

Consortium for High Energy Density Science (CfHEDS)

SSAP February 16-18, 2021



FLORIDA
AGRICULTURAL AND
MECHANICAL
UNIVERSITY



UNIVERSITY OF CALIFORNIA
MERCED

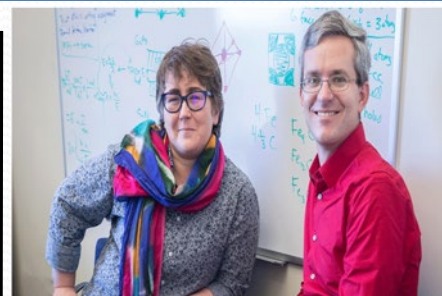


Charles A. Weatherford, PI
Florida A&M University

Introduction/Overview: CONSORTIUM FOR HIGH ENERGY DENSITY SCIENCE

Title:
Consortium for High Energy Density Science (CfHEDS)

Scientific Challenge: The CfHEDS participants are: Charles Weatherford, Ronald Williams (Florida A&M U.), David Strubbe, Aurora Pribram-Jones (U. California, Merced), Eddie Red, Wesley Sims (Morehouse C.), Frank Graziani, Tony Baylis, Ronnie Shepherd, David Rakestraw (Lawrence Livermore Natl. Lab) The goal of this project is to create and sustain a workforce pipeline to NNSA National Laboratories by increasing the number of students interested in science, by developing new scientists, and by building improved scientific educational and research capacity. This will be accomplished at three minority-serving institutions, enabling them to develop scientists who are well prepared to work in the NNSA-critical field of High Energy Density Science (HEDS).



Aurora Pribram-Jones and David Strubbe--UC Merced CfHEDS HED Scientists



FAMU STEM Day 4/6/19—800+ K-12 students and parents learn about and participate in STEM experiments.

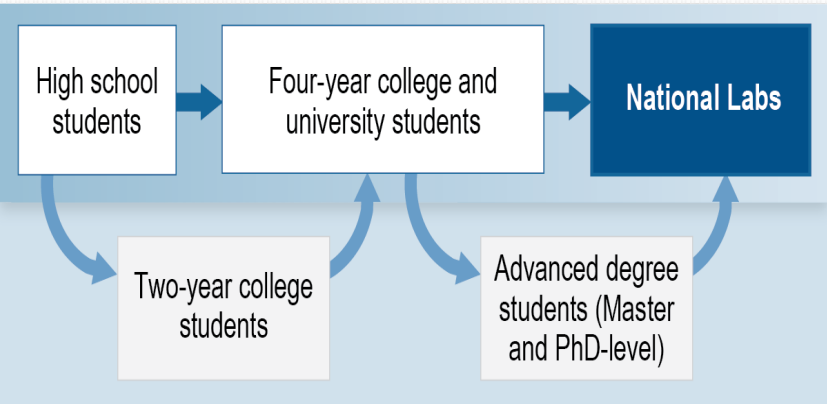


CfHEDS students at Morehouse workshop.



Trained students, postdocs, faculty
- HED expertise - Access to R&D facilities
LLNL and CfHEDS.

CfHEDS Pipeline



Project Period: 10/01/2018 – 09/30/2021

Research Topic Area: High Energy Density Science

Program: MSIPP

CfHEDS GOALS & OBJECTIVES

Objective 1: Enhance Educational Opportunities

Initiate joint curriculum building and develop LLNL-based internships.

Produce BS and PhD students from CfHEDS-participating students.

Institute extended professional training in experiment/theory at LLNL for CfHEDS students.

Teach newly developed HED and electronic structure-related courses.

Objective 2: Expand Research Collaborations

Initiate HEDS research collaborations between FAMU, UCM, MC, and LLNL.

Develop novel computational methods to enhance LLNL computing capabilities.

Benchmark proposed models/methods by comparison with LLNL experiments.

Apply models to systems of direct relevance to HEDS at LLNL and other NNSA Labs.

Objective 3: Enhance Awareness of HED Science Careers

Provide structured mentoring to CfHEDS participants and develop pre-college STEM initiatives.

Prepare CfHEDS students for applications to DOE-funded graduate/postdoctoral fellowships.

Add three CfHEDS alumni (postdoctoral fellow and/or PhD) to the NNSA Labs workforce.

Florida A&M U.

Historically Black University (HBCU) with a student body 84% African American--number one public HBCU.

