimum inhibitory concentration (MIC) against six bacterial strains. Both log(CMC) and ΔHmicelle for each series were found to be inversely proportional to chain length. While the identity of the third, non-tail bearing head group (trimethylammonium or pyridinium) did not have a drastic effect on the colloidal or antibacterial properties of the compounds, the number of tails did, when comparing the total length of the tails in each molecule. For example, the derivative with one 20 carbon tail has a CMC of 2.05 mM, while the derivative with two 10 carbon tails has a CMC of 12 mM. Additionally, the most biologically active double-tailed compounds were those with two 12 carbon chains, with MIC values of 1-2 μM for Gram-positive and 4-16 μM for Gram-negative bacteria. The most biologically active single-tailed compound was the 18 carbon chain derivative, with a MIC values of 2-16 μM for Gram-positive and 16-125 μM for Gram-negative bacteria. These novel amphiphiles could serve as useful antibacterials.

The characterization of the Ig58 domain of the giant muscle protein obscurin

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Obscurin (720-900 kD) is a giant sarcomeric signaling protein that is the only known link between the cytoskeleton and the surrounding membrane structure. Mutations to obscurin and to obscurin binding partners have been linked to human muscle diseases such as hypertrophic cardiomyopathies and muscular dystrophy. These diseases likely occur due to the abrogation of specific molecular interactions necessary for suitable function. To more fully understand how specific mutation lead to disease, here we have solved the high resolution structure of obscurin Ig58. The modular arrangement of independently folding domains of obscurin makes such studies feasible. An Arg8Gln mutation is associated with hypertrophic cadiomyopathy. Chemical shift changes of this mutation and MD simulations suggest that this mutation disrupts a large charge-charge surface of Ig58.

Structural Elucidation of the Ig59 Domain of Obscurin

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Obscurin (800-900 kDa) is a giant muscle protein vital to muscle cell maintenance and organization. It is the only known linker between the contractile apparatus and the sarcoplasmic reticulum of myocytes and may also bind to cytoskeletal, signaling, or membrane-associated proteins. One such interaction is the binding of obscurin domains Ig58/59 to titin domains ZIg9/10. This binding, which requires all four domains to be present, is hypothesized to stabilize the sarcomeric cytoskeleton. Mutations in this region of obscurin lead to malformed muscle architecture and may lead to hypertrophic cardiomyopathy (HCM). In order to better understand the molecular underpinnings of this disease, we solved a high-resolution structure (1.18 Å) of the Ig59 domain of obscurin. This domain folded into a classic Ig-like domain, consisting of two beta sheets and a well-defined hydrophobic core.

Mechanisms and Kinetics of Solvent loss in $Na[BH(C_2H_2N_3)_3]$

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The hydrotris(1,2,4-triazolyl)borate ligand was used to assemble frameworks to see the structural effects and kinetics of solvent loss in the framework. Three frameworks, $Na[BH(C_2H_3N_3)_3]\cdot$solvent (solvent = water, dimethylformamide, isopropanol), were synthesized under solvothermal conditions. Powder X-ray diffraction (PXRD) indicates the three solvates have different structures. The solvent of crystallization can be removed upon heating; isothermal thermal-gravimetric analysis (TGA) shows solvent loss by 1-D diffusion mechanism. Variable temperature PXRD shows a slight loss of crystallinity upon desolvation, indicating some framework decomposition. On solvent loss, the structures of the desolvated materials are identical. These activated frameworks adsorb water from the atmosphere. Details of the structural properties, thermal behavior, and kinetics of solvent loss of $Na[BH(C_2H_3N_3)_3]\cdot$solvent will be reported.

Synthesis and Characterization of New Low Band Gap Polymers Containing Ethyl and Phenyl Ester Fuctionalized Polythiophene Derivatives

