



Collation of Research and
Education in Materials
(NSF Grant No. DMR-0934142)

Dr. Xiao-Qian (Larry) Wang
Clark Atlanta University



Partnership: Atlanta University Center - Georgia Tech MRSEC

- AUC (Clark Atlanta, Morehouse, and Spelman)
Clark Atlanta: Profs. M. Williams and Wang
Morehouse: Profs. L. Muldrow and J. Mendenhall
Spelman: Prof. N. Ravi
- Georgia Tech MRSEC: The Georgia Tech
Laboratory for New Electronic Materials
- Profs: D. Hess (Director, MRSEC), M. Y. Chou
(Chair), E. Conrad (Facility Director), 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.

Research

- Experimental characterizations of epitaxially grown graphene
 1. Spectral characterization
 2. Magnetic properties
 3. Biosmart materials
- Simulation studies of the electronic structures of graphene-related nanodevices
 1. First-principles density-functional theory
 2. Molecular dynamics (multiscale modeling)

Clark Atlanta University

- Formed in 1988 by the consolidation of two historic institutions, Atlanta University (1865) and Clark College (1869), Clark Atlanta University, a United Methodist School is the largest of the United Negro College Fund institutions
- Major, urban, private, co-educational institution of predominately African American heritage located on 75 acres in downtown Atlanta, GA; part of the Atlanta University Consortium
- Broadly comprehensive at BS and MS level; doctoral programs in biological sciences, chemistry, systems sciences, education, psychology, English
- About 4000 students and over 170 FTE faculty from diverse backgrounds
- Several research centers and centers of excellence; CAU houses one of the largest research facilities in the southeast
 - Science Research Center complex - ~200,000 sq. ft. research and core lab facility
 - Center for Computational Intelligence for National Security
 - Center for Cancer Research and Therapeutic Development
 - High Performance Polymers and Composite Center
 - Center for Functional Nanoscale Materials
 - Environmental Justice Resource Center
 - Center of Excellence in Mass Media Arts
 - School of Business Administration
 - Center for Urban Educational Excellence
- Accredited by SACS, Clark Atlanta is among the top historically black colleges and universities receiving federal grants for science, prostate cancer and environmental justice, and is currently has a Carnegie classification of [Research University – High Research Activity](#)

Materials Research at Clark Atlanta



- Research
- Partnerships
- Education



- Conducting beneficial and innovative research for the benefit of the Nation and all humanity.
- Increasing the number of students pursuing graduate and undergraduate degrees in the natural and physical sciences.
- Enhancing the research productivity of its researchers.



- The development of a diverse, globally engaged science workforce.



Broader Impact

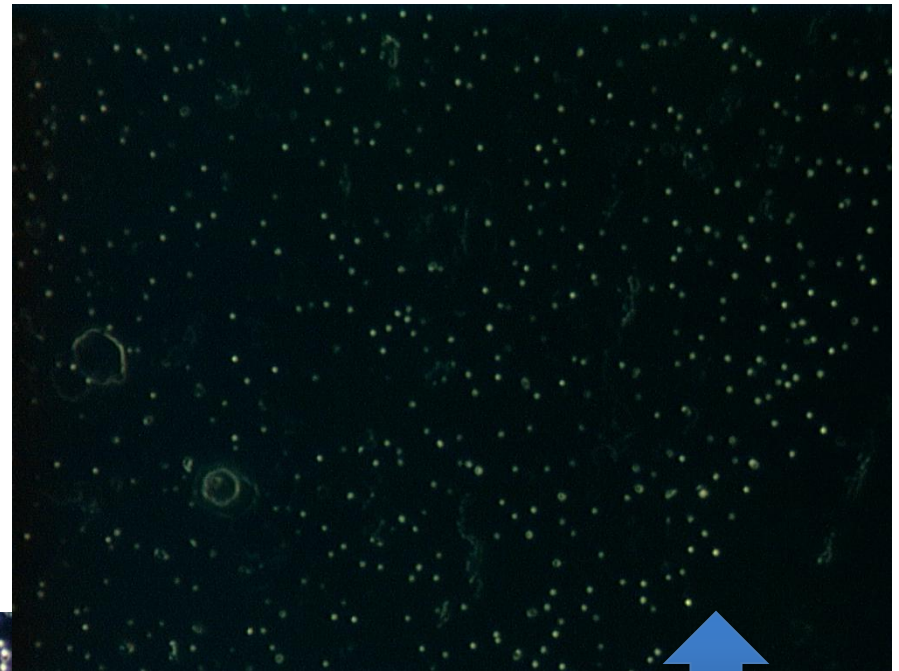
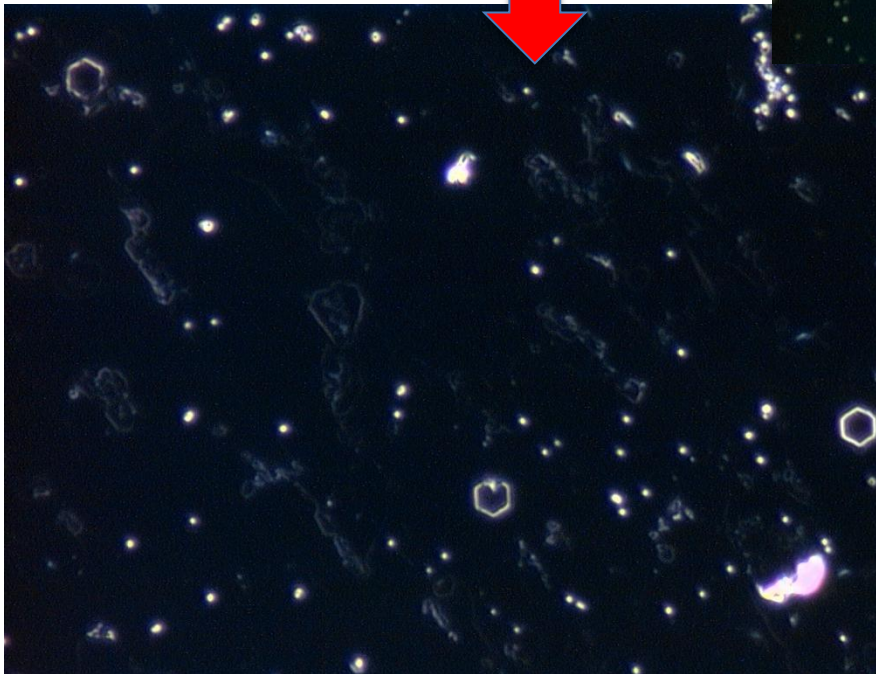
- A significant enhancement of the infrastructure of AUC for materials research, education, and technology transfer;
- Long-term, sustainable, synergistic impact on the GT diversity programs in science and engineering.
- The high school teachers program is designed to better-prepare and motivate high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

