Center for Computational Sciences
High Performance Computing Collaboratory
Mississippi State University
Annual Report FY2019

Mission

**To foster interdisciplinary research in both
the fundamental understanding of
and application of
all the natural sciences by modeling and developing
integrated computational environments and
crosscutting tools that allow a comprehensive, cross-disciplinary approach
to problem-solving.**

Vision

**To become the leader of interdisciplinary research and education
in science and technology**

Director's Note

The Center for Computational Sciences (CCS) at Mississippi State University is a College of Arts and Sciences center with a mission to foster interdisciplinary research in both the fundamental understanding of and application of all the natural sciences by modeling and developing integrated computational environments and cross-cutting tools that allow a comprehensive, cross-disciplinary approach to problem-solving.

The major research activities/initiatives of CCS include: (1) an NSF funded project "Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels" (2) a DOD funded project on quantum computing, machine learning and cybersecurity; (3) a DOE funded project "Nuclei in a relativistic framework: at and beyond density functional theory"; (4) An NSF funded project "Theory and simulations of unconventional superconductors"; (5) NRF funded project "First-principles design of functional electrides using a highly efficient computational platform"; (6) NSF funded project to develop new sensors to detect seawater contamination; (7) NSF funded "Research Experiences for Undergraduates (REU) in Computational Methods with Applications in Materials Science".

This report will provide synopsis of these activities/initiatives, the list of CCS Personnel, the recent awards and recognitions, and research publications. Also included in the report are the details on funding activity. Overall, this year has been another successful year for CCS. We look forward to building on this platform, to achieve greater excellence in coming years.

Seong-Gon Kim

Seong-Gon Kim
Director, Center for Computational Sciences
High Performance Computing Collaboratory
Mississippi State University

Personnel

Director: Seong-Gon Kim, Professor, Physics and Astronomy
Associate Director: Hyeona Lim, Associate Professor, Mathematics

Biological Sciences
Christopher Brooks, *Associate Professor*
Vincent Klink, *Associate Professor*

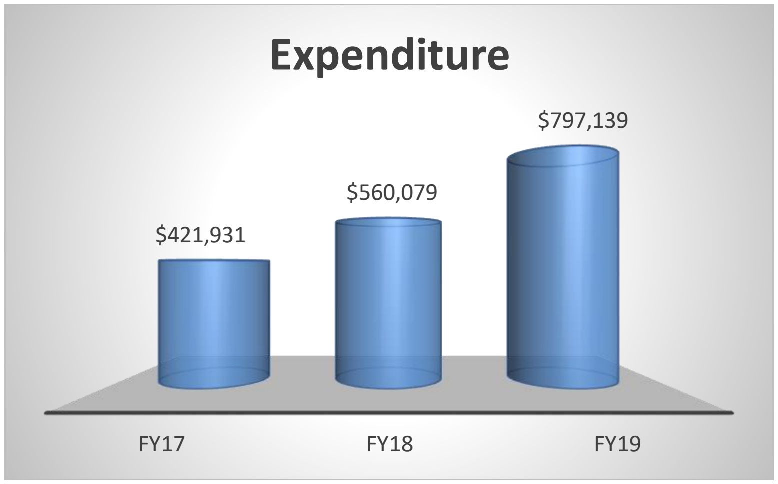
Chemistry
Steven Gwaltney, *Professor*
Keith Hollis, *Associate Professor*
Amanda Patrick, *Assistant Professor*
Charles Edwin Webster, *Professor*

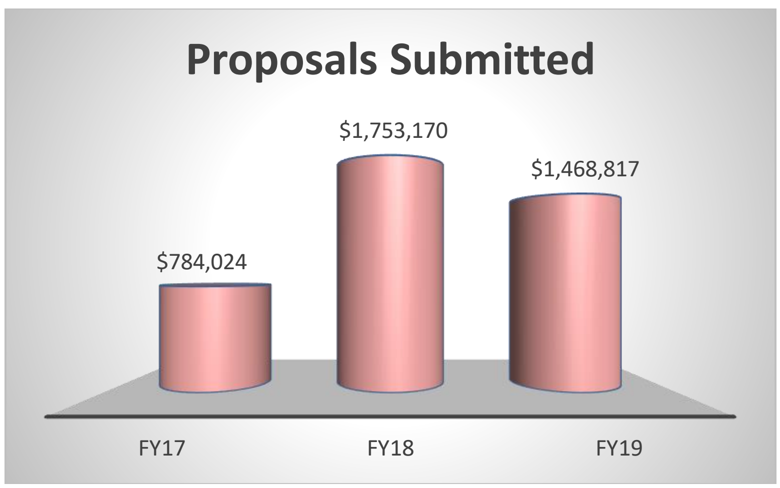
Computer Science and Engineering
Ioana Banicescu, *Professor*

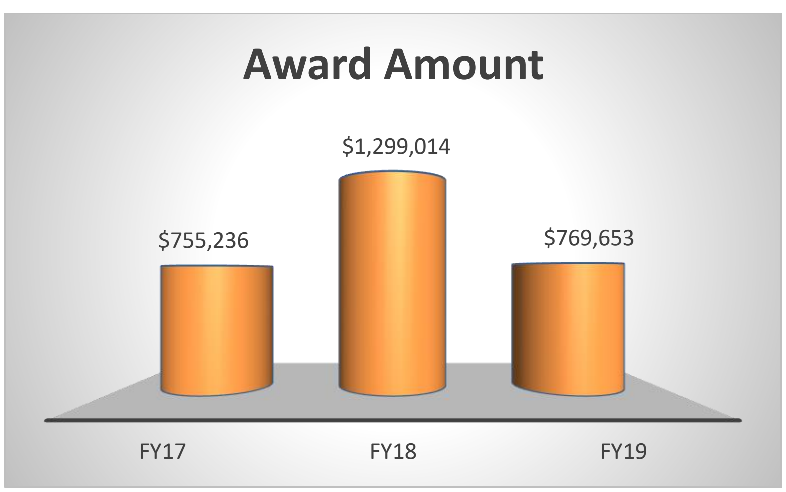
Mathematics and Statistics
Amanda Diegel, *Assistant Professor*
Seongjai Kim, *Professor*
Hyeona Lim, *Associate Professor*
Vu Thai Luan, *Assistant Professor*
Jingyi Shi, *Assistant Professor*
Tung-Lung Wu, *Assistant Professor*
Jialin Zhang, *Assistant Professor*
Michelle Zhou, *Assistant Professor*

Physics and Astronomy
Anatoli Afanasjev, *Professor*
Torsten Clay, *Professor*
Seong-Gon Kim, *Professor and Director*
Mark Novotny, *Professor and Head*
Gautam Rupak, *Associate Professor*
Jinwu Ye, *Professor*

Research Activities





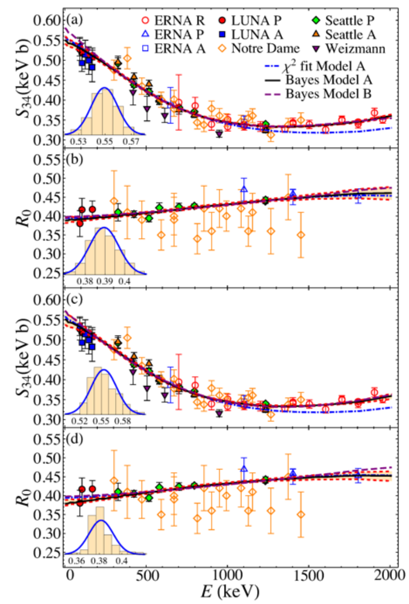


Research Highlights

Nuclear Structure and Reactions from Lattice Effective Field Theory

Researcher: Prof. Gautam Rupak (Physics & Astronomy)

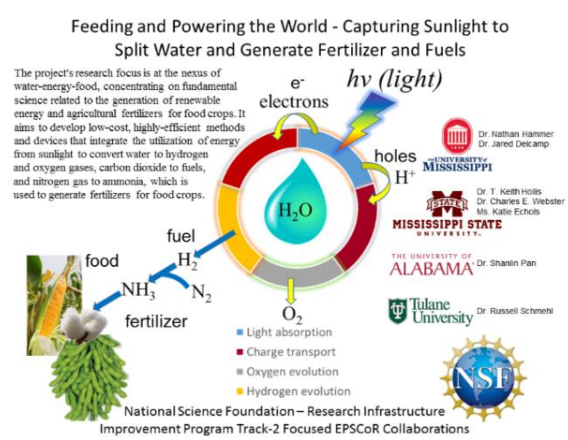
Prof. Gautam Rupak's research on nuclear structure and reactions from lattice effective field theory is partly supported by NSF grant PHY-1615092. Astrophysical models of Big Bang Nucleosynthesis (BBN) and stellar burning are greatly impacted by capture reactions that are often difficult to measure directly. Theoretical calculations become necessary to determine these reaction rates. In reaction calculations, one typically needs to describe the interaction between clusters of protons and neutrons. To develop the new techniques, the spin doublet neutron-deuteron n+d scattering would be calculated as a mixed channel problem. The n+d system is well studied in other methods and serves as a benchmark for the new lattice calculations. This would help develop the lattice techniques for charge exchange reactions. Radiative capture reactions 3He(□, □)7Be, 7Be(p, □)8B, that impacts the dominant source of high energy neutrinos detected in experiments probing physics beyond the Standard Model of particle physics would be calculated. These calculations would help develop lattice EFT techniques for electromagnetic currents from microscopic interactions. The electric polarizability of light nuclei would be calculated. Polarizability measures the distortion of atomic nuclei in a weak electric field, and provides information about nuclear structure. The projects in this proposal would advance the field of nuclear structure and reaction theory.



Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels

Researchers: Profs. Keith Hollis and Charles Webster (Chemistry)

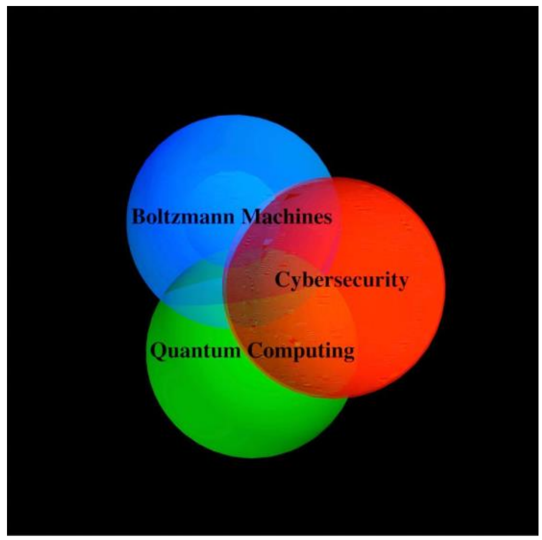
NSF RII Track-2 FEC awarded a collaborative $6 million, 4 year project to a team of researchers from Mississippi (University of Mississippi and Mississippi State University), Louisiana (Tulane University), and Alabama (University of Alabama, Tuscaloosa). **Profs. Keith Hollis and Charles Webster** are among the Principal Investigators. The project goals are anticipated to improve efficiency in the capture of sunlight, to develop new technologies to convert it to low-cost sustainable fuels and to develop a link to the preparation of synthetic fertilizer for food crops. The project's research focus is at the nexus of water-



energy-food, concentrating on fundamental science related to the generation of renewable energy and agricultural fertilizers for food crops. It aims to develop low-cost, high-efficiency methods and devices that integrate the utilization of energy from sunlight to convert water to hydrogen fuel, carbon dioxide to hydrocarbon fuels, and nitrogen gas to ammonia, which is used to generate fertilizers for food crops. The fundamental science focus of this project is anticipated to advance nowledge and technology and to produce trained scientists at the water-energy-food nexus in the US gulf coast region with an objective of connecting with the private sector for technology transfer and commercialization possibilities.

QuAnCo applied to Boltzmann Machines

Researchers: Prof. Mark A. Novotny (Physics & Astronomy) and Prof. Yaroslav Koshka (Electrical & Computer Engineering)

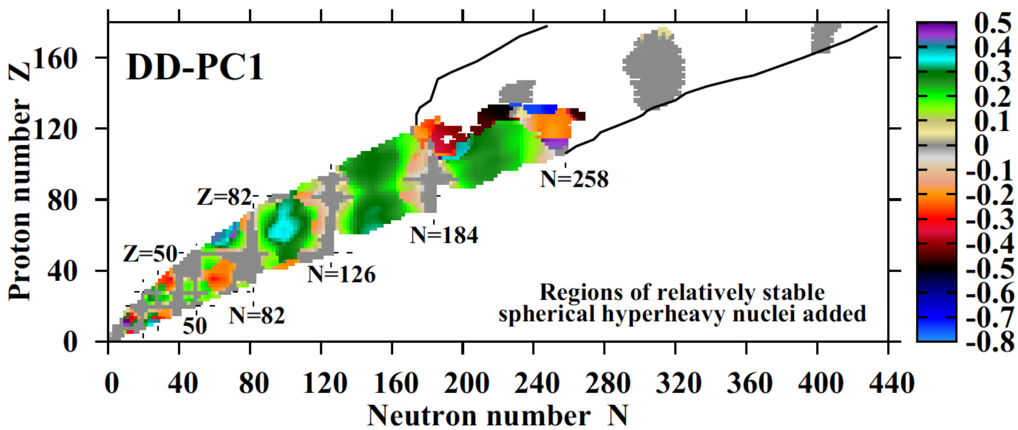


Prof. Mark A. Novotny and **Prof. Yaroslav Koshka**, together with their students, completed work related to quantum computing and machine learning. The project is funded by AFRL (Air Force Research Laboratory) under agreement FA8750-18-1-0096. The title of this award, QuAnCo applied to Boltzmann Machines, is difficult to parse. Basically the group is working at the intersection of three almost over-hyped fields, namely quantum computing, machine learning, and cybersecurity. For quantum computing the work is to test, advance, and utilize NISQ (Noisy Intermediate-Scale Quantum) devices, in particular quantum adiabatic computers (QuAnCo). The group utilizes 2000 qubit D-Wave machines, D-Wave 2000Q, in their research project. One question is how to utilize NISQ machines for machine learning paradigms. For this work, a Boltzmann Machine with one hidden and one visible layer fits onto the D-Wave 2000Q, and hence the majority of the studies are performed within the 64-visible and 64-hidden unit Restricted Boltzmann Machine which fits onto the current D-Wave architecture.

Nuclei in a relativistic framework: at and beyond density functional theory

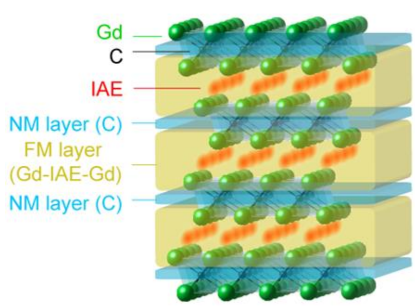
Researcher: Prof. Anatoli Afanasjev (Physics & Astronomy)

The research of the group of **Prof. Anatoli Afanasjev** has been supported by the grants from US Department of Energy, Office of Science, Office of Nuclear Physics and Department of Energy, National Nuclear Security Administration. The goal of these projects in the understanding of the properties of finite nuclei in covariant (relativistic) density functional theory. We studied fission properties of nuclei, the behavior and properties of nuclei under extreme conditions and their role in nuclear astrophysics processes. For the first time, systematic investigation of the properties of hyperheavy nuclei with proton number Z larger than 126 has been performed. It was shown that with increasing proton number the transition from ellipsoidal-like nuclear shapes to toroidal ones takes place. Many of such nuclei are expected to be unstable. However, three islands of stability of spherical hyperheavy nuclei have been predicted for the first time. The figure taken from Phys. Rev. C 99, 034316 (2019) shows the extension of nuclear landscape to hyperheavy nuclei. For the first time, nuclear reactions in the crust of accreting neutron stars have been investigated in a fully self-consistent network calculations including all nuclear reactions of relevance. It was found that nuclear heating is relatively robust and independent of initial composition, while cooling via nuclear Urca cycles in the outer crust depends strongly on initial composition. In addition, theoretical uncertainties (both systematic and statistical) in the description of different physical observables within the covariant density functional theory have been investigated. A special attention has been paid to these uncertainties in the fission process of superheavy nuclei. Another project involves the investigation of the clustering in light nuclei and the role of nodal structure of the single-particle wavefunctions in this phenomenon. In addition, the role of octupole deformation in superheavy nuclei and neutron rich actinides has been investigated.

