

CLARK ATLANTA UNIVERSITY

Presentation at the

10<sup>th</sup> Annual DOE MEI Small Business Conference

# CAU's Energy Related Research Capabilities



Ishrat M Khan Ph.D.

Director, Center for Functional Nanoscale Materials

[ikhan@cau.edu](mailto:ikhan@cau.edu)

[www.cau.edu/research](http://www.cau.edu/research)

Clark Atlanta University



Research and Sponsored Programs

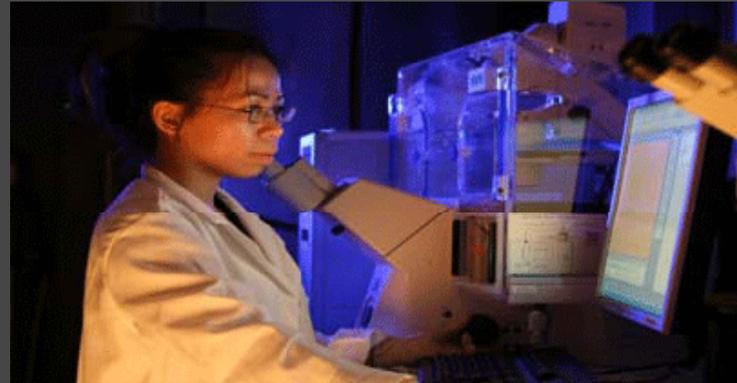


# Research @ CAU

Clark Atlanta University



Research and Sponsored Programs



"At Clark Atlanta University, we believe that research and education cannot be decoupled. Research at CAU is essential in providing a world-class educational experience for our students. We leverage the diverse skills and expertise of our faculty, researchers, staff and students to make significant discoveries and contributions to the knowledge of humankind."

-- Marcus W. Shute, P.E., Ph.D., Vice President

"Teaching without research is like confession without the sin..."



# About CAU

- 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**



# Awards by Agency

	FY2008	FY2007
Corporation and Private Foundations	\$9,968	\$7,891
Georgia State Agencies	\$508,447	\$483,056
Local Governments	\$279,800	\$0
National Aeronautics and Space Administration	\$789,859	\$1,796,850
National Science Foundation	\$2,341,889	\$3,513,096
National Geospatial-Intelligence Agency	\$500,000	\$500,000
National Oceanic and Atmospheric Administration	\$0	\$0
U.S. Agency for International Development	\$0	\$0
U.S. Department of Agriculture	\$39,400	\$135,000
U.S. Department of Commerce	\$0	\$0
U.S. Department of Defense	\$1,388,081	\$1,706,262
U.S. Department of Education	\$7,988,663	\$8,821,415
U.S. Department of Energy	\$576,541	\$274,827
U.S. Department of Health and Human Services	\$3,767,207	\$5,257,667
U.S. Department of Housing and Urban Development	\$0	\$0
U.S. State Department	\$0	\$0
U.S. Small Business Administration	\$0	\$0
U.S. Department of the Interior	\$0	\$0
U.S. Department of Labor	\$0	\$0
U.S. Department of Transportation	\$36,858	\$40,000
<b>Total</b>	<b>\$18,226,713</b>	<b>\$22,536,064</b>



# Promoting Research @ CAU

- Provide value-added, “one stop” support and management throughout the research process to PIs and research centers
  - Re-brand the organization: Division of Research and Sponsored Programs (RSP)
  - Pre- and post-award functions in house; strong coupling to grants acct.
  - Partnership with faculty, researchers, students, and admin. units
  - Streamline processes and improve efficiency w/o sacrificing compliance
  - World class research  $\leftrightarrow$  world class research management, processes, and facilities
- Grow the research enterprise at CAU; maintain Carnegie classification of Research Universities (high research activity) (RU/H)



## Promoting Research @ CAU - 2

- Identify and pursue opportunities in “high growth” areas across all disciplines
  - Info-, nano-, bio-technology, wireless comm., optical comm., learning sciences
  - Leverage existing research expertise in biological sciences, cancer, health, computational science, training, etc.
  - Increase level of basic and applied research funding/activities
  - Utilize RSP Advisory Council (Deans or designees, center directors, key faculty and industry advisors) to provide input in developing research initiatives, policies, etc.
- Collaborate with institutions with expertise in “high growth” areas



