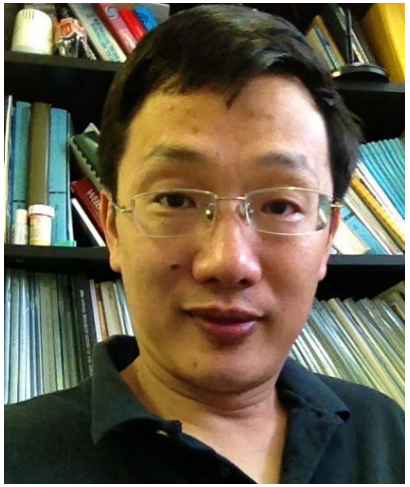
Coalition for Research and Education
Enhancement in Materials DMR-0934142

Research and Education on Graphene



X. Q. (Larry) Wang
(PI, Director)

Lycurgus Muldrow

Natarajan Ravi

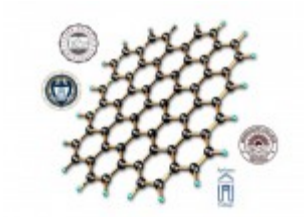
Dennis Hess
(Co-PI, MRSEC Director)

Clark Atlanta University

Morehouse College
Et Facta Est Lux
Georgia

Spelman College

Georgia Institute of Technology
Progress and Service
Seal · 1885



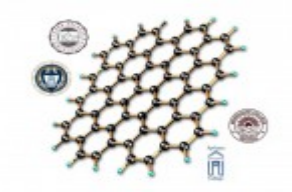
Coalition for Research and Education
Enhancement in Materials DMR-0934142

The Partnership
Atlanta University Center - Georgia Tech

- AUC (Clark Atlanta, Morehouse, and Spelman)
  Clark Atlanta: Profs. L.Wang and M. Williams
  Morehouse: Profs. L. Muldrow, and J. Hall
  Spelman: Prof. N. Ravi

- Georgia Tech MRSEC: The Georgia Tech Laboratory for New Electronic Materials

- Profs: D. Hess (Director, MRSEC), M. Y. Chou, E. Conrad (Facility Director), Dr. L. Conrad (Education/Outreach Director)



Key features of the partnership

(1) Establishing research collaboration between AUC and GT faculty, postdoctoral associates, and graduate students;

(2) Strengthening the research and education infrastructure of AUC;

(3) Providing research opportunities for AUC undergraduates during the academic year;

(4) Providing summer research experiences for AUC students at GT through the collaborative research program;

(5) Developing and hosting summer research institutes for high school teachers.

Graphene

- The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*.
- Epitaxial Graphene (EG) shows promise in high-performance electronics, could ultimately spawn a new generation of devices designed to take advantage of its unique properties.
- Graphene has been chosen as one of the European Commission's billion-euro flagship projects and has cemented its central position in European research.
- Development of reliable techniques to synthesize large quantities of high-quality graphene.
- Applications making use of the very high mobility of graphene.
- Absence of an intrinsic semiconductor bandgap.

Broader Impact

- A significant enhancement of materials research, education, and technology transfer;
- Long-term, sustainable, synergistic impact on the GT diversity programs in science and engineering;
- The high school teachers program is designed to better-prepare and motivate high school students from metro Atlanta to major in science or engineering upon entering college;
- The undergraduate student activities establish a pipeline of well-prepared and motivated undergraduate African American students.

Research Collaborations

Williams, Hess, Wang (GT-CAU, expt.-theory)
Williams, Hess (CAU-GT)
Ravi, Wang (Spelman-CAU, Theory)
Hall, Wang, Chou, Bongiorno (Morehouse-CAU-GT, Theory)
Williams, Conrad, Ravi (GT, Spelman, CAU, Expt.)
Rockward, Jiang (Morehouse, GT, experiment)

Education & Outreach

Seminars (GT, CAU, Morehouse)
Journal Club (GT)
Summer Programs (all)