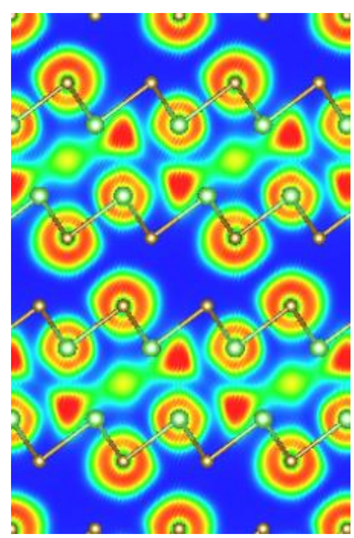


First-principles design of functional electrides using high-performance computers

Researcher: Prof. Seong-Gon Kim (Physics & Astronomy)



Electrides are unique ionic crystals in which electrons serve as anions. Similar to the fully delocalized electrons in metals, the electrons in electrides do not belong to any particular atom, molecule, or bond; however, unlike the former, these electrons are confined in the cavities within crystals and act as if they are anions by themselves. They have large non-reducible countercations that generate significant interstitial spaces within layers. Electrides have unique properties due to trapped electrons, such as high polarizabilities, high magnetic susceptibilities, highly variable conductivities, extremely low work functions, low temperature thermionic emission and very strong reducing character.

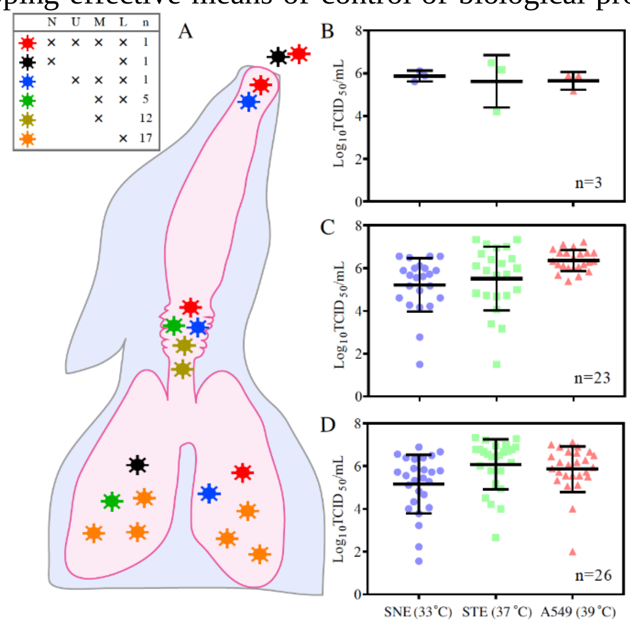


The combination of properties near metallic conductivity and weak electron binding can play a crucial role in solving problems based on electron emission due to light, heat or high electric fields. CCS researchers led by **Prof. Seong-Gon Kim** of Department of Physics and Astronomy use *ab-initio* computational methods to identify new candidate materials for electride and to investigate the material properties of newly designed candidate materials. This research is performed in international collaboration with researchers at Sung Kyun Kwan University in Korea.

Influenza Systems Biology

Researcher: Prof. Henry Wan (Basic Sciences, College of Veterinary Medicine)

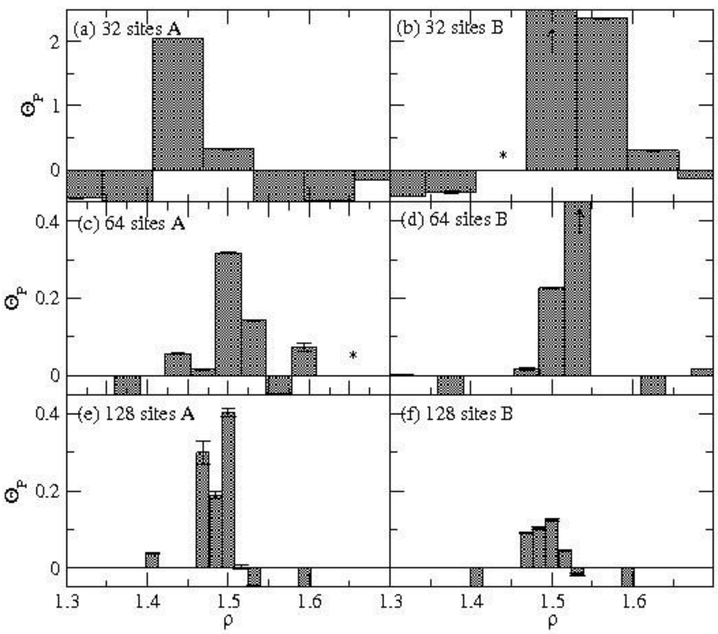
The mission of **Prof. Henry Wan**'s Influenza Systems Biology Lab is to study ecology, evolution, and host-pathogen interaction for emerging and re-emerging infectious diseases, especially influenza viruses, and to develop and apply systems biology based translational approaches to create influenza-less animal population and human communities. Translational systems biology is an integrated, multi-scale, evidence-based approach that combines laboratory, clinical and computational methods with an explicit goal of developing effective means of control of biological processes for improving human health and rapid clinical application. The current projects aim to 1) identify and predict emerging risks of influenza viruses for both human and animals (e.g. poultry and swine) using genomics sequences, big data and machine learning approaches; 2) develop a universal influenza vaccine, optimize vaccine production and vaccination strategies for disease prevention and quarantine; 3) develop machine learning methods to predict vaccine efficacy for each individual based on personal data, a move towards precision medicine; 4) understand molecular mechanisms for influenza evolution and influenza virus-host interactions, including host tropisms, pathogenesis, and transmission**.** These projects are currently supported through NIH, USDA, and NSF.



Theory and simulations of unconventional superconductors

Researcher: Prof. Torsten Clay (Physics & Astronomy)

Superconductivity, where the electrical resistance of a material vanishes below a critical temperature, is one of the least understood phenomena in materials. One of the greatest challenges in condensed matter physics is to understand the mechanisms driving superconductivity in several classes of materials that are known as *unconventional* superconductors. The well known BCS theory of superconductivity from 1957 is very successful at explaining the superconducting state found at very low temperatures in simple metallic elements and alloys. In the BCS model, superconductivity is due to the pairing of electrons, which is mediated by vibrations of the crystal lattice, phonons. In unconventional superconductors, the critical temperature is often far higher than can be explained by BCS, and in addition to superconductivity, unusual insulating states are often found. The mechanism behind these insulating states is the interaction between electrons themselves, which is ignored for simplicity in the BCS model. The superconducting pairing mechanism in these materials is however unknown. **Prof. Torsten Clay**'s group studies the quantum mechanics of interacting electrons in models for several of these materials. This requires using many-body numerical methods such as Quantum Monte Carlo. In recent work, we performed large-scale numerical calculations for a model of an organic unconventional molecular superconductor, $\kappa-(BEDT-TTF)_2$X. These calculations show that the superconducting pairing is enhanced by interactions between electrons *only* at a specific density of electrons, 0.5 per molecule. The fact that this same specific density of electrons is found in a number of unrelated unconventional superconductors points to a possible universal theory for superconductivity.



Hypothesis and Perspectives

Researcher: Prof. Tung-Lung Wu (Mathematics and Statistics)

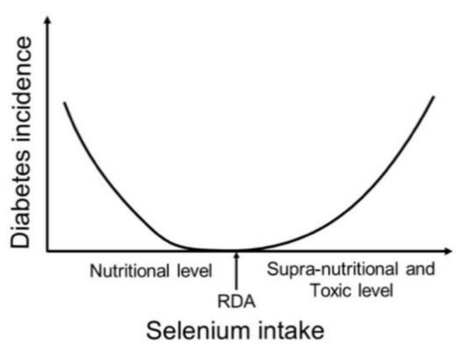


Figure 1. Impact of nutritional and supra-nutritional/toxic selenium on diabetes in normal individuals.

Although it is generally believed that body selenium (Se) status is adequate in the US, we argue that this may be overstated. Classic Se deficiency syndromes are very rare nowadays when body Se status reaches an extremely low level, but individuals with sub-optimal body Se status may be prone to certain chronic diseases such as diabetes. Here we ask whether and how sub-optimal Se status promotes diabetes. Published and our preliminary data indicates that Se insufficiency results in type-2 diabetes like syndromes and there is an inverse association between diabetes incidence and soil Se content in the US. Our long-term goal is to understand Se and selenoprotein functions in age-dependent degeneration including diabetes. **Prof. Tung-Lung Wu** is the main investigator on this National Institutes of Health (NIH)-R15 gramt and in this project, the central hypothesis (Figure 1), formulated and confirmed by the preliminary data, is that optimal body Se status at nutritional level prevents diabetes. Of note, we do not propose to study Se supplementation at supranutritional level. We propose to elucidate the optimal amount of Se and the protective mechanism for diabetes prevention (Aim 1) and the role of gut microbiota in diabetes prevention by nutritional Se (Aim 2). Thus, this project aims at addressing the serious diabetes issue in Mississippi and surrounding states, which is consistent with R15 funding mechanism.