Charles Weatherford—computational physicist working in atomic, molecular, plasma, and HED physics, and Quantum Chemistry (time independent and time dependent DFT).

Ronald Williams—experimental plasma physicist working in laser/plasma/electron beam interactions, plasma wave acceleration and undulators, and fusion/astrophysics studies using a spheromak plasma.

University of California, Merced

Hispanic-serving institution in California's Central Valley, 75% undergraduates are first-generation.

David Strubbe—computational condensed-matter physicist working on electronic and optical properties, response of non-equilibrium systems, time-dependent DFT.

Aurora Pribram-Jones—theoretical chemist working on developing finite-temperature DFT and TDDFT, for application to warm dense matter systems.

Morehouse College

The world's only all-male Historically Black College (HBCU).

Eddie C. Red--Materials Science Physics with Electrochemical Applications; Nuclear Science and Environmental Radiation Studies; Electron/Photon Interactions with Atoms & Molecules

Wesley D. Sims--Micro/Nano Optics and Lasers; Nanolithography; Meta-materials

Background—Why CfHEDS is a Part of MSIPP

- CfHEDS promotes the STEM disciplines in order to increase students' interest in obtaining degrees in both undergraduate and graduate programs, and to train the next generation workforce and in particular, the national laboratory workforce.
- The funding provided by the NNSA is critical to maintaining CfHEDS' success and will allow its members to leverage other funding agencies to support the NNSA vision.
- Activities conducted by CfHEDS members such as outreach, training workshops, short courses, and hands-on research, will increase awareness of STEM graduate, research, and career opportunities.
- CfHEDS activities will motivate students to pursue advanced degrees and increase their willingness and opportunities to work at the national laboratories.

PROJECT IMPACT

	Target Audience	Benefits
C O M M U N I T Y	Undergraduate Students	<ul style="list-style-type: none"> Access to enhanced HED curriculum 10-week summer research opportunities at LLNL
	Graduate Students	<ul style="list-style-type: none"> Access to enhanced HED curriculum 10-week summer and year-long research internships at LLNL Opportunities to pursue thesis work at LLNL, with LLNL staff serving as thesis co-directors
	Faculty	<ul style="list-style-type: none"> Research sabbaticals at LLNL Develop and teach new HED curricula Research collaborations with LLNL staff and faculty at partnering MSIs Serve on LLNL review and advisory committees
	Postdocs	<ul style="list-style-type: none"> Post-doctoral research appointments at LLNL Short and extended research visits to LLNL Access to world-class experimental and computational facilities Mentorship by leading HED experts at LLNL and partnering MSIs
L D O B E S	LLNL Staff	<ul style="list-style-type: none"> Develop enhanced HED curricula Serve as mentors and thesis advisors for HED physics students Expanded research collaborations with faculty at partnering institutions Opportunity to serve as adjunct faculty and teach HED courses

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www.llnl.gov/HighEnergyDensityScience

Capacity Building -CSF1

FLORIDA A&M UNIVERSITY

- **Curriculum:**

- Dr. Weatherford at FAMU developed a course in High Energy Density Physics and a course in Time Independent and Time Dependent Density Functional Theory
- A series of lectures was created by Ronald Williams targeted to undergrad and grad students introducing them to High Energy Density Science. Some of the topics of these lectures were inspired by the LLNL short course lectures on the Interaction of X-Rays with Matter.
- An X-Ray source was purchased and is being used in course work and demonstrations

- **Publications:**

- “Design, Properties, Operation, and Modelling of the STPX Plasma Device”, **R. Williams, J. Clark, M. Richardson, S. Evans, D. Ologunogba, A. Agjedo, J. Titus, C. Weatherford**, Pulsed Power & Plasma Science 2019 Conference, Orlando, FL, June 23-28, 2019.
- **Daniel Gebremedhin, Charles Weatherford**, and Brian Wilson, “Normalizing Cluster Wavefunctions in the Interstitial Region of the Watson Sphere”, In Philip Hoggan, editor: Novel Electronic Structure Theory: General Innovations and Strongly Correlated Systems, Vol 77, AIQ, UK: Academic Press, 2019.