Experimental Characterization

Profs. Williams and Hess

- CAU – 2 students
- GT – 1 graduate PhD student, 1 post-doc
- Spectral analysis of material quality in progress with preliminary publishable results
 - line shape modification
 - work function difference of 0.11 eV
 - C 1s binding energy difference of 0.51 eV
 - 0.4-0.5 higher work function than bulk graphite

low-quality
epitaxial graphene
sample

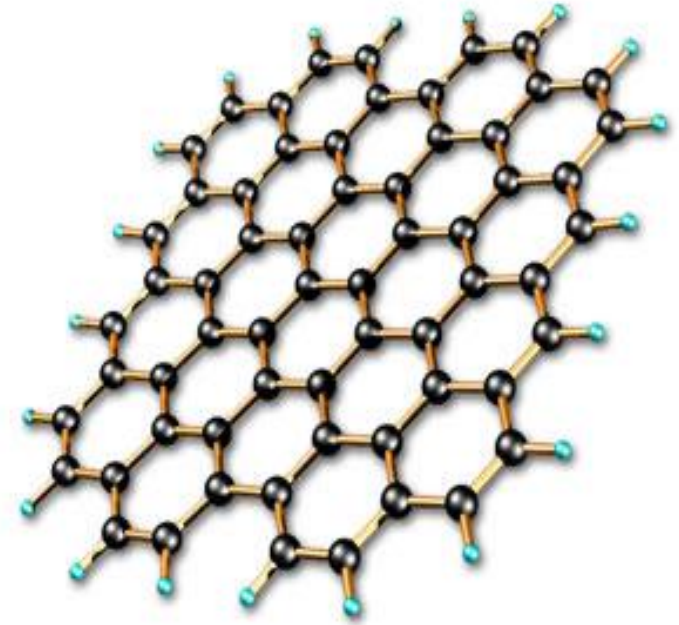


high-quality
epitaxial graphene
sample



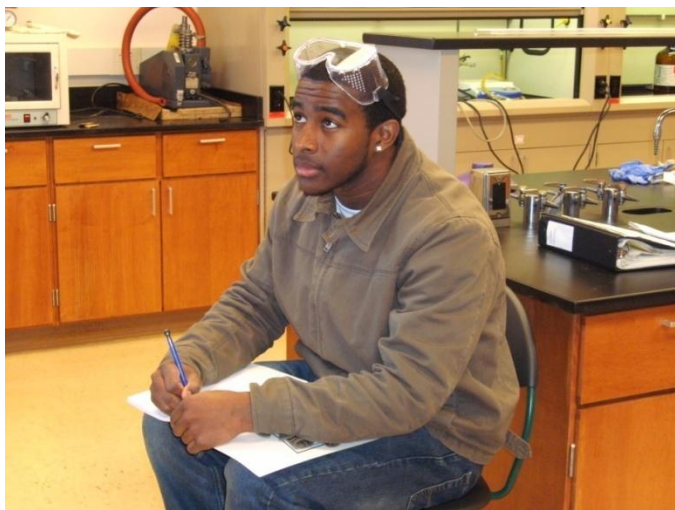
Prof. N. Ravi + 2 students (Spelman)

- Graphene is a single sheet of carbon atoms bonded together in a honeycomb structure
- Recent research studies have shown that metal incorporated graphene systems are promising semi-conductor at nanoscale
- Understanding the interaction of graphene with other molecules especially metal atoms will take us a step closer to graphene based devices. However, as a first step we have started looking at interaction of water and methanol with graphene from a theoretical standpoint.