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In an attempt to synthesize novel low band gap polymers, two new monomers 3-ethyl-2-(2,5-dibromothiophene)-3-ylacetate (1) and 3-pheylethyl-2-(2,5-dibromthiophene)-3-ylacetate (2) containing ester functionalities were synthesized. These monomers 1 and 2 were copolymerized with 2,5-bis(trimethylstannyl)thiophene to yield poly [3-ethyl 2-(thiophene-3-yl)acetate-2,2'-thiophene (PETAT) and poly [3-phenylethyl 2-(thiophene-3-yl)acetate-2,2'-thiophene (PPTAT). Additionally, these electron donating monomers 1 and 2 as well as 2,5-bis(trimethylstannyl)thiophene were incorporated with the electron withdrawing monomer, 4,7,dibromobenzo[c]-1,2,5-thiadiazole, to develop two new push-pull conducting polymeric systems; poly [3-ethyl 2-(thiophene-3-yl)acetate-2,2'-thiophene-2,6-diyl-alt-2,1,3-benzothiadiazole-4,7-diyl] (PETATBT) and poly [3-phenylethyl 2-(thiophene-3-yl)acetate-2,2'-thiophene-2,6-diyl-alt-2,1,3-benzothiadiazole-4,7-diyl] (PPTATBT). PETAT and PPTAT show a slight reduction in band gap at 1.9 and 2.0 eV as opposed to the standard poly-3-hexylthiophene (P3HT) at 2.3 eV, where as PPTATBT and PETATBT show a dramatic reduction in the band gap as low as 1.6 and 1.7 eV respectively. UV-Visible spectroscopy of films of PETAT and PETATBT show minimal changes in the λ max versus the polymers in solution. Alternatively, films of PPTAT and PPTATBT show significant bathochromic shifts as a result of the pendant phenyl moiety of 2. The impact of the phenyl moiety was further investigated using atomic force microscopy (AFM).

The Synthesis, Characterization, and Polymerization of Thienyl Phosphine Palladium(II) Complexes

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Palladium(II) complexes with functionalized thienyl phosphine ligands have been synthesized and polymerized. The synthesis of brominated thiophene ligands was performed by allowing 2,5-dibromothiophene to react with n-butyllithium, followed by the addition of chlorodiphenylphosphine or chlorodiethylphosphine to produce 2-bromo-5-diphenylphosphinothiophene (1) and 2-bromo-5-diethylphosphinothiophene (2) respectively.
Compounds 1 and 2 were allowed to react with dichloro(1,5-cyclooctadiene)palladium(II) to form either bis(2-bromo-5-diphenylphosphinothiophene)palladium(II)dichloride (3) or bis(2-bromo-5-diethhylphosphinothiophene)palladium(II)dichloride (4) respectively. Polymerizations of 3 and 4 were performed using 3-hexylthiophene and (2,5-bis-trimethylstannyl)thiophene as co-monomers. ^{1}H, ^{13}C, and ^{31}P NMR, ultraviolet-visible spectroscopy, and fluorescence spectroscopy were used to characterize the phosphine ligands and palladium complexes. UV-visible spectroscopy and ^{1}H NMR also confirm the incorporation of the palladium complexes into the polymer backbone.

Probing Buffer-specific Effects on Nucleotide Binding to RecA using Difference FTIR

Joshua E. Temple and Dr. Gina MacDonald
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The *Escherichia coli* protein RecA catalyzes the strand exchange reaction used in DNA repair and genetic recombination, and serves as a target for inhibiting microbial antibiotic resistance as well as understanding cancer propagation. Previous studies in our lab have shown buffer-specific changes in RecA stability and unfolding transitions. However, these studies suggest only minimal buffer-dependent changes in nucleotide binding and secondary structure that do not explain significant differences in RecA stability and unfolding profiles. These observations led to further investigations of how the four common biological buffers Tris, MES, HEPES, and Phosphate alter RecA structure and nucleotide binding. Here we have employed circular dichroism (CD) and infrared (IR) spectroscopy to further discern if buffers influence nucleotide binding to RecA. Global RecA structure is conserved across all buffers, yet unique aggregation states are observable in CD turbidity plots. RecA activity in HEPES buffer is also significantly decreased compared to Tris and MES buffers, and slightly depressed compared to Phosphate buffer. Laser-induced photolysis of caged nucleotides was used in conjunction with difference IR to generate RecA-ADP minus RecA difference infrared spectra in each of the four buffers. These studies detected buffer-specific changes in nucleotide binding to RecA including possible perturbations in Gln, Glu, Asp, Asn, Tyr, and Lys residues and unique secondary structural transitions. These differences between RecA-ADP *minus* RecA difference spectra may provide insight into possible mechanisms for buffer-specific stability profiles of RecA.