High Energy Density Optics and
the Materials and High Energy Density Science

Capacity Building -CSF1

FLORIDA A&M UNIVERSITY

- **Collaborative Research**

- **Jerry Clark and Dr. Ron Williams** are working with **Dr. Ronnie Shepherd (LLNL scientist)** on the experimental characterization of ionization potential depression in HED plasmas. Drs. Williams and Shepherd are co-directing Mr. Clark's PhD. Mr. Clark is in residence at LLNL.
- **Daniel Gebremedhin, Charles Weatherford, and Frank Graziani**--Density Functional Theory, Machine Learning, and Fluid Dynamics. Dr. Gebremedhin is in residence at LLNL
- **Ms. Jessica Tucker (Dr. Charles Weatherford's FAMU PhD student)** is working with **Dr. Jonathan DuBois and Dr. Frank Graziani (LLNL scientists)** on quantum control for quantum computing. Ms. Tucker is in residence at LLNL.
- **Mr. Yaye Badjo (FAMU PhD student of Bidhan Saha** is working with **Stanimir A. Bonev (LLNL)**. They are working on a computational study of the high-pressure properties of hydrogen iodide (HI). Mr. Badjo is in residence at LLNL. (Drs. Saha and Bonev are co-directing Mr. Badjo's PhD.
- **Adeola Aghedo, Carol Scarlett (FAMU), Felicie Albert (LLNL) and Candeias-Lemos, Nuno (LLNL)**-Analytical model for multi-MeV bremsstrahlung emission from interaction between short pulse, high intensity lasers and target metals. Adeola will be in residence at LLNL starting in summer of 2021.

Capacity Building - CSF1

University of California Merced

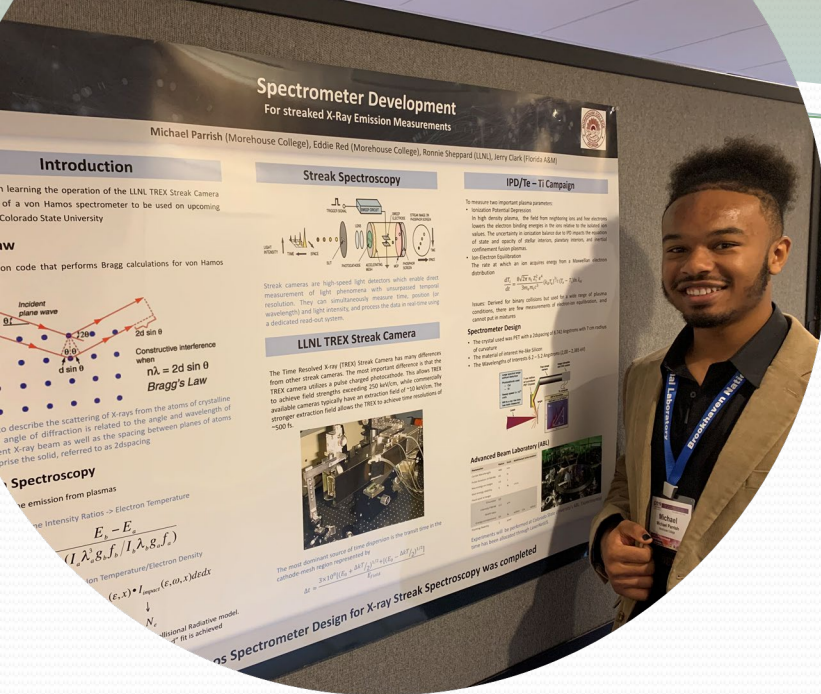
• Curriculum:

- Module on High Energy Density Physics for graduate “Condensed Matter Physics” class, including guest lectures by LLNL’s Dr. Jeff Colvin.
- Profs. Strubbe and Pribram-Jones spoke about HEDS, in Introduction to Graduate Research seminar series for first-year physics PhD students.
- HEDS content in general chemistry and graduate elective on density functional theory
- PhD student Md. Mehdi Masud took remote HEDS class from University of Nevada, Reno.