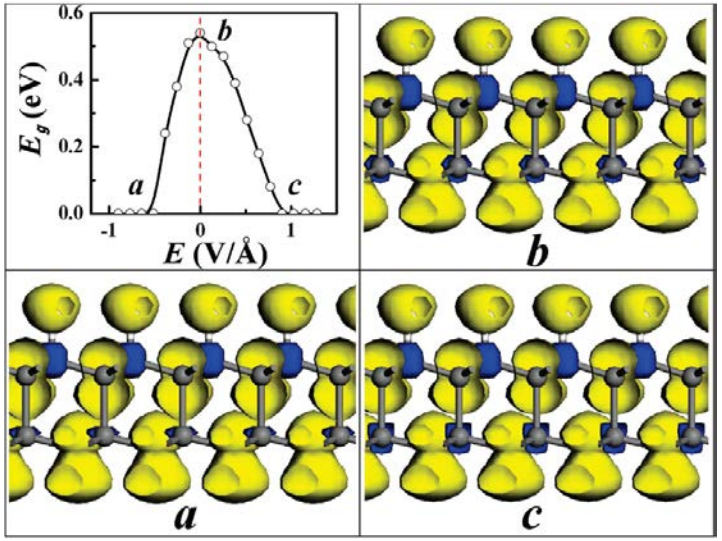
Pipelines

Graduates: Dr. Ogunro (faculty), Nathaniel (Drexel), Kah (Louisville), Suggs (CAU Chemistry); Carney (Boeing), Riche (Boeing), Quarles (Industry)
Undergraduates: Brown (Columbia), Harrison, Hargrove, Griffin (CAU, Physics)

Two Layers are Better than One: Engineering a Band Gap in Graphene

Xiao-Qian Wang, Michael Williams (Clark Atlanta University); Dennis Hess (Georgia Tech.) **DMR-Award #0934142**

The object of the PREM is to establish an integrated research, education, and student-mentoring in order to increase the number of underrepresented students pursuing graduate degrees and to increase their overall participation in the field of materials science and engineering.

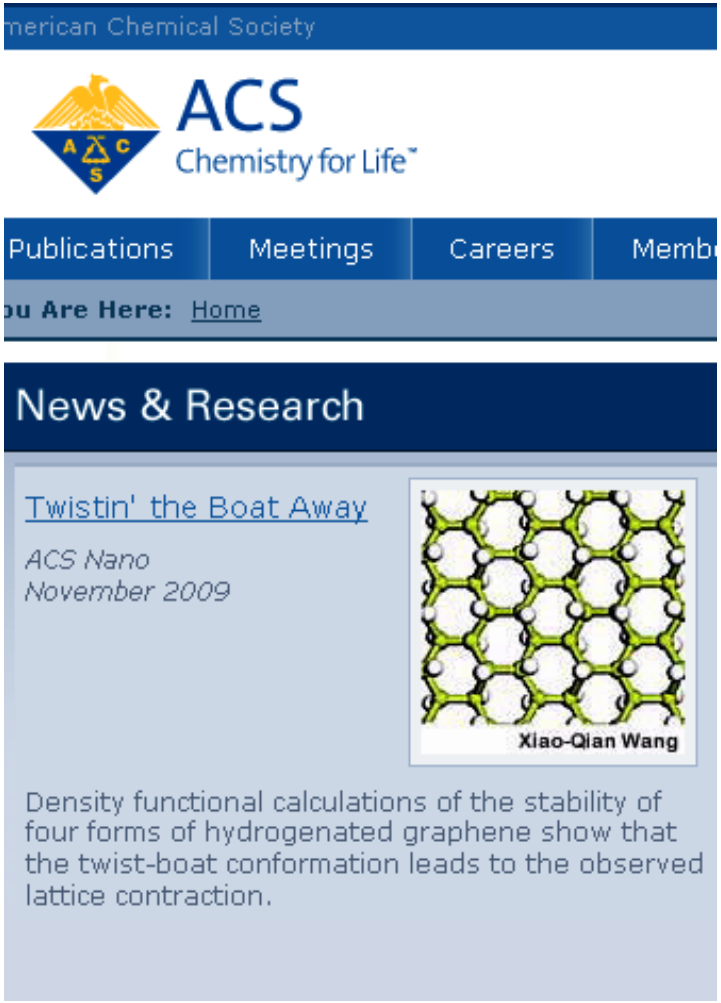


The PREM team explored the electronic and structural characteristics of hydrogenated graphene under an electrical bias. First-principles density functional calculations revealed tunable electronic properties, which are essential in the creation of more flexible nanodevices such as lasers that change color or electronic circuits that have the ability to rearrange themselves. The research result was published in ACS Nano (**2010**, *4*, 4126) and cited by the editors in *In Nano* (ACS Nano **2010**, *4*, 3540).

Twistin' the Boat Away: Structural and Electronic Properties of Graphene

Xiao-Qian (Larry) Wang (Clark Atlanta University); Dennis Hess (Georgia Tech.) DMR-Award #0934142

The Partnership for Research and Education in Materials (PREM) between three Atlanta University Center (AUC) schools and the Materials Research Science and Engineering Center (MRSEC) at Georgia Institute of Technology (GT) integrates research, education, and student-mentoring. One of our theoretical research results was published in *ACS Nano* **3**, 4017 (2009) and was cited by ACS as major research news on the ACS portal front page December 1-14, 2009.