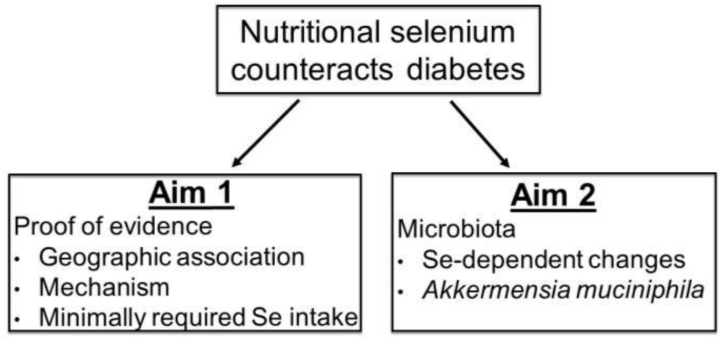
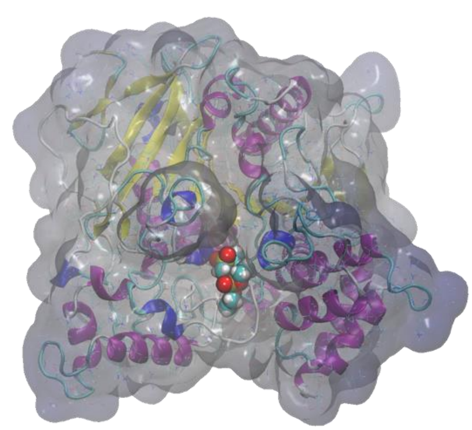


Figure 2. Aims Diagram.

Identification of novel brain-penetrating oxime antidotes for phorate toxicity

Researcher: Prof. Steven Gwaltney (Chemistry)

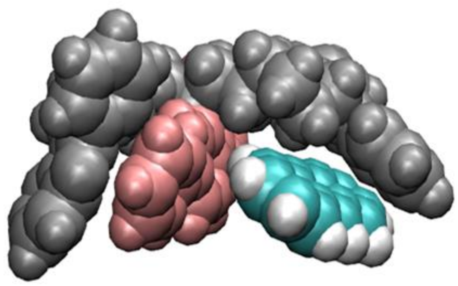
This work is sponsored by National Institutes of Health (NIH) CounterACT R21. The leading investigator is **Prof. Steven Gwaltney**. Phorate (O, O-diethyl S-ethylthiomethyl phosphorodithioate), is a highly toxic organophosphate (OP), and its active metabolites are potent inhibitors of acetylcholinesterase (AChE). Preliminary studies with a phorate metabolite phorate-oxon (PHO) have indicated a longer time delay and more violent signs of poisoning than with paraoxon (PXN), the active metabolite of parathion. Additionally, patterns of oxime-mediated cholinesterase reactivation differ between PHO and PXN, which is unexpected because both are diethyl phosphates, and would be expected to phosphylate cholinesterase with the same diethyl moiety and therefore display similar reactivation patterns. Estimates of binding energies and the unusual preliminary results observed thus far have suggested that there may be an ethoxy leaving group instead of the expected ethylthiomethyl group and that the slow bioactivation of PHO in the brain to PHO-sulfoxide and then to PHO- sulfone might be responsible for the unexpected preliminary observations. The aims of the project are to confirm the leaving group of PHO or PHO metabolites through a mass spectral analysis of AChE-phosphylated peptides and through computational modeling, to determine bioactivation efficiency through analysis of brain and hepatic bioactivation kinetics for phorate to its several metabolites, and to identify more effective oxime reactivators than the treatments currently in use. Above is an image of phorate-oxon sulfone, the most toxic phorate metabolite, bound to its target enzyme, acetylcholinesterase.

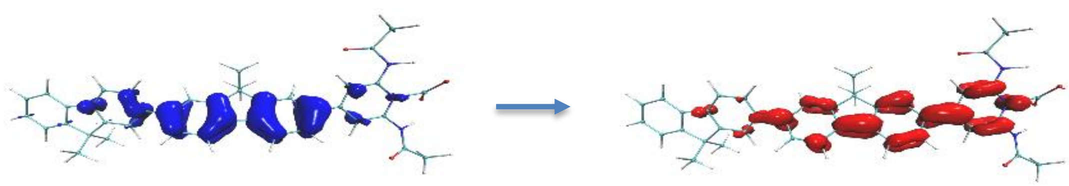


Developing new Sensors to Detect Seawater Contamination

Researcher: Prof. Steven Gwaltney (Chemistry)

The Gulf of Mexico is critical to the wellbeing of the United States, with substantial food and energy production, as well as its role in shipping and transportation. Protecting the health of the Gulf of Mexico requires monitoring the levels of pollutants such as polycyclic aromatic hyrdocarbons (PAH's), heavy metals, nitrates, and phosphates, along with monitoring carbon dioxide and oxygen levels. **Prof. Steven Gwaltney**'s group is using computational modeling to understand and develop new sensor technology to meet this challenge. Collaborators at the University of Southern Mississippi and the University of Alabama have been synthesizing and testing new polymer-based sensors. The Gwaltney group's computational modeling is providing useful insight into the behavior and performance of these new sensors. For example, the figure on the left shows the binding of the PAH anthracene with a PBP monomer. Unlike other PAH's, anthracene fits into a pocket in the PBP, causing a large shift in the PBP's fluorescence. The figure below shows the way the electron density changes during absorption when a carbon dioxide is interacting with a CO_2 detector. This change in electron density leads to a very intense excitation in the near UV with a large change in the absorption wavelength when a carbon dioxide molecule binds to the detector. This work is supported by the NSF through an EPSCoR Track II grant.

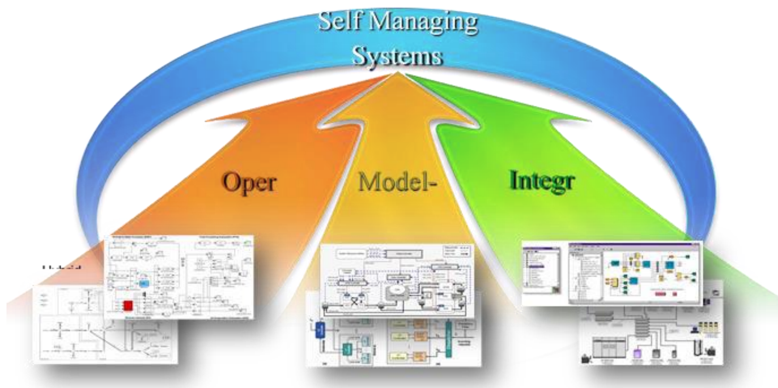




Autonomic Security for Next Generation Health Care Systems

Researcher: Prof. Ioana Banicescu (Computer Science and Engineering)

Effectively protecting computing infrastructures and networks from internal and external threats is a challenging task, due to their complexity, their large scale, and to the heterogeneity of the hardware and software components. On the field of Internet of Things (IoT), these characteristics are even more emphasized due to the presence of a plethora of sensors and actuators. Manually managing and protecting in real-time all these devices is tedious and error-prone, sometimes becoming even unfeasible. Together with **Prof. Stefano Iannucci** from Computer Science department, **Prof. Ioana Banicescu** is leading an international research collaboration initially sponsored by a Global Discovery Seed Grant from the International Institute at MSU. The goal of this international collaboration is to explore automatic cyber-defense in the field of Medical IoT (IoMT), which recently is gaining interest due to the increased capability of remotely analyzing in real time the health parameters of patients. Any cyber-attack in this domain has the potential to not just cause economic loss, but even loss of life. The project's objective is to advance the state-of-the-art on IoMT by proposing novel approaches for the automatic protection of large-scale distributed systems. Efforts have been made to establish a long-term collaboration with experts from institutions worldwide. This year, an international collaborative team has been initiated with experts from the University of Florida, Virginia Commonwealth University, University of Sapienza (Italy), University of Rome Torr Vergata (Italy), Blekinge Institute of Technology (Sweden), University of Basel (Switzerland). The proposed research is multidisciplinary and requires expertise in several areas such as, autonomic computing, performance modeling, cyber-security, big data. The group holds regular meetings and seeks external funding through applications to national and international funding agencies.