• Speaking Engagements:

- Seminars at UCM by Dr. Tammy Ma, Frank Graziani, Félicie Albert from LLNL
- Seminars at LLNL by Profs. Strubbe and Pribram-Jones in 2019 and 2020
- Seminars (virtually) for Morehouse by Profs. Strubbe and Pribram-Jones
- Seminar at UCM by Prof. Red from Morehouse
- Talk about UC Merced grad programs at High-Energy Density Science University Partners Day 2019 at LLNL

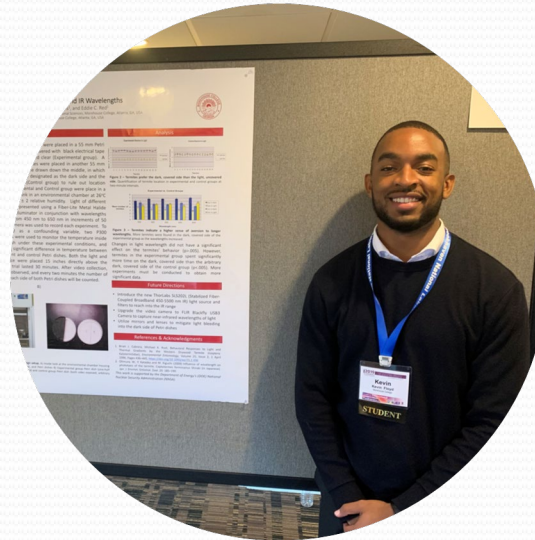




Morehouse Students Supported by CfHEDS

Research

- All physics majors are required to participate in at least two undergraduate research experiences.
- Students are highly encouraged to attend national conferences to present their research.



Recent Conferences

- CfHEDS has supported Morehouse participation at the National Society of Black Physicists (NSBP) Conference (2018-2020). MC has a strong presence with an average of 10 student participants annually.
- Two students received awards for outstanding undergraduate research presentation: Kevin Jameson Floyd and Michael Parrish.

Morehouse is the nation's #1 producer of underrepresented males who earn a B.S. in Physics.

Morehouse College

- Morehouse supported 11 undergraduate students presenting STEM research at the 2018 National Society of Black Physicists (NSBP) Conference in Columbus, OH, and 8 undergraduate students at the 2019 NSBP Conference in Providence, RI, where Kevin Jameson Floyd and Lettrell Harris received awards for outstanding undergraduate research presentations in 2019.
- Morehouse PI and 2 students (John Ali and Omar Tafiti) attended the Oak Ridge National Laboratory Research Collaboration Workshop, to present their research and learn more about opportunities at ORNL.



Morehouse undergraduate researchers at 2019 NSBP conference.

Morehouse-LLNL Summer Internships and Collaborative Research

- Summer 2018
 - Two students, Eric Carter and Quahhar Fletcher, participated in a 10-week summer research experience at LLNL. Eric and Quahhar were both part of the pilot internships with LLNL.
 1. Student: Quahhar Fletcher
 - Mentor: Dr. Vanessa Peters
 - Project: “Investigating ways to improve the deposition process used for electroplating gold on spheres”
 2. Student: Eric Carter
 - Mentor: Dr. Steven Hawks
 - Project: “Developed a custom translation stage that would be used to calibrate multi-channel magnetic probes used in capacitive desalination”

Morehouse-LLNL Summer Internships and Collaborative Research

- Summer 2019

- 5 undergraduate Morehouse students completed a 10-week summer research experience at LLNL. Similar to summer 2018, each student was paired with a lab mentor to guide their summer research projects related to High Energy Density Science.
 - Student: Eric Carter
 - Mentor: Dr. Chantel Aracne Ruddle
 - Project: “Carbon Nanotube Yarns”
- 2. Student: Quahhar Fletcher
 - Mentor: Dr. Vanessa Peters
 - Project: “Electrodeposition of high-z capsules for Inertial Confinement Fusion (ICF)”
- 3. Student: Trent Malone
 - Mentor: Dr. Juana Mendenhall, Dr. James Kelly, Dr. Marcus Worsley
 - Project: “Fabrication of Diatomaceous Earth (DE) Mini-tubes Based on Their Effectiveness and Use for Filtration”
- 4. Student: Michael Parrish
 - Mentor: Dr. Ronnie Shepherd
 - Project: “Spectrometer Development for X-ray Emission Measurements in Support of IPD Campaign”
- 5. Student: Jassiem Robinson
 - Mentor: Dr. Edwin Quashie
 - Project: “Using Machine Learning to Predict Microscopic Properties of Materials”