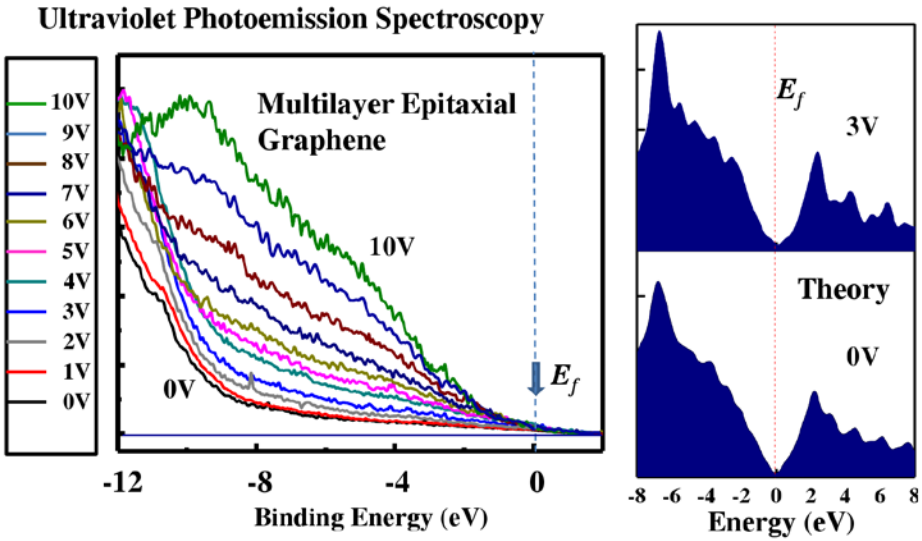


Tunable bands in biased multilayer epitaxial graphene

M. D. Williams, D. K. Samarakoon, X.-Q. (Larry) Wang (Clark Atlanta University) D. W. Hess (GaTech) **DMR-Award #0934142**

Clark Atlanta University and Georgia Tech. researchers supported by the NSF PREM project studied the electronic characteristics of multilayer epitaxial graphene under a perpendicularly applied electric bias.

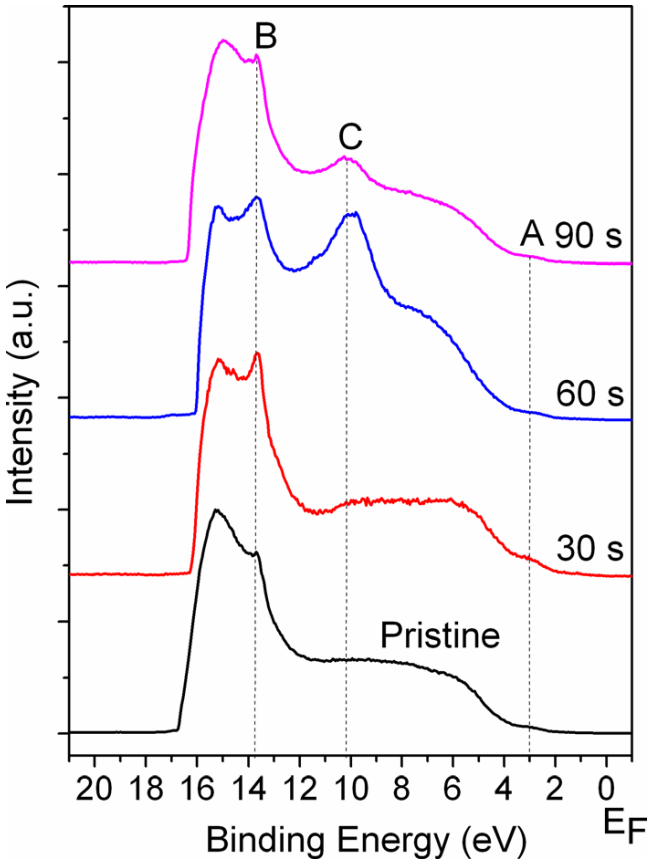
The experimental and theoretical results demonstrate that the tailoring of electronic band structure correlates with the interlayer coupling tuned by the applied bias. The controllable electronic structure of rotationally fault-stacked epitaxial graphene grown on the C-face of SiC provides promising routes for future device applications.