Prof. J. Mendenhall + 2 students (Morehouse)

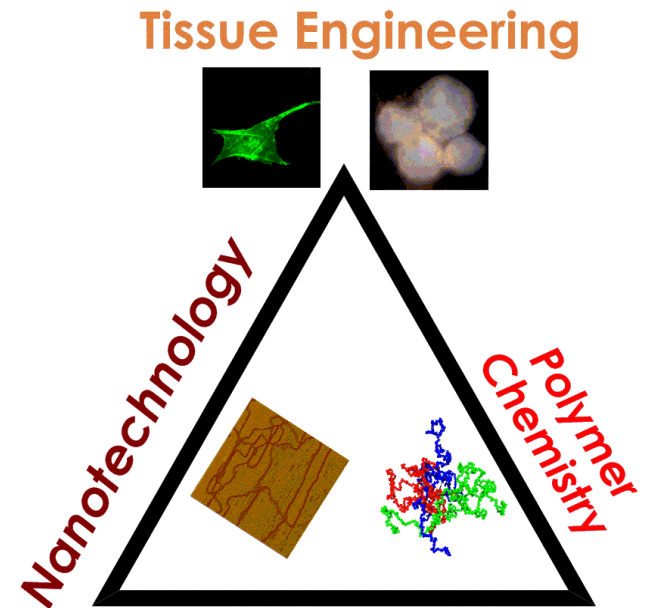
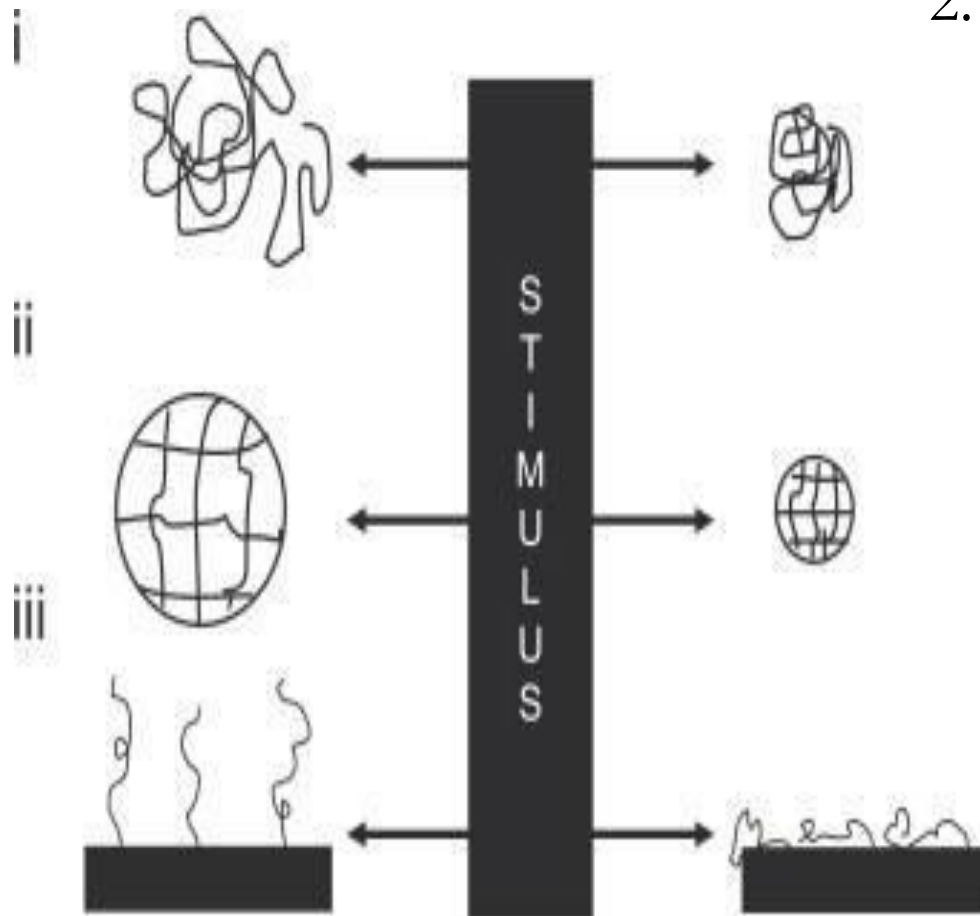
Brandon Lynch