Cation Effects on Caffeine Partitioning Thermodynamics

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This project is studying specific cation effects on the thermodynamics of caffeine partitioning between the aqueous and cyclohexane phases. The standard Gibbs free energy for caffeine partitioning is measured in the presence of a series of thirteen chloride salts in the aqueous phase at varied concentrations. Cations seem to have less effect overall than the anions studied previously. It is found that all monovalent cations studied generally produced linear dependence on salt concentration, while the divalent alkaline earth and transition metal cations have shown non-linear dependence. The standard Gibbs free energy for caffeine partitioning as a function of temperature will be investigated in the near future to obtain the enthalpy and entropy for caffeine partitioning.

Synthesis and Study of Polycationic Amphiphiles as Potent Antiseptics and Novel Colloids: Exploring Structure Activity Relationships

Brenna J. C. Walsh[1], Kirstie Thompson[1], John N. Marafino[1,2], Kristin McKenna[1], Louis Damiano[1], Tara M. Gallagher[2], Matt Schmachtenberg[1,2], Kunny Kou[1,2], Mark Wenzel[1], Dr. Kyle Seifert[2] and Dr. Kevin L. Caran[1]
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Several series of novel amphiphilic molecules have been designed and synthesized in an effort to develop novel and efficient antiseptics. Each of the new series include amphiphiles with non-conventional structures; molecular architectures include compounds with multiple hydrophilic head groups and one or two hydrophobic tails. The synthesis, purification, colloidal analyses, and results of antibacterial assays of these molecules will be presented. Relationships between amphiphile structure, colloidal properties and biological properties will be discussed. We will also present progress on current research directions including bolaamphiphiles (with three charged groups on each end of a non-polar linker), amphiphiles with hexasubstituted hydrophilic head groups, and single-tailed amphiphiles with a cis double bond in the hydrophobic tail. In addition, we will present progress on the effect of adding or exchanging anionic counterions on colloidal and antibacterial properties.

Molecular Dynamics Studies of the Ubiquitin Conjugation Mechanism

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Post-translational modification of proteins can have drastic effect on their structure and function. One such modification involves the attachment of a small protein, ubiquitin. An important function of ubiquitination is to signal proteins for cellular degradation. This process occurs in three enzymatic steps. In the second step, ubiquitin transfers to a conjugating enzyme, called E2, which then transfers ubiquitin to a lysine in the target protein. However, the mechanistic details for this final transfer remain obscured. Although it is clear that ubiquitin does bind, there are no studies that show exactly how this happens. The two most favored proposals involve a step-wise mechanism with a tetrahedral oxyanion intermediate and concerted mechanism. This work probes the accuracy of the oxyanion hypothesis. In particular, if the oxygen on the observed carbonyl carbon can form a stable hydrogen bond with the hydrogen on the nitrogen of the asparagine side chain, then oxyanion intermediate is plausible. By using molecular dynamics (MD), combined with umbrella sampling, a free energy profile of the formation of the breaking and forming of the hydrogen bond is constructed to see if its creation is thermodynamically favorable. Furthermore, information about the hydrogen-bonding environment in the active site is extracted.

2015 Department of Chemistry and Biochemistry Student Award Winners

Amenta Award	Jessica L. Shott
R.D. Cool Award	Kathleen T. Krist
J.W. Chappell Scholarship	Anthony P. Allsbrook
Palocsay Award in Undergraduate Research	Kirstie A. Thompson
Service Award	Santina S. Cruz
J. W. Chappell Award	Heather M. Rucker
American Institute of Chemists	Matthew C. Oehler
Degesch America Award	Brenna J. C. Walsh
ACS-Award	Joshua E. Temple
Hypercube Scholar	Tracy A. Caldwell
Casali Scholarship (2014)	Kelsey L. Berrier
Outstanding Student Researcher Award	*to be announced*

American Chemical Society Divisonal Awards

ACS Analytical	Kelsey Berrier
ACS Environmental	Kelsey Berrier
ACS Inorganic	Santina Cruz
ACS Organic	Devon Shircliff
POLYED Award in Organic Chemistry	Daniel Corbin

The cover art is a composite of select Spring Symposium covers:

We gratefully acknowledge the following for their support:

American Chemical Society – Petroleum Research Fund
Camille and Henry Dreyfus Foundation
Department of Defense – ASSURE
The Extreme Science and Engineering Discovery Environment (XSEDE)
Institute for Infrastructure Assurance
International Society for Chemical Ecology
Jeffress Memorial Trust
James Madison University Center for Materials Science
James Madison University College of Integrated Science and Engineering
James Madison University College of Science and Mathematics
National Institute of Standards and Technology
National Science Foundation – OCI, REU, RUI
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