The research result was published in *Nanoscale* **4**, 2962 (2012).

Photoelectron spectroscopy studies of plasma-fluorinated epitaxial graphene

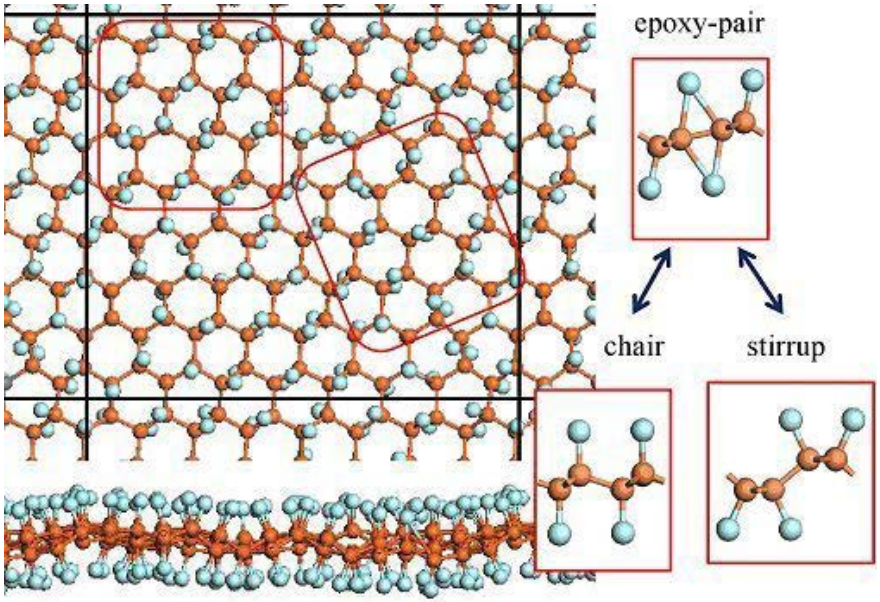
Sonam D. Sherpa, Sergio A. Paniagua, Galit Levitin, Seth R. Marder, Dennis W. Hess (Georgia Tech.), M. D. Williams (Clark Atlanta)



Fluorination of graphene has emerged as an attractive approach toward manipulating its physical, chemical, and electronic properties. Georgia Tech. and Clark Atlanta University researchers have demonstrated the viability of sulfur hexafluoride plasmas to fluorinate graphene as a safer alternative to the commonly reported techniques of fluorination that include exposures to fluorine and xenon difluoride gas. Modifications in the valence band states of graphene after plasma-treatment were characterized by ultra-violet photoelectron spectroscopy. An increase in the work function of plasma-treated graphene estimated demonstrates the ability of plasma-assisted fluorination to modify the electron emission characteristics of graphene. Raman spectroscopy reveals that the sp^2 configuration of graphene survives the plasma-treatment. Published in J. Vac. Sci. Technol B, **30** (2) 03D102 (2012.)

Electronic and Optical Properties of Fluorographene

Chantel Nicolas, Z. Chen, D. K. Samarakoon, K. Suggs, O. Ogunro, X.-Q. Wang (**DMR-Award #0934142)**



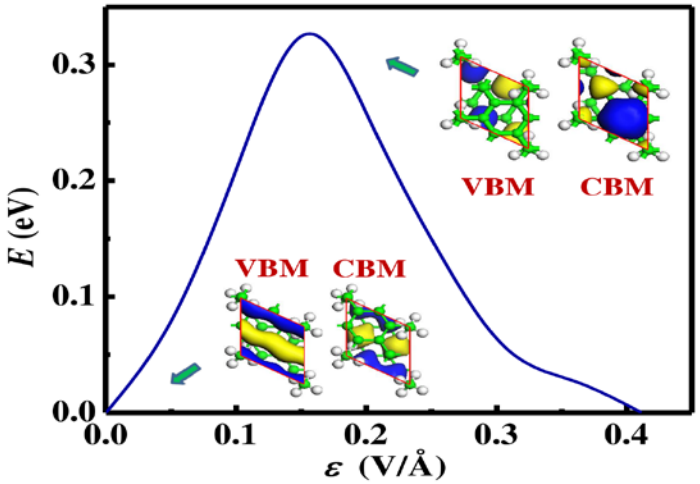
Following the synthesis of graphane, recent experimental work has successfully created fully fluorinated graphene. The single-layer fluorographene exhibits a wide-gap semiconducting behavior. Being a stoichiometric derivative with high thermal and chemical stability, fluorographene is poised to provide a promising platform for applications.