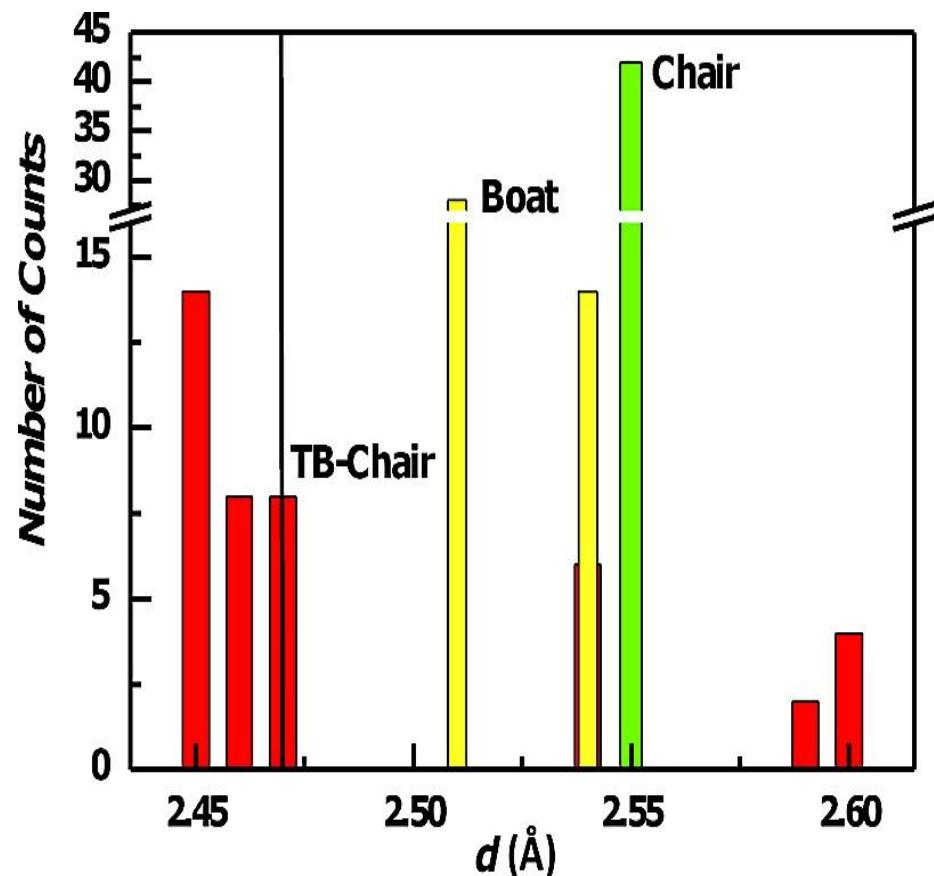
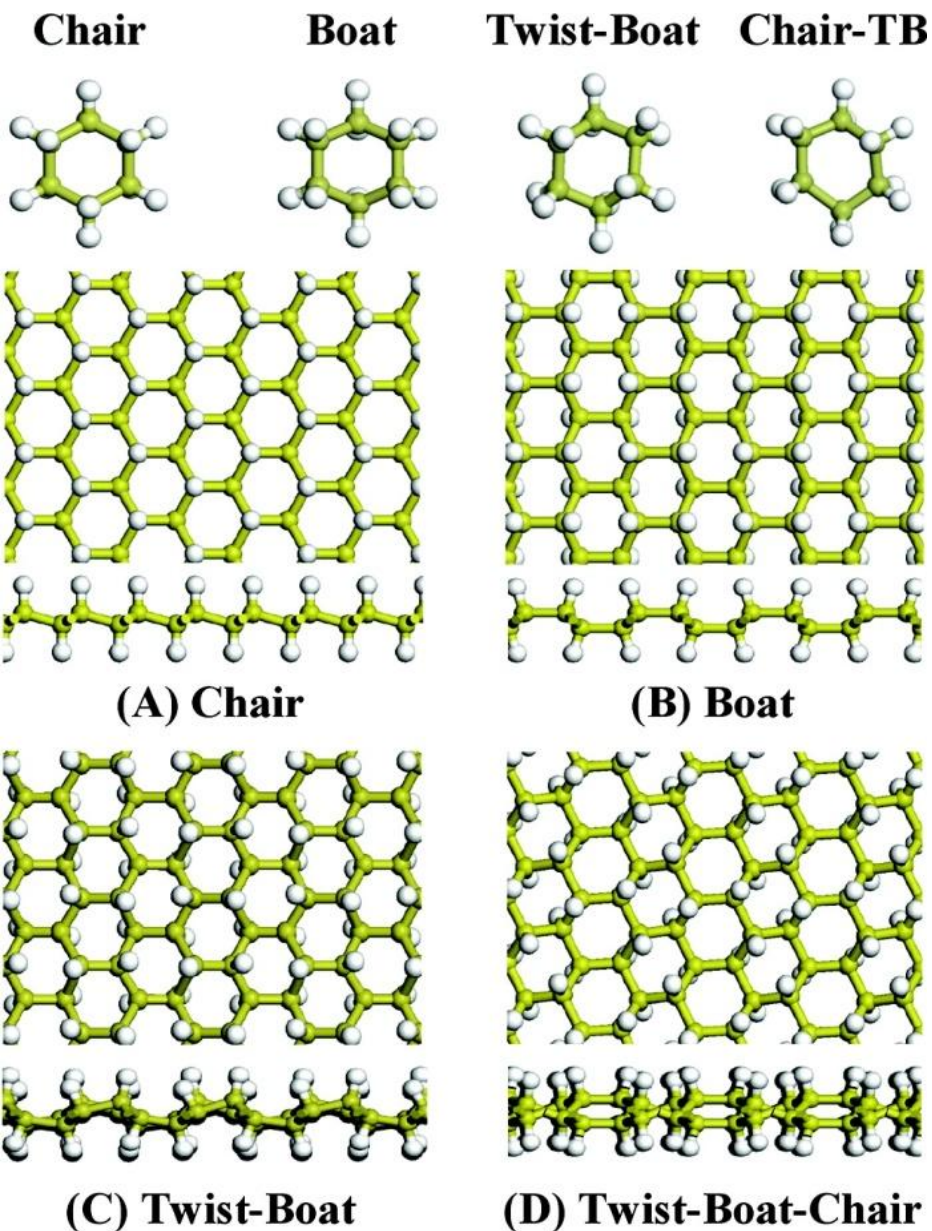
Matthew Moore