# Promoting Research @ CAU - 3

- Establish and reevaluate existing research centers and capability in biomedical research/biotechnology, nanotechnology, computational science, materials, and learning sciences
- Non-profit research organization affiliated with CAU - CAURC
  - Vehicle for contract research and services; minimizes restrictive contracting and financial procedures
  - Facilitates collaboration with industry
  - Technology transfer/commercialization
  - Develop high tech incubator and “research park” @ CAU
- CAU Research Complex
  - Facilities for existing centers and sponsored programs
  - Initial buildings - ~200,000 nsf; site can accommodate add'l. ~27,000 nsf
    - core facilities to support research across disciplines
    - research facilities for cancer research, cell biology, computational science, bio-nanoscience, etc.
  - **2<sup>nd</sup> phase – additional ~27,000 nsf of research labs and facilities**
    - animal facility to enhance biomedical research effort



# Clark Atlanta University Research and Sponsored Programs



- ~200,000 sq. ft. research facility; Phase II – add'l. 27,000 sq. ft.; efficient/effective space allocation
- Office of the Vice President
- Office of Research & Sponsored Programs
- Center for Cancer Research and Therapeutic Development
- Center for Functional Nanoscale Materials
- Environmental Justice Resource Center
- Core and research lab facilities
- High Performance Polymers and Composites Center
- Center for Academic Excellence in National Security



# CAU SRC Facility



- State-of-the art central core user facilities and labs for biomedical/biotechnology and nanoscience research
  - collaborative R&D  $\Rightarrow$  technology breakthroughs  $\Rightarrow$  start-ups/entrepreneurial efforts
  - applications to human health, energy, defense, homeland security, environment, etc.
- Resource for high-tech industry and federal government  $\Rightarrow$  stimulate economic growth
- Resource for local schools, community colleges and universities  $\Rightarrow$  highly skilled STEM workforce in GA  $\Rightarrow$  stimulate economic growth
- Several examples of investment in research infrastructure  $\Rightarrow$  increased external funding  $\Rightarrow$  stimulate economic growth (GA, NC, KY, NV, etc.)



# CAU Strategic Response

- Future needs??
  - Infrastructure – annex including animal facility or renovate satellite facility or both?
  - Equipment
  - Personnel
- Leverage existing programs and expertise
- Well positioned for future growth
- Proposal development for institutional initiatives requires input and leadership from researchers and faculty





# Partnership w/ CAU and Collaborators

- Mutually beneficial and rewarding partnership
- Lots of synergy and potential
  - Opportunity to expand our research scope and funding; leverage our unique positioning
  - Biomedical and cancer research
  - Nanoscale science and technology; materials research
  - Environmental research
    - Expertise in diverse issues involving environmental justice
    - Water quality and assessment
    - Fate and transport of contaminants
    - Chemical lab analysis/trace analysis
  - Computational sciences/modeling
  - Learning sciences and training
  - Homeland security (border security, sensors, intelligence, biosecurity, etc.)
- Possible partner in expanding research complex and research initiatives
- Support student, faculty, and infrastructure development
- Positioned as prime and sub-contractor for corporate and federal R&D opps.



# Promoting Research @ CAU - 5

- Requires commitment and partnership from University, Board of Trustees, government and corporate partners
  - Funding for infrastructure, research initiatives, equipment, and personnel, i.e. expanding research complex @ CAU, etc.
  - Recruit and retain students, faculty, and researchers with expertise in high growth areas
- Enhanced research reputation @ CAU ⇒ intangible benefit to our students, the State of GA, our partners, and community
- Stimulate growth of “high-tech” industry and economic development in GA
- <http://www.cau.edu/research>
- Thank you for your continued support!