Researchers at Clark Atlanta University researchers investigated the structural and electronic characteristics of fluorinated graphene based on first-principles density-functional calculations. The appearance of bounded excitons in the ultraviolet region can result in an excitonic Bose–Einstein condensate in fluorographene. The work was published in *Small*.

Band Gap Opening in Methane Intercalated Graphene

Jasmine Hargrove, H. B. M. Shashikala, X.-Q. Wang (Clark Atlanta) L. Guerrido, N. Ravi (Spelman) (DMR-Award #0934142)

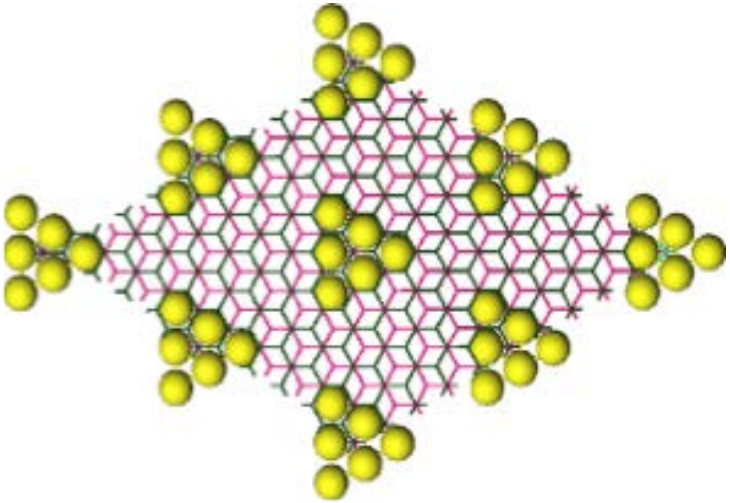
Recent experimental work has demonstrated production of quasi free-standing graphene by methane intercalation. The intercalation weakens the coupling of adjacent graphene layers and yields Dirac fermion behaviour of monolayer graphene.



Researchers at Clark Atlanta University and Spelman College have investigated the electronic characteristics of methane intercepted graphene bilayer under a perpendicularly applied electric field. Evolution of the band structure of intercalated graphene as a function of the bias is studied by means of density-functional theory including interlayer van der Waals interactions. The findings suggest a controllable band gap opening in methane-intercalated graphene for future device applications.

Tunable Band Gap in Gold Intercalated Graphene

I. Sapkota, K. Suggs, X.-Q. Wang (Clark Atlanta); M. Roundtree, J. Hall (Morehouse) (**DMR-Award #0934142)**



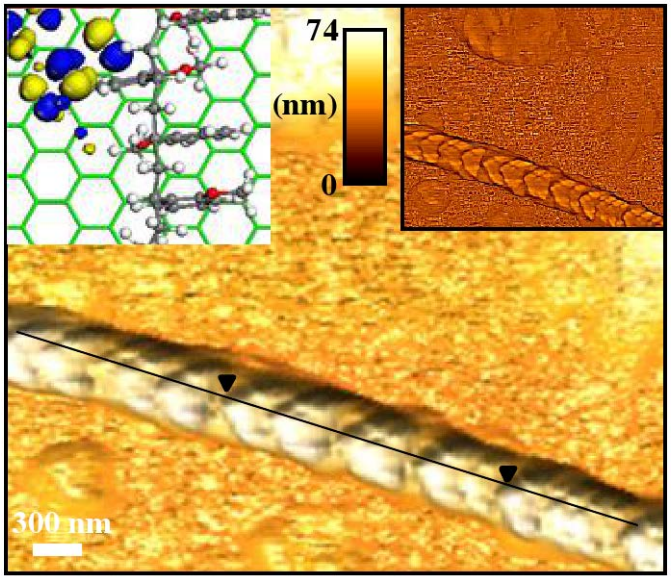
Recent experimental work has demonstrated production of quasi free-standing graphene by gold intercalation. The intercalation weakens the coupling of adjacent graphene layers and yields Dirac fermion behavior of monolayer graphene.