Morehouse-LLNL Summer Internships and Collaborative Research

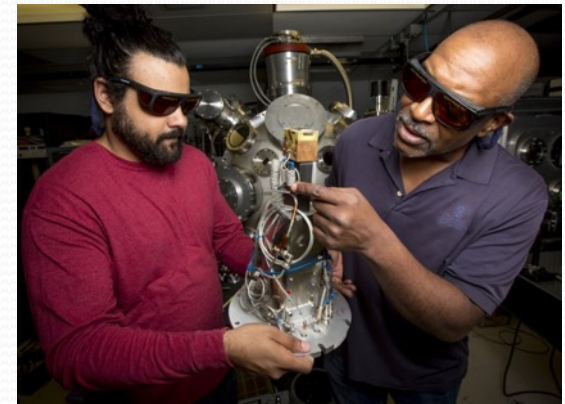
- Summer 2020
 - 3 undergraduate Morehouse students completed a 10-week virtual summer research experience at Lawrence Livermore National Laboratory (LLNL). Again, each student was paired with a lab mentor to guide their summer research projects related to High Energy Density Science.
 1. John Ali
 - LLNL Mentor: Dr. David Rakestraw
 - Project: “Physics Education: Designing New Projects for High School Physics using Smart Phones”
 2. Letrell Harris
 - LLNL Mentor: Dr. Daniel Gebremedhin
 - Project: “Fundamental Basis Sets for Electronic Structure Calculations
 3. Omar Tafiti
 - LLNL Mentor: Dr. Jeffrey Greenough
 - Project: “Creating a Structure Dictionary and Using Maestro Code to Run Variations”

Morehouse Publications

- C. Kyaw, R. Yahiaoui, J. Burrow, V. Tran, K. Keelen, W. Sims, E. C. Red, W. S. Rockward, M. A. Thomas, A. Sarangan, I. Agha, and T. Searles. “Polarization-selective modulation of supercavity resonances originating from bound states in the continuum.” *Commun Phys* 3, 212 (2020).
- C. Kyaw, R. Yahiaoui, J. Burrow, V. Tran, K. Keelen, W. Sims, E. Red, M. Thomas, A. Sarangan, I. Agha, and T. Searles, “Polarization Dependence of Friedric-Wintgen Bound States in the Continuum form THz Metasurfaces,” in *Conference on Lasers and Electro-Optics, OSA Technical Digest (Optical Society of America, 2020)*, paper FM4B.1.

Capacity Building -CSF1

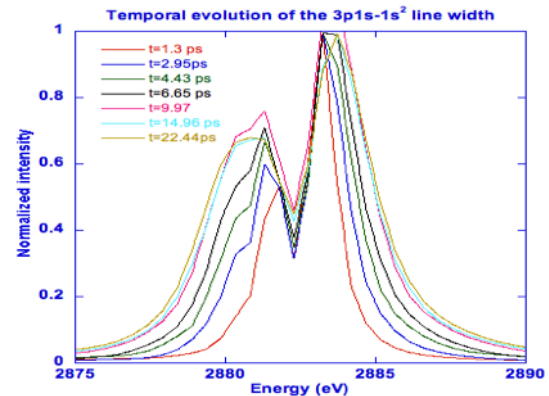
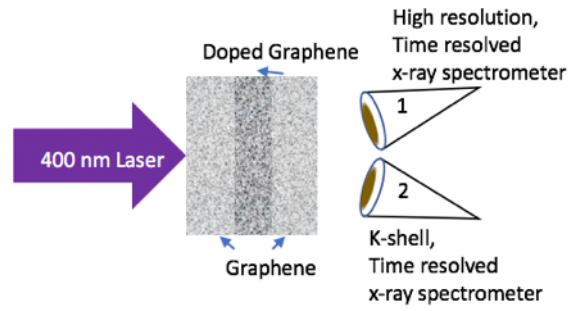
- **LLNL points of contact**
 - Tony Baylis, Strategic Diversity and Inclusion Programs
 - Dr. Frank Graziani, Director, HEDS Center
 - Dr. Ronnie Shepherd, Atomic physics in dense plasmas,
 - Dr. David Rakestraw--LLNL scientist
- **HED curriculum supports CfHEDS academic programs**
 - LLNL HED short courses were offered to CfHEDS
 - CfHEDS will contribute to national curriculum concept
- **CfHEDS experimental and computational collaborative projects (4)**
 - Drs. Daniel Gebremedhin (Weatherford's FAMU postdoctoral fellow) is conducting research at LLNL
 - Jerry Clark is doing thesis research under Dr. Shepherd conducting experiments at Colorado State University
 - Yaye Badjo, Jesica Tucker, working on PhD while at LLNL
 - Dr. Charles Weatherford will be on LLNL NIF Advisory Board
- **Internship opportunities (4) at LLNL for CfHEDS students**
 - Zach Mauri (UC Merced)-TDDFT
 - Adeola Aghedo (FAMU) JLF experiments
 - Quahbar Fletcher (Morehouse)
 - Shalton Evans (FAMU)