- **Semiconductor Nanowires, Functionalized Nanotubes, and Epitaxial Graphene**

**Xiao-Qian (Larry) Wang**  
**Department of Physics, Clark Atlanta**  
**University, Atlanta, GA 30314**



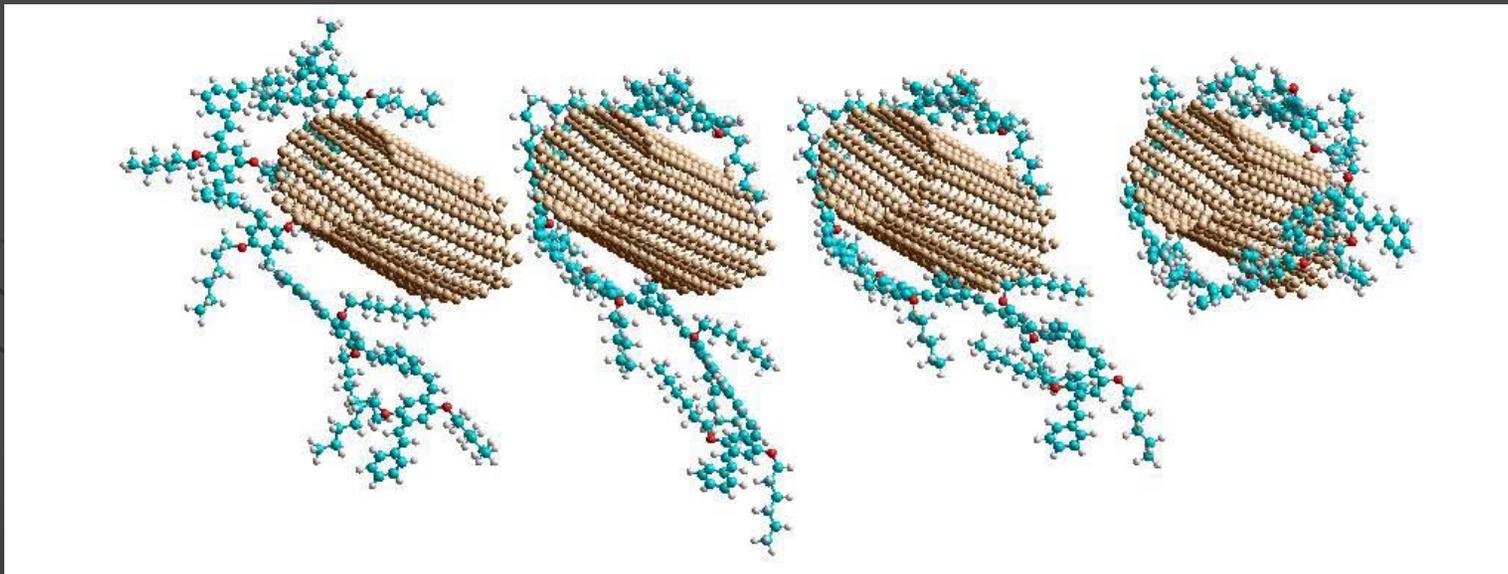
# Simulation Studies of Nanostructures

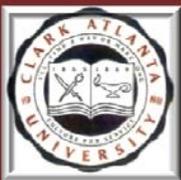
- Multiscale modeling: first-principles density-functional calculations, molecular dynamics, and continuum models
- Nanostructures up to 1,000 atoms studied by first-principles calculations
- Molecular dynamics simulations: polymer matrices, conjugated polymer interacting with carbon nanotubes, epitaxial graphene structures
- Quantum phenomena: shape memory alloys (NASA, ARO); semiconducting nanowires (NSF); functionalized nanotubes (NSF, NASA); epitaxial graphene (NSF)