Researchers at Clark Atlanta University and Morehouse College have investigated the electronic characteristics of gold intercepted graphene bilayer under a perpendicularly applied electric field. Evolution of the band structure of intercalated graphene as a function of the bias is studied by means of density-functional theory including interlayer van der Waals interactions. The findings suggest a controllable band gap opening in gold intercalated graphene for future device applications. The work was published in *Phys. Chem. Chem. Phys.*

Self-Assembly of Biofunctional Polymer on Graphene Nanoribbons

D. G. Reuven, Kelvin Suggs, M. D. Williams, X.-Q. (Larry) Wang
(Clark Atlanta University) **DMR-Award #0934142**

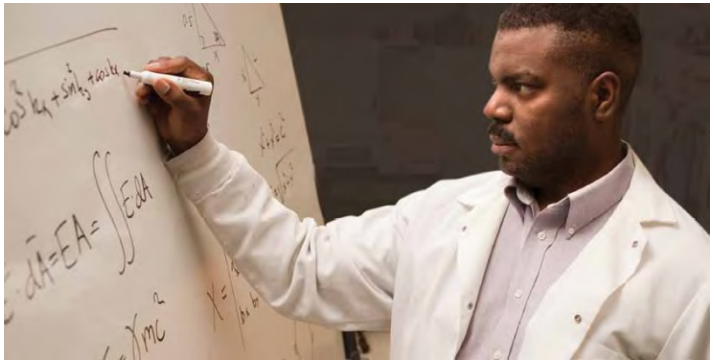
Clark Atlanta University researchers supported by the NSF PREM project worked on supramolecular self-assembly of biofunctional-modified poly(2 methoxystyrene) on graphene nanoribbons. The bioactive polymer has attracted a considerable interest owing to its versatile properties as a bisosensor. However, the formation of regular patterned structures for the polymer is difficult, which greatly hampers its applications. The combined experimental and theoretical work demonstrates that the glycol modified polymer can self-assemble into structured nanopatterns on graphene nanoribbons with preserved bioactivity. The findings demonstrate that the assembly yields a prospective route to novel nanomaterial systems.



The research result was published in *ACS Nano* **6**, 1011 (2012).

No Problem is Too Big to Solve

Xiao-Qian Wang, M. D. Williams (Clark Atlanta University),
D. Hess (Georgia Tech.) **DMR-Award #0934142**



For the United States to lead the world in the critical fields of science, technology, engineering and math (STEM) , it is important to recruit a great deal more women and minorities in STEM. Eighteen underrepresented minority students took part in the PREM projects involving experimental and theoretical studies of nanostructured materials, as well as summer programs.

The PREM team published 14 refereed journal publications in this fiscal year. One of the minority graduate students, Mr. Kelvin Suggs, gave an invited talk at the Materials Research Society meeting in Boston, December, 2010.

Scientific Literacy Pre-Freshman Bridge Summer Science Program

Lycurgus L. Muldrow (Morehouse College)