Increase Access to DOE/NNSA STEM Resources -CSF2

Florida A&M University

- FAMU has three PhD students and one postdoc who are using LLNL facilities including the Jupiter Laser, the LLNL Superconducting Circuit Quantum Computer, and the LLNL High Performance Computer network. All four are conducting research while on extended stays at LLNL and at FAMU.
- Two other FAMU interns will work with LLNL mentors this summer, for a total of six.
- Jerry Clark (FAMU PhD student) is the PI on a proposal to LaserNetUS2019 titled “The utilization of time resolved x-ray spectroscopy to measure two important plasma processes: 1) The electron-ion temperature relaxation and 2) ionization potential depression.”

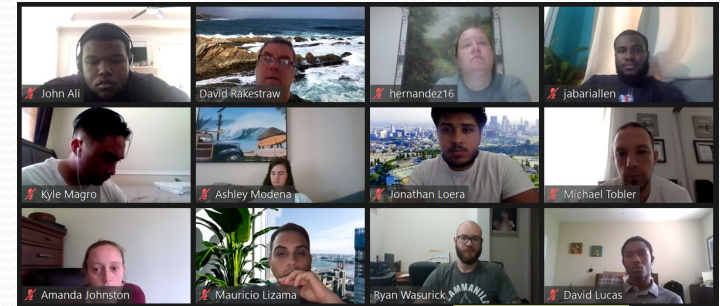


- Dr. Eddie Quashie (LLNL Postdoc) gave seminar at FAMU April 10: “Vicinage Effects in the Stopping Power of Molecular Hydrogen in Aluminum”.

University of California Merced

- **Internships:**

- Undergraduate physics major Zachary Mauri, advised by Prof Pribram-Jones, working at LLNL with Dr. Xavier Andrade.
- Four undergraduate students from UC Merced (David Lucas, Fnu Azma, Jonathan Loera, and Kyle Magro) worked remotely with Dr. Dave Rakestraw at LLNL on physics education activities using smartphone sensors



- **Career development:**

- LLNL visit in 2019 for PhD students, to see the National Ignition Facility and facilities
- Strubbe organized symposium about MSIPP program research at SACNAS conference, 2019
- Strubbe spoke at National Society of Black Physicists on CfHEDS
- Webinars on fellowship applications
- Graduate recruiting fairs at SACNAS, PhysCon, APS March Meeting, CUWiP





Increase Access to DOE/NNSA STEM Resources – CSF2

University of California Merced

• Student Conference Presentations:

- Brittany Harding, Zachary Mauri, and Aurora Pribram-Jones, “Adiabatic Connection Approaches to Thermal Density Functional Theory,” SACNAS, 22-24 Oct 2020
- Estefania Cuevas-Zepeda, Christopher Perez, Ryan P. Brisbin, Ryan D. Baxter, and Aurora Pribram-Jones, “Substituent Effects on Microcapsule Ligand Self-Assembly From Density Functional Theory Calculations,” SACNAS, 22-24 Oct 2020, poster. (**won prize**)
- Emily Junez and Aurora Pribram-Jones, “Validation of Water Contaminant Structure Libraries for Activated Charcoal Filtering Models Relevant to Atwater, California,” SACNAS, 22-24 Oct 2020, poster.
- Sheindel Gamerberg, Attila Cangi, Raphael F. Ribeiro, and Aurora Pribram-Jones, “Semiclassical approximation of heat capacities for model systems,” SACNAS, 22-24 Oct 2020, poster.
- Brittany Harding, Zachary Mauri, and Aurora Pribram-Jones, “Adiabatic Connection Approaches to Thermal Density Functional Theory,” “New Horizons in Density Functional Theory” Faraday Discussion, 2-4 Sept 2020, poster. (**won prize**)
- Zachary Mauri, Brittany Harding, and Aurora Pribram-Jones, “Connections to Ground-State Approximations with the Generalized Thermal Adiabatic Connection”, “New Horizons in Density Functional Theory” Faraday Discussion, 2-4 Sept 2020, poster.
- Md. Mehdi Masud, Bradford A. Barker, and David A. Strubbe, “Optical Effects of Extreme Pressure on Silicon,” Virtual Electronic Structure Workshop, UC Merced, 3 June 2020, poster
- Mojdeh Banafsheh, Leeor Kronik, Tim Gould, David A. Strubbe, and Tomasz A. Weselowski, “Analytic inversion procedure for the exact non-additive kinetic potential functional Vnad,” American Physical Society March Meeting, 3/3/20 – presented locally due to COVID-19 conference cancellation
- Md. Mehdi Masud, A. H. Bhuiyan, and David A. Strubbe, “Investigation of the Structural, Thermal and Electrical Properties of Plasma Polymerized o-Methoxyaniline Thin Films,” IEEE Pulsed Power and Plasma Science, Orlando, FL, 26 June 2019. poster