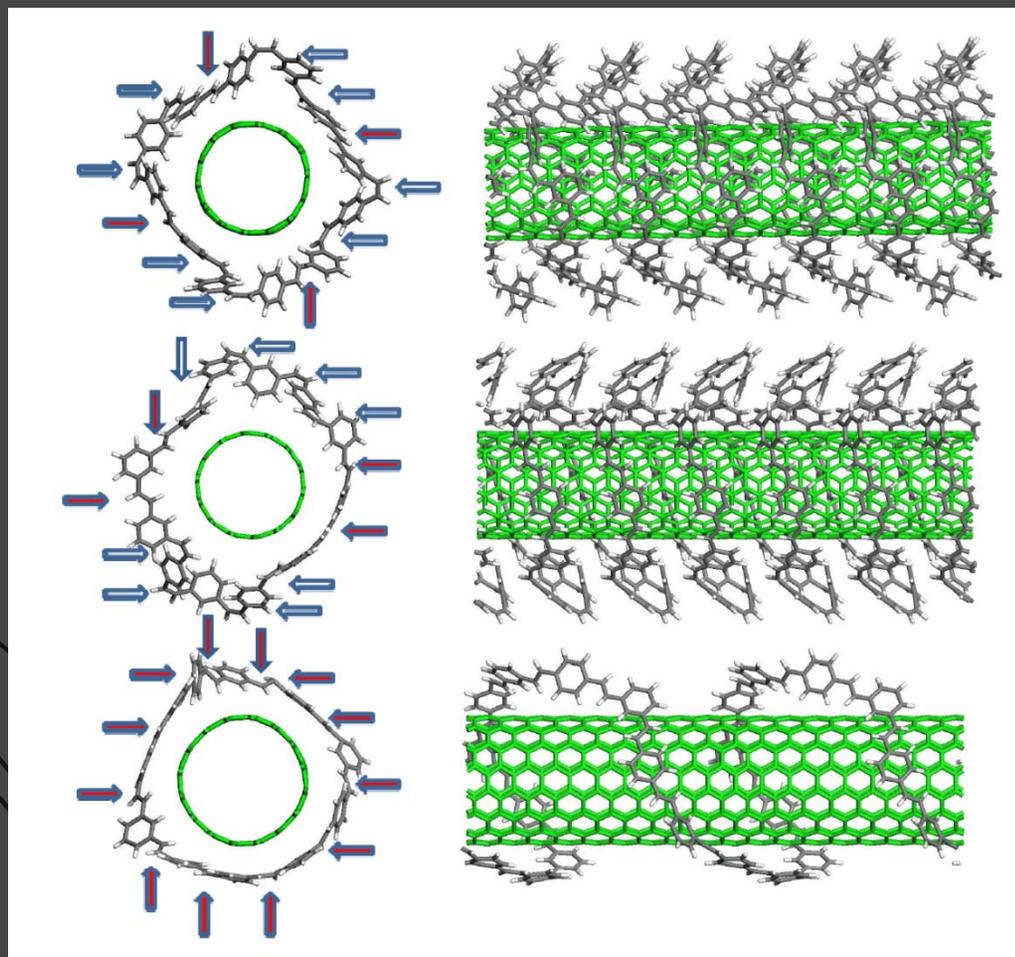
# Multiscale Modeling of Nanocomposites

- Interface chemistry and interactions
- Molecular dynamics and density-functional calculations





# Polymer Conformation Assisted Helical Wrapping: The Impact of *cis*-Linkage





## Energy-Related Research

### Alfred Z. Msezane

Low-energy electron collisions with lanthanides [1] and rare earths are investigated using novel theoretical methods for a fundamental understanding of the attachment process. Oscillator Strengths and Lifetimes of multiply charged ions are investigated, as well as the interaction of radiation with matter. The objective is to uniquely and unambiguously identify the constituent atoms in the design and synthesis of novel functional compounds and exotic ultracold molecules and realization of high temperature superconductivity and Bose-Einstein condensation. Their importance and relevance to DOE mission are summarized below:

Transition metal atoms are technologically important in plasma physics (e.g. impurities in fusion devices), Atomic Trap Trace Analysis (detection of minute quantities of radioactive species), astrophysical abundance and atmospheric studies, deep level traps in semiconductors, hydrogen storage devices, etc. The complicated rare earths are important in lasers, high temperature superconductivity, Bose-Einstein condensation, advanced lighting sources, magnets, etc.

Emission lines from multiply charged ions are frequently observed in the spectra of astrophysical and laboratory plasmas. Accurate absorption oscillator strengths for these ions are needed in astrophysical observations and in the study of laboratory plasmas both for diagnostic purposes and for the determination of the effects of impurities on controlled thermonuclear fusion [2].