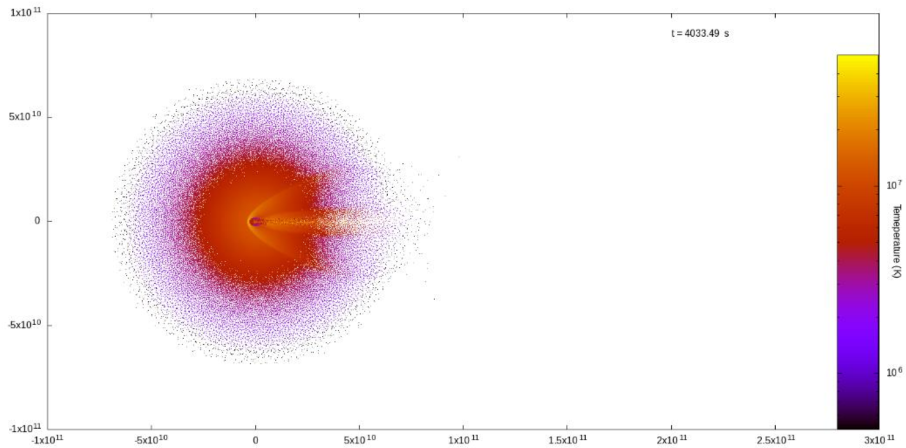


SPH-EXA: Optimizing Smoothed Particle Hydrodynamics for Exascale Computing

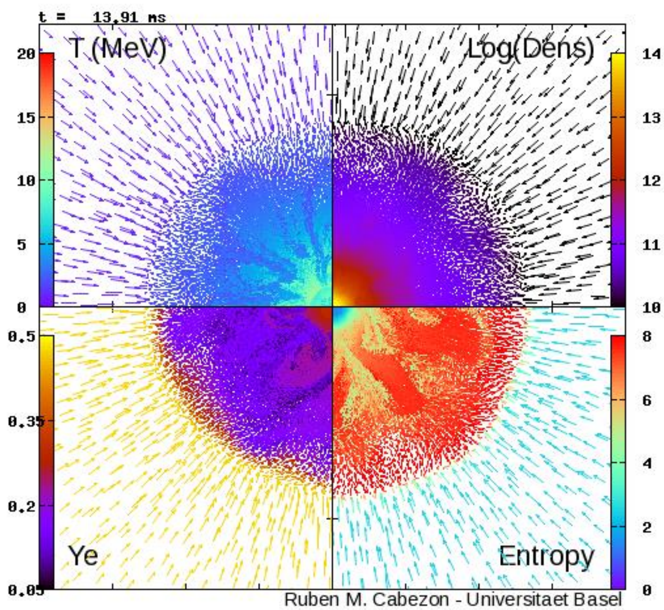
Researcher: Prof. Ioana Banicescu (Computer Science and Engineering)

The SPH-EXA is in international collaborative research project funded by the Swiss Platform for Advanced Scientific Computing in which **Prof. Ioana Banicescu** has an important contribution. The project brings together expertise in High Performance Computing, Astrophysics, and Computational Fluid Dynamics from universities and research laboratories in the United States and Europe. The goal of the project is optimizing the smoothed particle hydrodynamics technique for exascale computing, the next frontier in high performance computing. The efforts to achieve this goal are bring together a collaborative team of researchers from the University of Basel, University of Zurich, Mississippi State University, University of Washington and University Politecnica de Catalunya, Nextflow Software (France). The Smoothed Particle Hydrodynamics (SPH) technique is a purely Lagrangian method, used in numerical simulations of fluids in astrophysics and computational fluid dynamics, among many other fields. SPH simulations are among the most computationally-demanding calculations, in terms of sustained floating-point operations per second, or FLOP/s. It is expected that these numerical simulations will significantly benefit from the future Exascale computing infrastructures, that will perform 10^{18} FLOP/s. The performance of the SPH codes is, in general, adversely impacted by several factors, such as multiple time-stepping, long-range interactions, and/or boundary conditions. SPHYNX, ChaNGa, and SPH-flow, three SPH implementations, are the starting point of an interdisciplinary co-design project, SPH-EXA, for the development of an Exascale-ready state-of-the-art implementation. The goal is to understand the scalability limitations of today's state-of-the-art SPH implementations and use such knowledge to create the Exascale-ready implementation that includes efficient parallelization methods, fault-tolerance mechanisms, and load balancing approaches, to sustain the scalable execution of massively parallel SPH codes. The

SPH-EXA implementation targets reproducibility and portability by using continuous integration systems, and containerization techniques.



Head-on collision of a brown dwarf star with a (much bigger) solar-mass star.



Prompt convection in a newly born proto-neutron star 14 ms after bounce happened in the core-collapse Supernova scenario.

Education and Outreach

Co-sponsorship for the Institute for Mathematics and its Applications (IMA) Participating Institution Membership

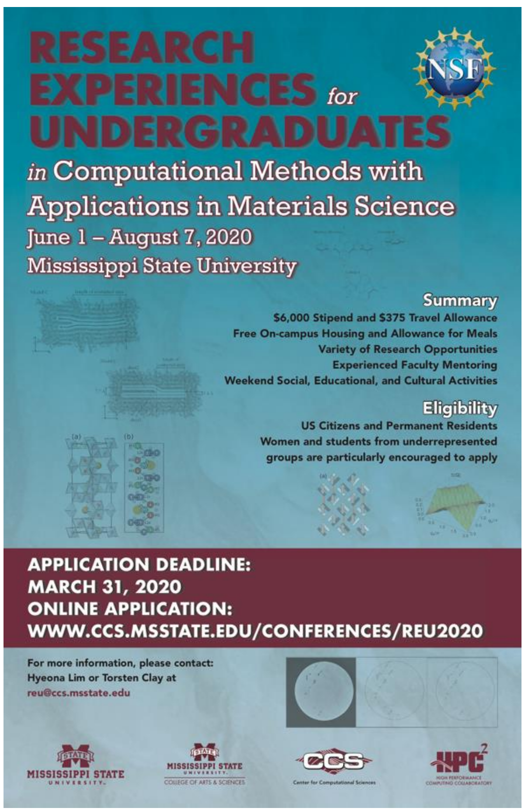
The CCS is one of the proud sponsors for the Institute for Mathematics and its Applications (IMA) Participating Institution Membership. Other sponsors are Department of Mathematics and Statistics, Center for Advanced Vehicular Systems (CAVS), Arts & Sciences Dean's Office, and The Office of Research and Economic Development (ORED) at MSU. The IMA, housed at the University of Minnesota, Minneapolis, MN, connects scientists, engineers, and mathematicians in order to address scientific and technological challenges in a collaborative, engaging environment, developing transformative, new mathematics and exploring its applications, while training the next generation of researchers and educators. With a history dating back to 1982, the IMA is an NSF-funded visitors' institute that has grown to become among the most influential math institutes in the world. The IMA facilitates groundbreaking research and provides a forum for collaboration and intellectual discourse. The IMA identifies rapidly developing areas of research and offers workshops in various interdisciplinary fields. MSU has been one of nearly 40 IMA participating institutions since 1999 many MSU faculty and students have participated in the IMA workshops and graduate summer schools. In 2018, MSU was named as the most active participating institution during the IMA PI Council Meeting. Prof. Hyeona Lim is the MSU representative for the IMA.

The Second International Conference on Computational Methods and Applications in Engineering (ICCMAE 2021)

With the Department of Mathematics and Statistics at MSU, the CCS will co-host *The Second International Conference on Computational Methods and Applications in Engineering (ICCMAE 2021)* in May, 2021. The conference was originally scheduled to be held on May 7-9, 2020 but it is postponed to 2021 due to COVID-19. The conference will also be jointly organized with the Universitatea Politehnica Timisoara (UPT), Romania. Main organizers are Profs. Mohsen Razzaghi (Math, MSU), Radu Vasiu (UPT), Hyeona Lim (Math & CCS, MSU), Amanda Diegel (Math & CCS, MSU), and Vu Thai Luan (Math & CCS, MSU). The main goal of the ICCMAE 2021 is the fostering of close interaction and networking opportunities between the participants in the interdisciplinary fields of computational mathematics, sciences and engineering with their real world applications. Our conference will facilitate the exchange of ideas and information among mathematicians, scientists and engineers in these areas. The ICCMAE 2021 will also provide many benefits to participants as it will create a unique and collaborative relationship between the United States institutions and other European universities. In addition to 5 plenary talks, the conference program will consist of mini-symposium sessions by the experts in the focused areas, interactive parallel contributed sessions, panel discussion, and informal discussions to promote conversation between the participants. With **Profs. Mohsen Razzaghi and Amanda Diegel, Prof. Hyeona Lim** secured the IMA seed funding to organize the conference. NSF proposal was also recently funded (DMS-1952848, PI: Hyeona Lim, Co-PIs: Mohsen Razzaghi, Amanda Diegel, and Vu Thai Luan) to mainly support the travel expenses of young researchers to attend this conference.