Increase Access to DOE/NNSA STEM Resources – CSF2

Morehouse College

- Five undergraduate Morehouse students completed a 10-week summer research experience at LLNL. Eric Carter worked on carbon nanotube yarns with Dr. Chantel Aracne Ruddle; Quahhar Fletcher worked on electrodeposition of high-Z capsules for inertial confinement fusion with Dr. Vanessa Peters; Trent Malone worked on fabrication of diatomaceous earth mini-tubes for filtration with Drs. Juana Mendenhall, James Kelly, and Marcus Worsley; Michael Parrish worked on spectrometer development for X-ray emission measurements in support of the IPD campaign with Dr. Ronnie Shepherd; and Jassiem Robinson worked on using machine learning to predict microscopic properties of materials with Dr. Edwin Quashie.



L- Morehouse students Kyron Keelen and Eric Patterson presenting posters. R- Fabrication of diffractive materials by these students using Georgia Tech cleanroom facilities.



Beyond the Borders of
Morehouse

Recruiting, and K-12
Outreach



- Morehouse PIs and CfHEDS students participated in annual Prospective and Admitted Students events.
- The Physics & Dual-Degree Engineering Program hosts the NuMaSS Summer Program for rising 9th-12th graders. This is a 5-week enrichment program exposing students to college-level courses in physics, mathematics, and English.
- NuMaSS participants enjoy weekly enrichment trips in the areas of Nuclear, Materials, and Space Sciences. They also present a research topic at the conclusion of the program.

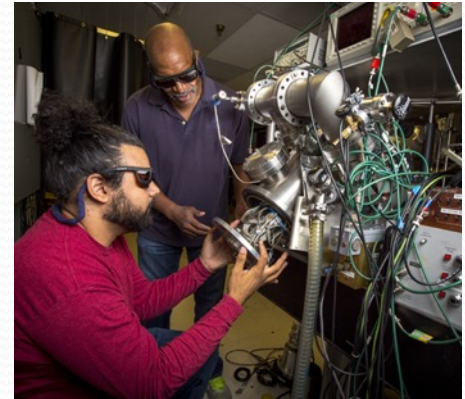
Increase MSIPP Students Who Graduate With STEM Degrees-CSF3



This program is supported by the Office of Defense Programs, National Nuclear Security Administration, U.S. Department of Energy.

Florida A&M University

- The structure of CfHEDS will allow for FAMU’s PhD students to work on PhD projects, co-mentored by LLNL experts, on some of the most current and exciting projects in science and technology, and will allow for the use of state-of-the-art LLNL facilities that are not available at their home institutions.
- These opportunities will increase the number and quality of FAMU’s STEM PhD students.
- Florida A&M is doing significant outreach to K-12 in the Tallahassee area to expose students to STEM and to encourage them to go into STEM areas in college.
- **Jerry Clark**--FAMU graduate student who is knowledgeable in experimental, computational and theoretical physics; thesis research with Drs. Ronnie Shepherd (LLNL) and Ronald Williams (FAMU) on dense plasma effects on bound states; Ph.D. expected in 2020.
- **Jessica Tucker** working on Quantum Control for Quantum Computing with Dr. Jonathan DuBois and Frank Graziani (LLNL) and Charles Weatherford (FAMU), using the LLNL superconducting circuit quantum computer. PhD expected in 2021.
- **Yaye Badjo** calculating the high-pressure properties of hydrogen iodide, working with Drs. Bonev (LLNL) and Saha (FAMU). PhD expected in 2021.
- Outreach to K-12 in FAMU vicinity—STEM Day (800 K-12 students)





Florida A&M University

- **Edwin Quashie**
 - 4 publications in Physical Review (2015, 2017, 2018, 2019), 1 more manuscript to be submitted this year
 - Research with Dr. Alfredo Correa using time dependent density functional theory.