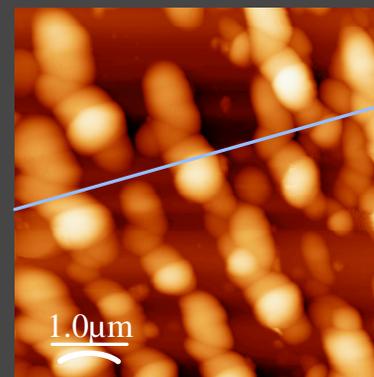
Z. Felfli, A.Z. Msezane and D. Sokolovski, Phys. Rev. A **79**, 012714 (2009)

2. N.C. Deb, A. Hibbert, Z. Felfli and A. Z. Msezane, J. Phys. B **42**, 015701 (2009)



## Michael Williams (Physics)

- This research effort is focused on achieving a fundamental understanding of the physical processes occurring at the surfaces and interfaces of epitaxially grown semiconductors for application to microelectronic and integrated device structures. Impacted devices include high-speed laser diodes, photovoltaics, modulators for fiber optic communications and field emitters for flat panel displays. Phenomena of interest are strain effects on electronic structure, the interfacial migration of constituent materials, surface reaction kinetics and valence band offsets. Capabilities include photoemission spectroscopy (ultraviolet and X-ray), Auger spectroscopy, scanning electron microscopy, secondary ion mass spectrometry, temperature programmed desorption spectroscopy, and epitaxial crystal growth.





# ● Research Program: Nanoporous Multifunctionalized Organosilicates

- Conrad Ingram, Ph.D.
- Principal Investigator
- Chemistry Department-CAU

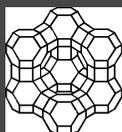
## ● Other Senior personnel:

- Eric Mintz, Ph. D. - Professor of Chemistry-CAU
- Liao Liang, Ph. D. - Research Associate
- Yi Lu - Professor of Chemistry, UIUC



# Zeolites and nanoporous silicates

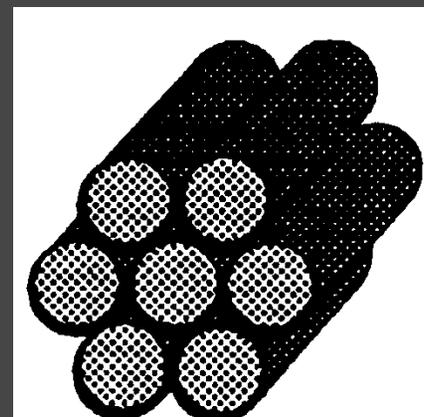
## History



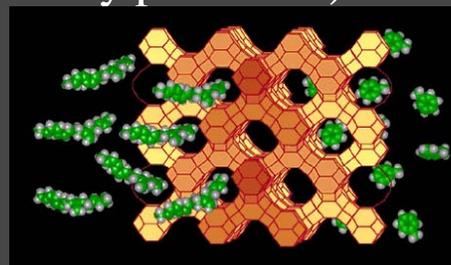
Up 1980 zeolites  
1980s  
aluminophosphates  
(crystalline, < 1 nm  
pore)

## Applications

- heterogeneous selective catalysts (mainly petroleum)
- adsorbents
- bio-separation agents
- optical and electronic devices
- structural composites



Since 1990s-  
Larger pores & surface area  
silicas/aluminophosphates  
(ordered, but non crystalline, > 2 nm pore)