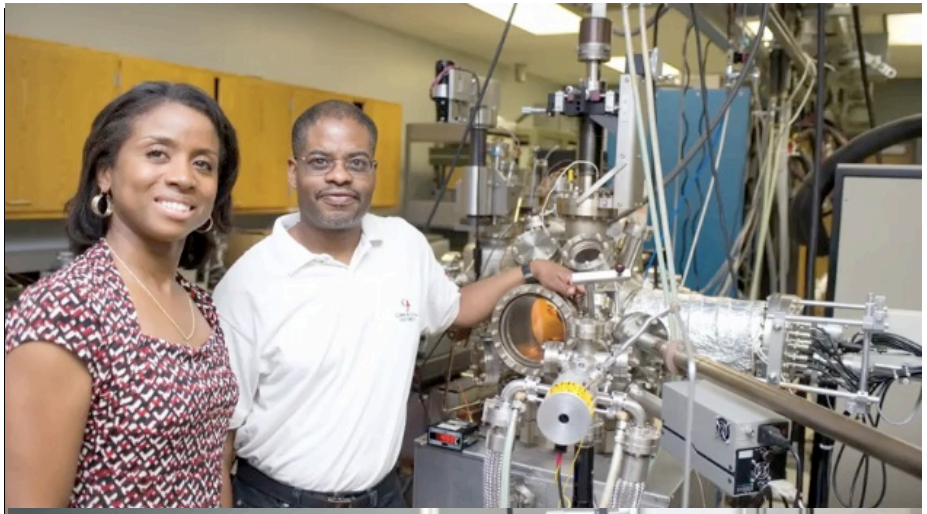
DMR-Award #0934142

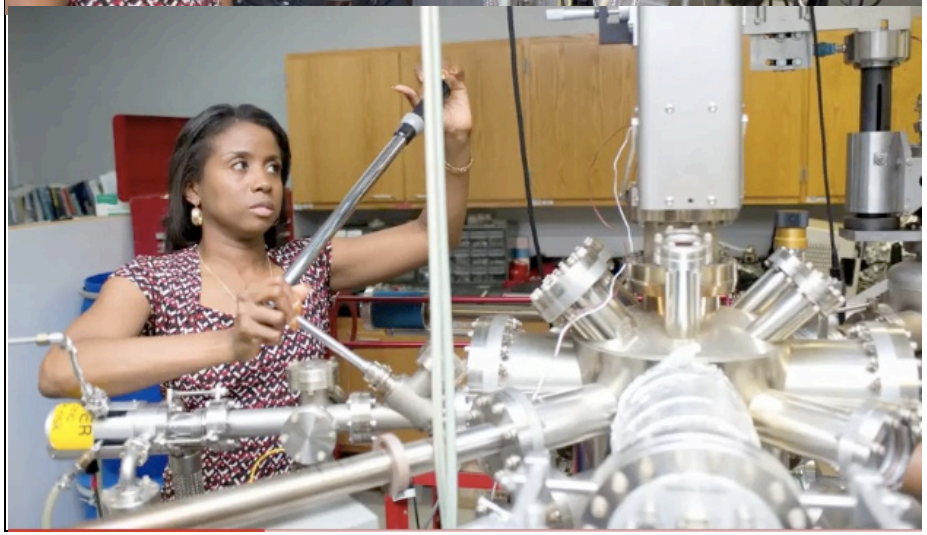
A Pre-Freshman Bridge Summer Science Program at Morehouse College was designed to develop an advanced level of scientific literacy among pre-freshmen science majors with the goal of increasing the number of graduates who enter graduate school in pursuit of research careers.

This innovative summer program incorporated a unique combination of proven components that increases success, builds academic skills, exposes students to the scientific method and research methodology, as well as promotes an enhanced interest in the pursuit of careers in science and research. In this six-week summer experience students participate in scientific literacy building, applied mathematics, guided inquiry laboratories in materials science, scientific field trips, as well as personal and professional development.

Research Experience for High School Teacher

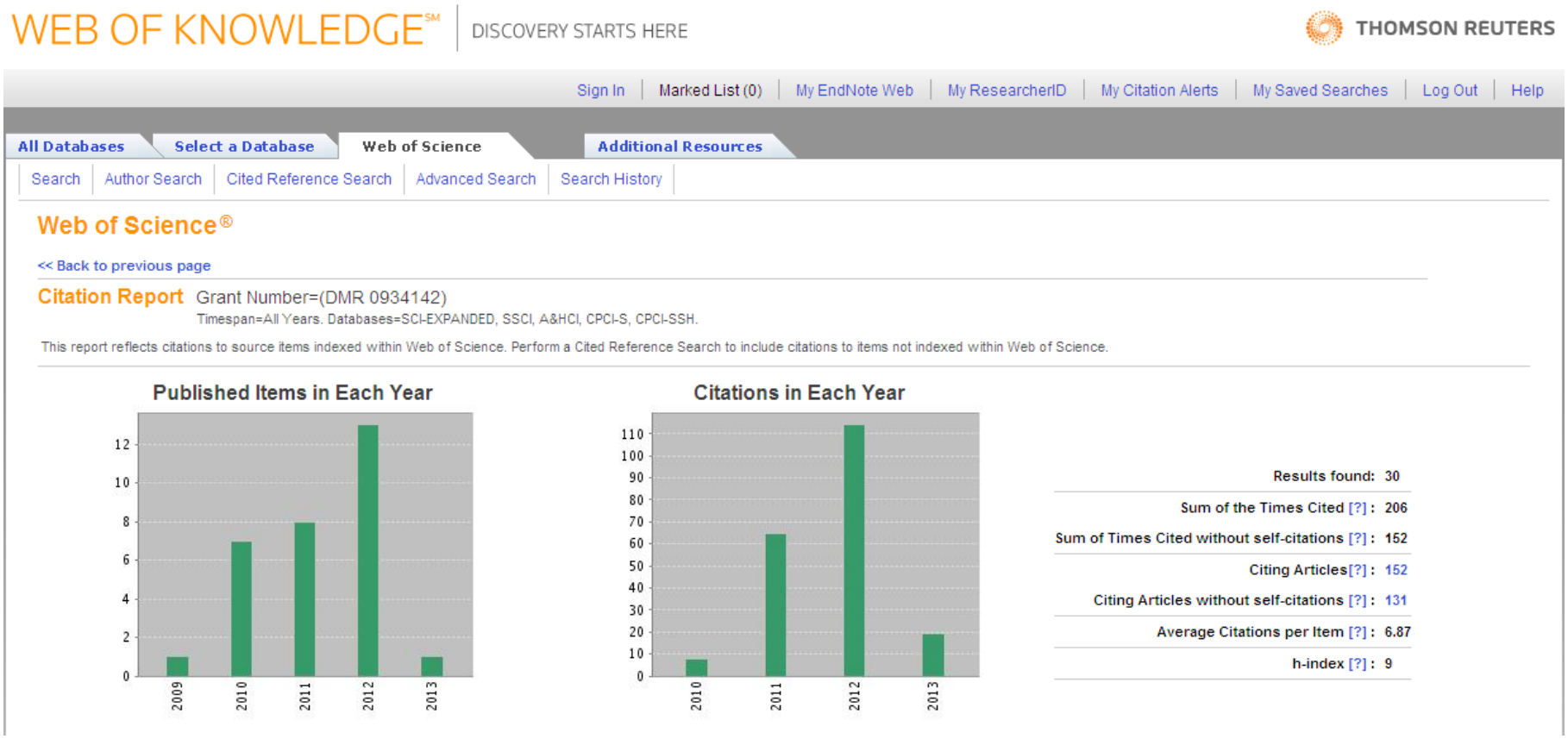
M. E. Walker (N. Cobb High), M. D. Williams (Clark Atlanta University),
D. Hess (Georgia Tech.) DMR-Award #0934142