Research Experiences for Undergraduates (REU) in Computational Methods with Applications in Materials Science

The CCS will be hosing "Research Experiences for Undergraduates (REU) in Computational Methods with Applications in Materials Science" starting in the summer of 2021. This summer research program for undergraduates is recently funded by the NSF (DMR- 1950208) for 3 years. The REU program was supposed to start during the summer of 2020 but due to COVID-19 outbreak, it has been postponed to the summer of 2021. The director for this 10-week summer research program is **Prof. Hyeona Lim**. **Prof. Torsten Clay** is the Co-Director and faculty mentors are **Profs. Amanda Diegel, Steven Gwaltney, Gautam Rupak, Charles Edwin Webster, and Tung-Lung Wu.** This NSF's most prestigious undergraduate research program is among the three current REU programs at MSU. The REU will involve undergraduate students in research activities with a group of researchers in Mathematics, Statistics, Physics, and Chemistry from the CCS. We aim to show the students the enjoyment of doing research. The student participants recruited for this REU will spend 10 weeks over the summers of 2021-2023 in multidisciplinary research with faculty mentors in Mathematics, Statistics, Physics, and Chemistry from CCS. The students are first trained in the basic science and computational techniques necessary for their research projects. Additional training activities improve the participants' computational skills as well as written and oral presentation skills. REU participants are given access to supercomputing resources at the MSU High Performance Computing Collaboratory (HPCC). The students participate in weekly group meetings, seminars and training sessions on scientific and computational topics, and a Graduate Record Exam workshop. At the end of the summer they present the results of their project to the REU group and at the MSU Summer Undergraduate Research Symposium.



Grants

1. **I. Banicescu (Co-PI),** SPH-EXA: Optimizing Smooth Particle Hydrodynamics for Exascale Computing Sponsor: Swiss Platform for Advanced Scientific Computing, Investigators: F. Ciorba (U. Basel), Lucio Mayer (U. Zurich), D. Garcia-Senz (U. Politecnica de Catalonia), Thomas Quinn (U. Washington), Collaborators: International Proposal, 7/1/2017- 6/30/2020, $549,009.66
2. **I. Banicescu (Co-PI),** "Global Discovery Seed Grant Program" Mississippi State University, 1/1/2018-12/31/2018, $15,000
3. **C. E. Webster (PI)**, NSF CHE 1800201 Collaborative Research: SusChEM: Atomistic Switches on Pyridinol Based Pincer Ligated Catalysts for Carbon Dioxide Reduction, $115,566.00
4. R. King, **S. Zhang (Co-PI)**, E. Swan, TJ Jankun-Kelly, D. W. Carruth, G. W. Burgreen, C. L. Bethel, J. A. McGinley, M. A. Hamilton, R. Jones, Analytics and Data Sciences - Big Data Visualization, DoD, $4,017,172, 7/1/17-6/30/20
5. R. King, **S. Zhang (Co-PI)**, Marufuzzaman Mohammad, Brian Smith, Michael A. Hamilton, Randy Jones, Daniel Carruth, Analytics and Data Sciences - Big Data Analytics, DoD, $4,741,994, 7/1/17-6/30/20
6. **H. Lim (PI), Amanda Diegel (Co-PI),** IMA conference proposal, The second ICCMAE, $1,000, 01/15/19-01/14/21
7. **H. Lim (Co-PI),** DOD- ERDC T3: ROM Design Space-Advancing Design Space Exploration Through Surrogate Modeling, 4/28/17-4/27/20, $1,684,515.00
8. **H. Lim (Senior Personnel),** US Army ERDC WD 67 Topic 7-1 (360714); 09/30/2016 – 08/30/2018. PI: Mark Horstemeyer, $599,371.66
9. **H. Lim (Senior Personnel),** US Army ARL ICME (360645); 8/16/2017 – 8/16/2018. PI: Mark Horstemeyer, $468,546
10. **M. Novotny (PI),** Air Force Research Lab (AFRL), "QuAnCo Applied to Boltzmann Machines", co-PI Yaroslav Koshka, $484,819 for 12 months starting May 1, 2018
11. **H. Wan (PI),** USDA ARS, Wan, P.I. and Pharr, Co-PI, USDA ARS 310327-182090-021000 (G00003087) "Environmental management and animal health as they relate to processing yields and food safety of broiler meat and table eggs—Development of broadly protective E. Coli vaccine", $750,000. 10/1/2017-9/30/2022
12. **H. Wan (PI),** USDA, Arzt, Co-PI, "Inferred antigenic emergence associated with Quasispecies Dynamics and Subconsensus Variants of FMDV", $235,401 (direct cost). 05/14/2018-05/13/2020
13. **H. Wan (PI),** NIH NIAID R21AI135820, Wan, P.I., "Risk Assessment of Influenza A Viruses", $400,125. 05/02/2018 – 04/30/2020

14. **H. Wan (Senior Personnel),** DBI-1659630, Perkins, P.I., “REU Site: Undergraduate Research in Computational Biology at Mississippi State University”. $327,470. 04/15/2017- 03/31/2020
15. **H. Wan (PI),** NIH NIAID 1R01AI116744-01, “Genome Based Influenza Vaccine Strain Selection using Machine Learning”, $1,869,842. 01/13/2015-12/31/2019
16. **H. Wan (PI),** Firstline Biopharmaceuticals Corporation, “Test the vaccine efficacy of a novel influenza vaccine candidate.” $208,519. 12/1/2017-11/30/2019
17. **H. Wan (PI),** USDA APHIS, Wan, P.I., 16-740-1219-CA, 17-7440-1219-CA, 18-7440-1219-CA “Emergence and spread of avian influenza viruses in Poyang Lake”, $895,000. 9/1/2016-9/29/2019
18. **H. Wan (PI),** USDA APHIS, 16-7428-1264-CA, 17-7428-1333-CA, “Identifying microbes causing fish disease outbreaks in Mississippi Delta Using Metagenomics.” $120,000. 9/1/2015-8/31/2019
19. **H. Wan (PI)**, USDA APHIS, 18-7428-1382-CA, “Pathogenesis and transmission of the H1N1 and H3N2 avian origin influenza virus in feral swine”. $149,999. 08/15/2018 – 08/14/2019
20. **S.-G. Kim (PI),** “Discovery of New Functional Electride through the Dimensional Control of Interstitial Electron Arrays, Period 5”, National Research Foundation, Republic of Korea, PI, $90,090, 02/04/2019 – 02/03/2020
21. **S.-G. Kim (PI),** “Discovery of New Functional Electride through the Dimensional Control of Interstitial Electron Arrays, Period 4”, National Research Foundation, Republic of Korea, PI, $109,399, 02/04/2018 – 02/03/2019
22. **A. Afanasjev (PI),** U. S. DOE, ``Nuclei in a relativistic framework: at and beyond density functional theory'' $264,000, 01/2017-12/2019
23. **S. Gwaltney (Co-PI),** NIH CounterACT R21, “Identification of novel brain-penetrating oxime antidotes for phorate toxicity” PI: Janice Chambers, $394,764, 9/1/2018-8/31/2020
24. **S. Gwaltney (Senior Personnel),** NSF, OIA-1632825: RII Track-2 FEC: Emergent Polymer Sensing Technologies for Gulf Coast Water Quality Monitoring, 09/01/16 - 08/31/20, $4,000,000
25. **Yuan Liu (PI),** Simons Foundation Collaboration Grant “High order numerical methods on complex geometries”, $35,000, 9/1/16-8/31/21
26. **T. K. Hollis (Co-PI),** National Science Foundation, EPSCoR Track 2 – Co-PI - 09/01/2015 – 08/31/2019, $917,490 (Hollis portion of total $2.16M MSU portion of the budget of a total $6 million award for the 4 year period), “Feeding and Powering the World - Capturing Sunlight to Split Water and Generate Fertilizer and Fuels.” PI – Nathan Hammer, Co-PIs – T. Keith Hollis, C. Edwin Webster, Shanlin Pan, Russell Schmehl, Senior Personnel – Jared Delcamp
27. **G.Rupak (PI),** NSF PHY-1615092, awarded $264,138 from July 2016 - July 2019. Title: Nuclear Structure and Reactions from Lattice Effective Field Theory
28. **J. Ye (PI),** AFOSR, Atomic, Molecular and Optical Physics, “Quantum, topological phases and phase transitions of interacting cold atoms with spin-orbit couplings in optical lattices”, 9/15/16-9/15/19, $406,321