- **Daniel Gebremedhin**
 - Visiting FAMU postdoc working on cluster wavefunctions with LLNL opacity group
 - kinetic simulation of laser-plasma interaction in a 4 model.
 - New version of Kohn Sham DFT with state energies (Weatherford and Gebremedhin).

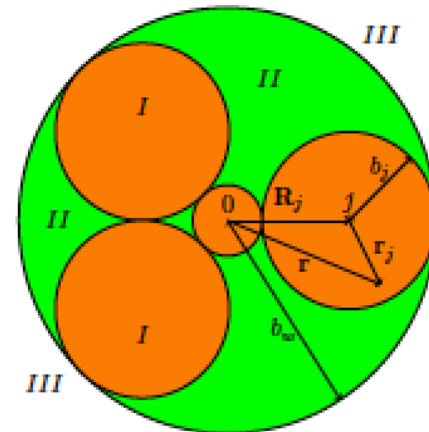
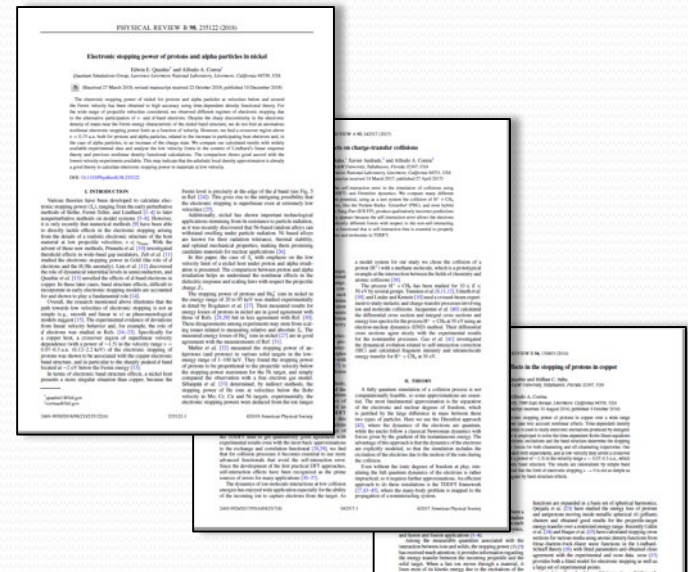


Figure 1: Partitioning of space into (I) ionic, (II) interstitial and (III) extramolecular regions.



Expanding Science Through Opportunities
The Office of Basic and High Energy Density Science

K-12 OUTREACH—USE OF SMARTPHONE

- Dr. David Rakestraw (LLNL) is helping CfHEDS introduce the use of smartphones into the K-12 curriculum as a scientific instrument.
- The remarkable advances in microelectronics and communication technologies provide an unprecedented opportunity for a sea change in high school STEM education.
- This is now possible by exploiting the “supercomputers” and powerful sensor systems that most students carry to class every day.
- The suite of sensors, computational power, and real-time visualization capabilities on a smartphone can revolutionize the student learning experience using a sophisticated interface that they have already mastered.
- All common smartphones include: 3-axis accelerometer (Fig. 23), 3-axis gyroscope (Fig. 24), 3-axis magnetometer, barometric pressure transducer, microphone, speaker system, GPS system, high-resolution optical video camera, high-resolution timer, exceptional computational power for fast data processing and analysis, high-resolution graphical interface with touch screen, blue-tooth and Wi-Fi that enable data communication and transfer.

K-12 OUTREACH—USE OF SMARTPHONE

Example Experiments to be Designed:

- Measurement of walking velocity
 - Distance vs. time graphing (introducing data tables, graphing, line fitting, error analysis)
 - Calculating walking speed and time to reach distant classrooms (identification of potential variations in walking time algorithm)
- Measurements of distance using GPS data
 - Introducing longitude and latitude
 - Understanding how GPS works
- Measuring height of buildings using precise phone orientation and trigonometry
- Characterization of smartphone 3-axis accelerometer
- Exploring 3D sensor concept and phone axis relationships
- Microelectromechanical systems (introduction of electron microscope, lithography and basic principles of MEMS system)
- Specific design of accelerometer

Gyroscope data collected during a 7-minute car ride near LLNL.