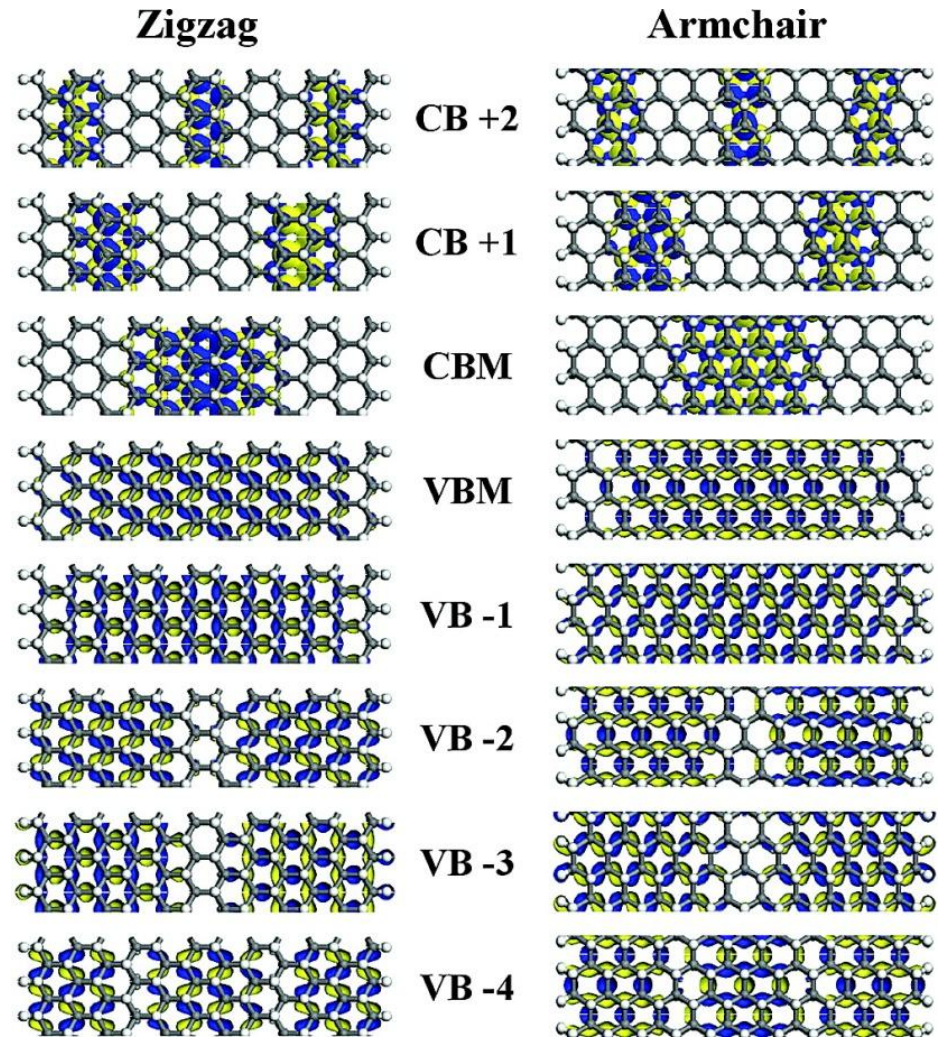
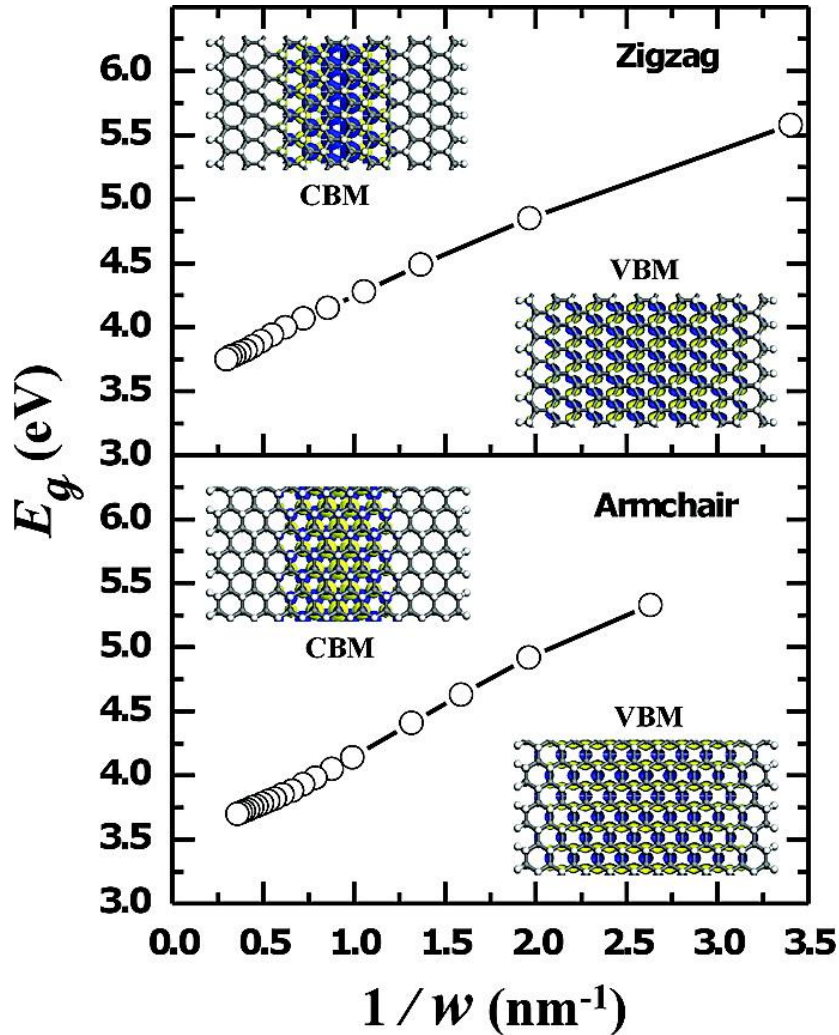
1. Poly(N-vinyl caprolactam) is a water-soluble, synthetic, biocompatible, temperature-sensitive polymer.
2. The LCST of PVCL is known to be tunable depending on molecular weight ranging from 32-37°C.