29. **T.-L. Wu (Co-PI)**, NIH-R15, "Optimized Selenium Intake, Gut Microbiota, and Diabetes" PI: Wen-Hsing Cheng, $421,185, 1/1/19 - 12/31/21
30. **V. Clink (PI)**, Agriculture and Food Research Initiative Competitive Grants Program USDA-NIFA, "A1701: Genetics and RNA Marker Development for FOV4 Resistance Breeding in Cotton" $294,216, 1/1/19-12/31/22
31. **V. Clink (PI)**, Cotton Incorporated, "Utilization of Genetic Resistance Mechanisms against Parasitic Nematodes of Cotton" $40,000, 1/1/19-12/31/20

Publications

1. K. P. Faseela, Ye Ji Kim, **S.-G. Kim**, S. W. Kim, and S. Baik, "Dramatically Enhanced Stability of Silver Passivated Dicalcium Nitride Electride: Ag-Ca2N", Chemistry of Materials, 30 (21), 7803-7812 (2018) (DOI: 10.1021/acs.chemmater.8b03202)
2. V. Dixit, D. Thapa, B. Lamichhane, C. N. Nandadasa, Y.-K. Hong, and **S.-G. Kim**, "Site preference and magnetic properties of Zn-Sn-substituted strontium hexaferrite", J. Appl. Phys. 125, 173901 (2019) (DOI: 10.1063/1.5084762).
3. D. L. Duong, S. J. Yun, Y. Kim, **S.-G. Kim**, and Y. H. Lee, "Long-range ferromagnetic ordering in vanadium-doped WSe2 semiconductor", Appl. Phys. Lett. 115, 242406 (2019)
4. **A. Diegel**, S. W. Walker. "A Finite Element Method for a Phase Field Model of Nematic Liquid Crystal Droplets", Comm. Comput. Phys., Volume 25 (1), Pages 155-188 (2019), (DOI: 10.4208/cicp.OA-2017-0166)
5. Kasielke, F., Ronny, T., Iwainsky, C., Velten, M., Ciorba, F. M., **Banicescu, I.** (2019). "Exploring Loop Scheduling Enhancements in OpenMP: An LLVM Case Study", (pp. 131--138). Proceedings of the 18th International Symposium on Parallel and Distributed Computing, ISPDC 2019. https://doi.org/10.1109/ISPDC.2019.0002
6. Sanders, W. S., Srivastava, S., **Banicescu, I.** (2019). "A Container-Based Framework to Facilitate Reproducibility in Employing Stochastic Process Algebra for Modeling Parallel Computing Systems", (pp. 373--381). Proceedings of the IEEE International Parallel and Distributed Processing Symposium IPDPSW 2019. https://doi.org/10.1109/IPDPSW.2019.00070
7. Iannucci, S., Barba, O. D., Cardellini, V., **Banicescu, I.** (2019). "A Performance Evaluation of Deep Reinforcement Learning for Model-Based Intrusion Response", 2019 IEEE 4th International Workshops on Foundations and Applications of Self* Systems (FAS*W).
8. **Banicescu, I.**, Strazdins, P., Aubanel, E., Raphael C., Shontz, S. M., Rauber, T., Gudula , R. Yang, L. T. (2019). "Introduction to Proceedings of the IEEE International Parallel and Distributed Processing Symposium", IPDPSW-PDSEC 2019 (pp. 673--674). Proceedings of the IEEE International Parallel and Distributed Processing Symposium IPDPSW 2019 / IEEE Computer Society. https://doi.org/10.1109/IPDPSW.2019.00113
9. Ciorba, F. M., L. Mayer, R. M. Cabezón, D. Imbert, D. Guerrera, A. Cavelan, A. Mohammed, D. S. Reed, J.-G. Piccinali, **I. Banicescu**, D. Garciá-Senz, and T. R. Quinn, "SPH-EXA: Optimizing Smoothed Particle Hydrodynamics for Exascale Computing", Project poster presented at the International Supercomputing Conference (ISC), Frankfurt, Germany, June 17-20, 2019.
10. Ciorba, F. M., L. Mayer, R. M. Cabezón, D. Imbert, D. Guerrera, A. Cavelan, A. Mohammed, D. S. Reed, J.-G. Piccinali, **I. Banicescu**, D. Garciá-Senz, and T. R. Quinn, "Design and Imple-

mentation of an Exascale-Ready Mini-App for Smoothed Particle Hydrodynamics Simulations", presented at the 6th ACM SIGHPC Platform for Advancing Scientific Computing Conference (PASC 2019), Zurich, Switzerland, June 12-14, 2019.

11. Mohammed, A. Cavelan, F. M. Ciorba, R. M. Cabezón, **I. Banicescu**, "Identifying Performance Challenges in Smoothed Particle Hydrodynamics Simulations", presented at the 6th ACM SIGHPC Platform for Advancing Scientific Computing Conference (PASC 2019), Zurich, Switzerland, June 12-14, 2019.
12. **A. V. Afanasjev**, "Cluster structures, ellipsoidal shapes and nuclear molecules in light A=12-50 nuclei", European Physical Journal, Web of Conferences 194 (2018) 06001: 1-6
13. S. E . Agbemava, **A. V. Afanasjev**, and A. Taninah, "Propagation of statistical uncertainties in covariant density functional theory: Ground state observables and single-particle properties", Physical Review C 99, 014318 (2019): 1-24
14. S. E. Agbemava, **A. V. Afanasjev**, A. Taninah, and A. Gyawali, "Extension of the nuclear landscape to hyperheavy nuclei", Physical Review C 99, 034316 (2019): 1-26
15. **A. V. Afanasjev**, N. Itagaki and D. Ray, "Rotational excitations in near neutron-drip line nuclei: the birth and death of particle-bound rotational bands and the extension of nuclear landscape beyond spin zero neutron drip line", Physics Letters B 794 (2019) 7-13
16. Z. Shi, **A. V. Afanasjev**, Z. P. Li and J. Meng, "Superheavy nuclei in microscopic collective Hamiltonian approach: the impact of beyond mean field correlations on the ground state and fission properties", Physical Review C 99 (2019) 064316: 1-10 and supplemental material
17. **T.-L. Wu** (2018). Boundary Crossing Probabilities for Jump Diffusion Processes to Time-Dependent Boundaries, Methodology and Computing in Applied Probability. DOI: 10.1007/s11009-018-9685-5
18. **T.-L. Wu** (2018). Conditional Waiting Time Distributions of Runs and Patterns and Their Applications, ANNALS OF THE INSTITUTE OF STATISTICAL MATHEMATICS. DOI: 10.1007/s10463-018-0696-3 3.
19. **T.-L. Wu** (2018). A note on Erdös and Kac's identity: boundary crossing probability of Brownian motion to constant boundary, Methodology and Computing in Applied Probability. DOI: 10.1007/s11009-018-9686-4
20. **Q. Zhou**, S. Zhang, and H. Lin (2019) "Goodness-of-fit Test of Copula Functions for Semi-parametric Univariate Time Series Models." Statistical Journal, to appear. https://doi.org/10.1007/s00362-019-01153-4.
21. A. Robertson, **Q. Zhou**, A. Tatch, and M. Walsh (2019). Gender-Specific Predictors of Recidivism among DUI Offenders. Journal of Studies on Alcohol and Drugs, 80(6), 641-650.
22. S. Zhang, **Q. Zhou**, D. Zhu, and P. Song. (2019) "Goodness-of-Fit Test In Multivariate Jump Diffusion Models." Journal of Business & Economic Statistics, 37(2), 275-287.