The electronic structure characteristics of graphene epitaxial-layers as a function of surface morphology and thickness is investigated using ultraviolet photoemission spectroscopy. Elizabeth Walker participated in a summer program for High School Physics Teachers. She could spend her time at Clark Atlanta University through our collaboration with Dr. Dennis Hess. She determined the surface electronic structure of epitaxial graphene with ultraviolet photoemission spectroscopy. Work published in *Graphene* **2**, 55 (2013).

43 Publications in Refereed Journals, 65 Presentations



Citations: 206 (152 excluding self-citation) *h*-index: 9

ACS Nano (3, IF: 11.4), Small (2, IF 8.3), ACS Macro Lett., JPCL, APL, Nanoscale, PRB (Rapid Comm.), JPCC, CPL

Papers Published

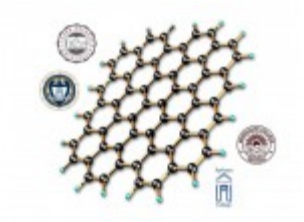
43 publications

- 32 theoretical; 10 experimental; 8 joint experiment/theory
- 3 joint publications with GaTech
- 6 publications involving two or more groups
- 38 with postdoc/students (88%)
- **28 with African American postdoc/students (65%)**
- **6 with undergraduate African American students as co-authors (14%)**

65 representations (invited talks, contributed talks, posters)

- 60 with African American postoc/students

- Increased integration between theory and experiment in joint projects
- Increased interaction between AUC and GaTech

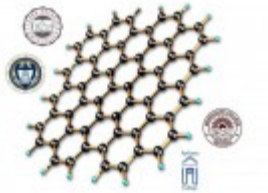


New Courses

Ron Mickens, Biophysics (2012 Summer)
M. D. Williams, Surface Physics (2011)
X. Q. Wang, Solid State Physics (2010)

M. D. Williams, Seminar (2011)
N. Ravi, Module for Materials Research

Mini-workshop (Summer 2010, 2012) Dr. A. Nduwimana
NSF XSEDE Collaboration: High-performance computing; programming
Workshop: Visualization (VisIt, Feb. 2013)
Workshop: Molecular dynamics (Fall 2013)



Coalition for Research and Education Enhancement in Materials DMR-0934142

Development of Strong Research Culture through Cross-fertilization Across Disciplines and Institutions

- Institution of Weekly AUC Research Meeting
- Student Attendance at MRSEC Journal Club
- Participation in MRSEC IRG Meetings, Retreats
- Participation of MRSEC students in AUC Experiments and Vice-Versa
- Utilization of NSF NNIN Facilities at GT
- Participation of PREM Undergraduates in MRSEC REU
- Participation in MRSEC STEG Conferences

External Advisory Board Committee

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Georgia State University
Dr. Susan Sinnott
University of Florida

- The EAB highly commends the PREM project team's extraordinary effort in producing high quality papers since its short inception.
- The education component aimed at material science pipeline has a good start and looks promising.
- Clearly PREM is making positive impact in both research and education components. It has increased the UMI research output and is shaping the education pipeline in material sciences.
- The new equipment and computational facilities at CAU obviously benefits the research and education missions as does shared use of the Georgia Tech facilities.