Dr. Wang + 3
students



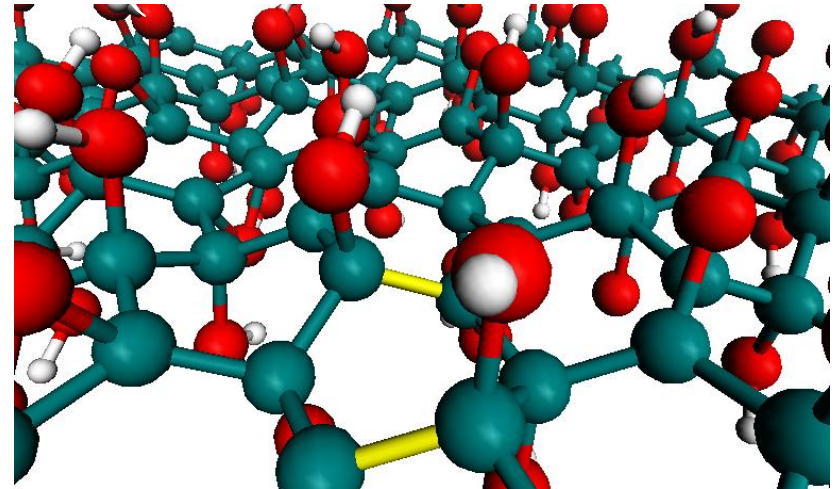
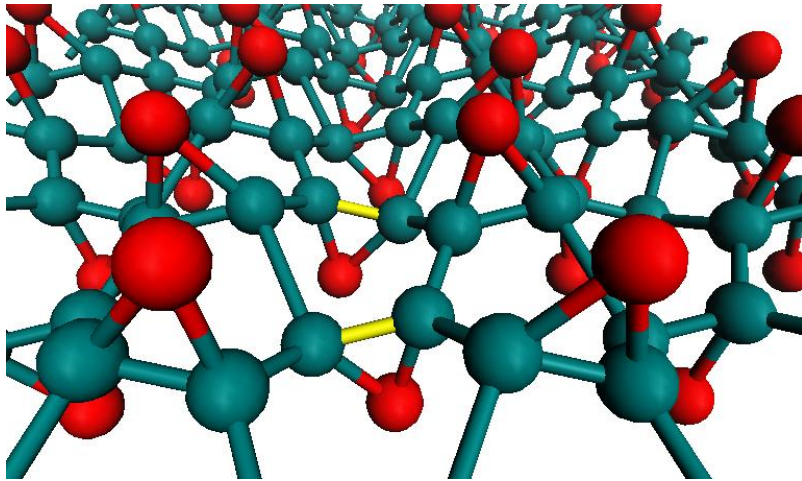
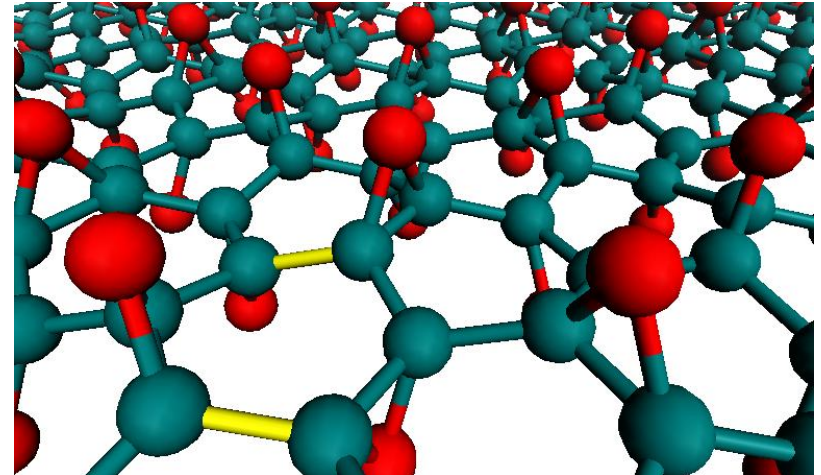
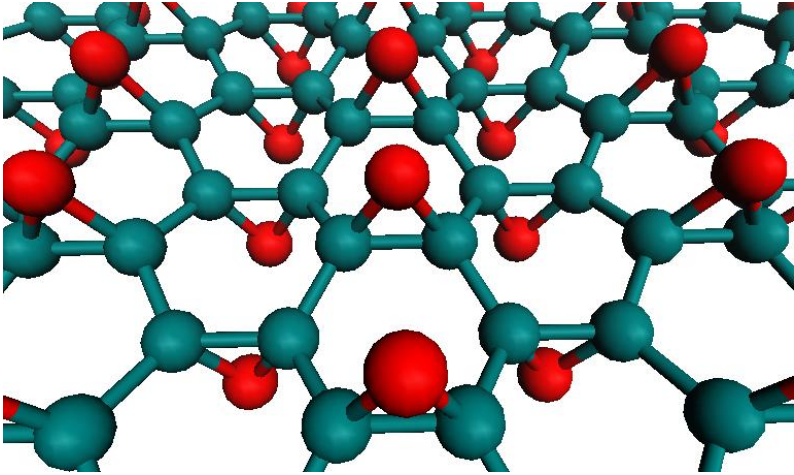
Graphane nanoribbons