23. Chen, S., Sun, S., Li, C., Pittman Jr., C. U., Lacy, T. E., Hu, S. and **Gwaltney, S. R.** 2018. “Molecular dynamics simulations of the aggregation behavior of overlapped graphene sheets in linear aliphatic hydrocarbons”, Mol. Simul. 44: 947-953.
24. Dickel, D., **Gwaltney, S. R.**, Mun, S., Baskes, M. I., and Horstemeyer, M. F. 2018. “A Dispersion-Corrected Modified Embedded-Atom Method Bond Order Interatomic Potential for Sulfur”, J. Phys. Chem. A 122: 9572-9578.
25. Jinasena, D., Bowleg, J., Simmons, R., Zhang, Y., **Gwaltney, S. R.,** and Fitzkee, N. C. 2019. “Using Histone H1 Derived Peptides to Investigate Binding Affinity and Inter-Domain Dynamics in Human Pin1”. Biophys. J. 116: 463a.
26. Murphy, M. A., Mun, S., Horstemeyer, M. F., Baskes, M. I., Bakhtiary, A., LaPlaca, M. C., **Gwaltney, S. R.,** Williams, L. N., and Prabhu, R. 2019. “Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths”, J. Biomolecular Struct. Dyn. 37: 1346-1359.
27. Bowman, A., Mun, S., Nouranian, S., **Gwaltney, S. R.,** Huddleston, B. D., Baskes, M., and Horstemeyer, M. F., 2019. “Free Volume and Internal Structural Evolution During Creep in Amorphous Polyethylene by Molecular Dynamics Simulations”, Polymer 170: 85-100.
28. S. Das, R. R. Rodrigues, R W. Lamb, F. Qu, E. Reinheimer, C. M. Boudreaux, **C. E. Webster**, J. H. Delcamp, E. T. Papish "Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction" Inorg Chem, 2019, 58, 8012-8020.
29. P. Wang, G. Liang, C. L. Boyd, **C. E. Webster**, X. Zhao "Catalytic H2 Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand" Eur J Inorg Chem, 2019, 2134-2139.
30. Y. O. Wong, L. A. Freeman, A. D. Agakidou, D. A. Dickie, **C. E. Webster**, R. J. Gilliard, Jr. "Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents" Organometallics, 2019, 38, 688-696.
31. G. K. Kosgei, D. Breen, R. W. Lamb, M. Y. Livshits, L. A. Crandall, C. J. Ziegler, **C. E. Webster**, J. J. Rack. "Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes" J Am Chem Soc, 2018, 140, 9819-9822.
32. P. Wang, G. Liang, M. R. Reddy, M. Long, K. Driskill, C. Lyons, B. Donnadieu, J. C. Bollinger, **C. E. Webster**, X. Zhao. "Electronic and Steric Tuning of Catalytic H2 Evolution by Cobalt Complexes with Pentadentate Polypyridyl-Amine Ligands" J Am Chem Soc, 2018, 140, 29, 9219-9229.
33. “Universal behavior of p-wave proton-proton fusion near threshold”, B. Acharya, L. Platter and **G. Rupak**, Phys. Rev. C 100, 0210001 (R), 2019.
34. “Bayesian analysis of capture reactions $^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$”, P. Premarathna and **G. Rupak**, arXiv:1906.04143. Accepted for publication in Eur. Phys. J A.

35. A. B. Misra and **H. Lim**, “Compare Speckle denoising models based on total variation and filtering methods”, Communications in Computer and Information Science, Vol. 1030, pp. 257 – 270, 2019
36. A. B. Misra, C. Jones, and **H. Lim**, “Edge Enhancing Accelerated Diffusion Model for Speckle Denoising in Medical Imagery”, Proceedings of the 1st International Conference on Computational Methods and Applications in Engineering, ITM Web Conf. Vol. 29, 01009, 2019, https://doi.org/10.1051/itmconf/20192901009;
37. M. Judson, T. Viger, and **H. Lim**, “Efficient and Robust Non-Local Means Denoising Methods for Biomedical Images”, Proceedings of the 1st International Conference on Computational Methods and Applications in Engineering, ITM Web Conf. Vol. 29, 01003, 2019, https://doi.org/10.1051/itmconf/20192901003.
38. **R. T. Clay** and S. Mazumdar, “From charge- and spin-ordering to superconductivity in the organic charge-transfer solids," Physics Reports 788 (2019) 1-89.
39. Wen, F, and **X.-F. Wan**. “Influenza Neuraminidase: Underrated Role in Receptor Binding”. Trends in Microbiology, 27(6): 477-479, 2019.
40. Cunningham, F. L., K. C. Hanson-Dorr, L. Ford, R. Middleton, A. Crain, L. Durst, C. Ware, M. J. Griffin, C. C. Mischke, **X.-F. Wan** and L. A. Hanson. “Environmental Factor(s) and Animal Vector(s) Associated with Atypical Aeromonas hydrophila Abundance and Dissemination among Channel Catfish Ponds”. Journal of the World Aquaculture Society, 2019, https://doi.org/10.1111/jwas.12608.
41. Uher-Koch, B., T. Spivey, C. V. Hemert, J. Schmutz, K. Jiang, **X.-F. Wan**, and A. Ramey. “Serologic evidence for influenza A virus exposure in three loon species (Gavia spp.) breeding in Alaska”, Journal of Wildlife Diseases, 55(4):862-867, 2019.
42. You, W., Z. Yang, G. Guo, **X.-F. Wan**, and G. Ji. 2019. “Prediction of DNA-binding proteins by interaction fusion feature representation and selective ensemble”, Knowledge-based systems, 163: 598-610.
43. Han, L., L. Li, F. Wen, L. Zhong, T. Zhang, and **X.-F. Wan**. 2019. “Graph-Guided multi-task sparse learning model: a method for identifying antigenic variants of influenza A(H3N2) virus”, Bioinformatics, 2019 Jan 1; 35(1):77-87 doi: 10.1093/bioinformatics/bty457.
44. Zhang, X., H. Sun, F. L. Cunningham, L. Li, K. Hanson-Dorr, M. W. Hopken, J. Cooley, L.-P. Long, J. A. Baroch, T. Li, B. S. Schmit, X. Lin, A. K. Olivier, R. G. Jarman, T. J. DeLiberto, and **X.-F. Wan**. 2018. “Tissue tropisms opt for transmissible reassortants during avian and swine influenza A virus co-infection in swine”, PLoS Pathogens, 14(12):e1007417.
45. Li, L. T. J. DeLiberto, M. L. Killian, M. K. Torchetti, and **X.-F. Wan**. 2018. “Evolutionary Pathway for the 2017 Emergence of a Novel Highly Pathogenic Avian Influenza A(H7N9) Virus among Domestic Poultry in Tennessee, United States”, Virology, 525: 32-39.

46. Wen, F., S. Blackmon, A. K. Olivier, L. Li, G. Guan, H. Sun, and P. Wang, and **X.-F. Wan**. 2018. “Mutation W222L at the receptor binding site of hemagglutinin could facilitate viral adaption from equine influenza A(H3N8) virus to dogs”, Journal of Virology, 92(18). pii: e01115-18.
47. Li, L., A. S. Bowman, T. J. DeLiberto, M. L. Killian, S. Krauss, J. M. Nolting, M. K. Torchetti, A. M. Ramey, A. B. Reeves, D. E. Stallknecht, R. J. Webby, **X.-F. Wan**. 2018. “Genetic evidence supports sporadic and independent introductions of low pathogenic H5 avian influenza A viruses from wild birds to domestic poultry in North America”, Journal of Virology, 92(19). pii: e00913-18.
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49. Austin H. W., McNeece B. T., Sharma K, Niraula P. M., Lawrence K. S., **Klink V. P.,** “An expanded role of the SNARE-containing regulon as it relates to the defense process that Glycine max has to Heterodera glycines”, Journal of Plant Interactions 14:276-283.
50. Alshehri H. A., Alkharouf N. W., Darwish O., McNeece B. T., **Klink V. P.**, “MAPKDB: A MAP kinase database for signal transduction element identification”, Bioinformation 15:338-341, 2019.
51. McNeece B. T., Sharma K., Lawrence K. S., Lawrence G. W., **Klink V. P.**, “The mitogen activated protein kinase (MAPK) gene family functions as a cohort during the Glycine max defense response to Heterodera glycines”, Journal: Plant Physiology and Biochemistry 137:25–41, 2019.
52. **A. Patrick**, “Dissociation pathways of protic ionic liquid clusters: Alkylammonium nitrates”, Journal of Mass Spectrometry, Vol 54, Pages 371-377.
53. **A. Patrick**, “Mechanistic insights into intramolecular phosphate group transfer during collision induced dissociation of phosphopeptides”, Journal of Mass Spectrometry, Vol. 54, pages 449-458.
54. **A. Patrick**, “Electrospray Ionization Enters the Final Frontier: Mass Spectrometry's Role in Understanding Electrospray Thrusters and Their Plumes”, Rapid Communications in Mass Spectrometry (in press)
55. **J. Shi, J. Zhang**, and Y. Ge. "CASMI—An Entropic Feature Selection Method in Turing’s Perspective" Entropy, 2019, 21(12), 1179. (doi: https://doi.org/10.3390/e21121179)