ZGNR 12

AGNR 21

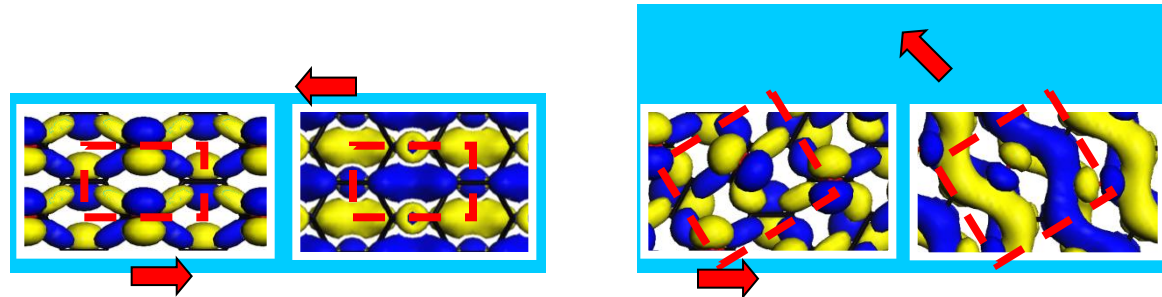
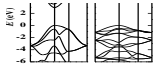
Twist-Boat Conformation in Graphene Oxides



Electronic Structure

Boat

Twist-boat



W

Γ

L

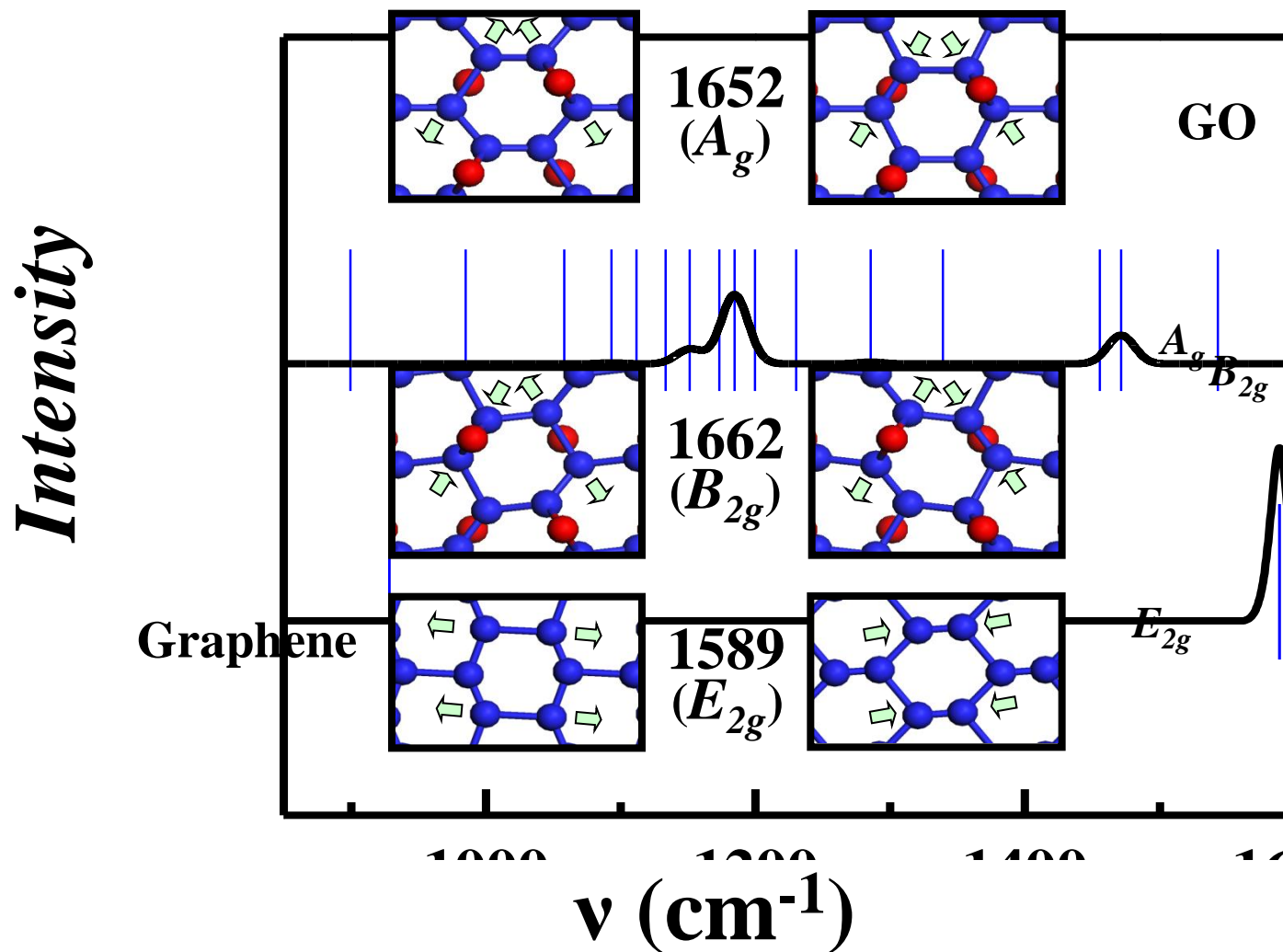
W S

Γ

D

S

Raman Spectrum



Planned Education & Outreach

- Four new courses will be developed for AUC students
 - Introduction to Materials Science
 - Nanomaterials
 - Biological Materials
 - Seminar in Materials Science
- Summer Bridge Program

10 incoming students' math and science knowledge will be enhanced through instructional modules and research
- Academic year undergraduate research at AUC & GT
- 10 week research REU positions @ GT
- PhD bound AUC grad students will be supported @ GT
- RET experience for 4 teachers @ AUC & 2 teachers @ GT

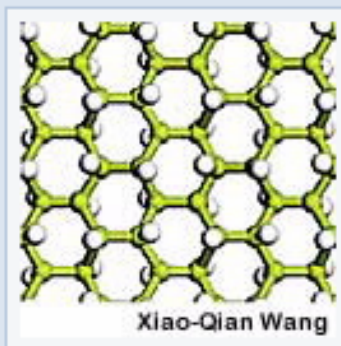

[Publications](#)
[Meetings](#)
[Careers](#)
[Members](#)

 You Are Here: [Home](#)

News & Research

[Twistin' the Boat Away](#)

ACS Nano
November 2009



Density functional calculations of the stability of four forms of hydrogenated graphene show that the twist-boat conformation leads to the observed lattice contraction.

1. Duminda K. Samarakoon and Xiao-Qian Wang, "Chair and twisted boat membranes in hydrogenated graphene", *ACS Nano* **3**, 4017-4022 (2009).
2. Olayinka O. Ogunro, Kayode Karunwi, Ishrat M. Khan and Xiao-Qian Wang, "Chiral Asymmetry of Helical Polymer Nanowires", *J. Phys. Chem. Lett.* **1**, 704-707 (2010).
3. W. Yi, A. Malkovskiy, Y. Xu, X.-Q. Wang, A. P. Sokolov, M. Lebron-Colon, M. A. Meador, and Y. Pang, "Polymer conformation-assisted wrapping of single-walled carbon nanotube: The impact of *cis*-vinylene linkage", *Polymer* **51**, 475-481 (2010).
4. Kelvin Suggs and Xiao-Qian Wang, "Structural and electronic properties of carbon nanotube-reinforced epoxy resins", *Nanoscale*, 2010, **2**, 315.
5. O. O. Ogunro and X.-Q. Wang, "Charge transfer in noncovalent functionalized carbon nanotubes", *New J. Chem.*, in press, 2010.