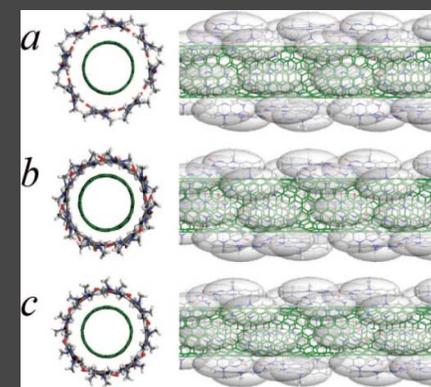
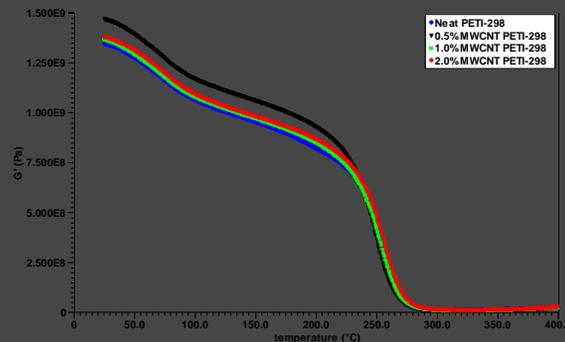
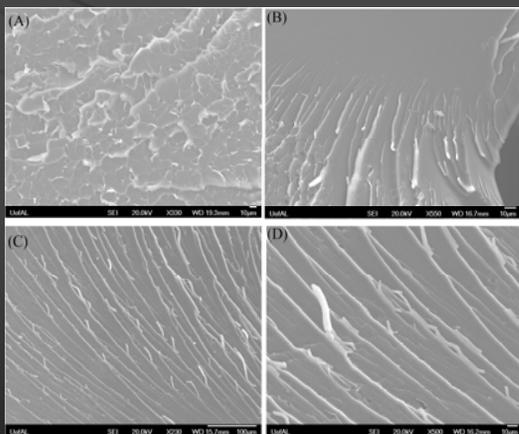


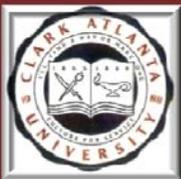
## Research Program: Synthesis and Property Studies of Functionalized Carbon Nanotubes

Principal Investigators: I. Harruna and X. Bu

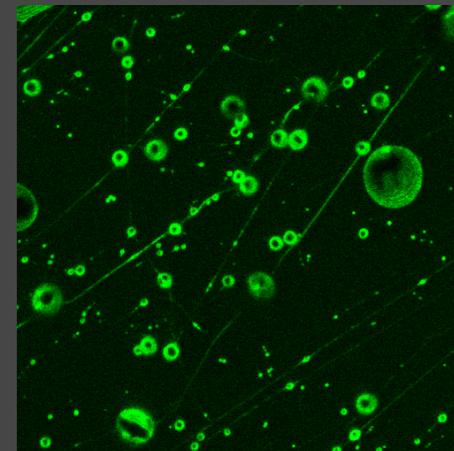
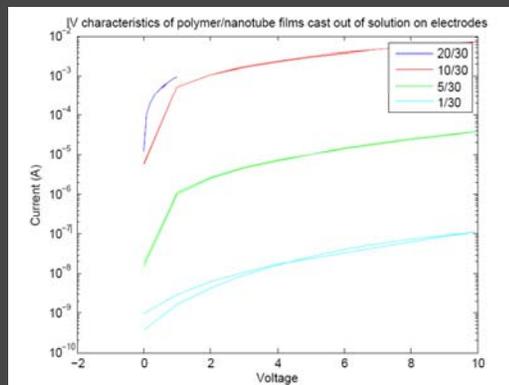
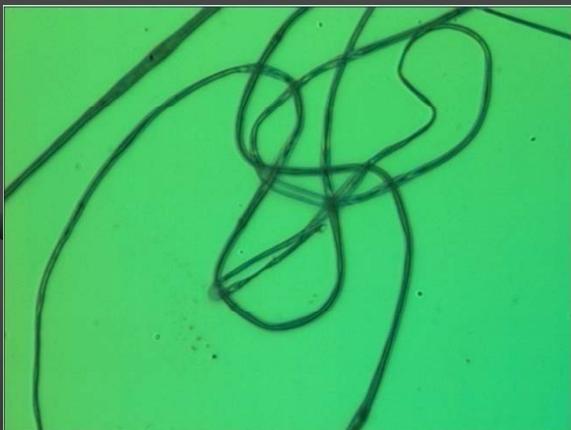
Collaborate with NASA Labs

- Nanomaterials are anticipated to play an increasing role in the development of advanced materials that will offer superb performance otherwise unobtainable with conventional materials.
- Our long-term goal is to develop, characterize, and **utilize nano-structured materials for electro-optical, opto-electric, and anti-corrosion applications.** The particular foci are on single wall carbon nanotubes(SWNTs) materials. The approach includes (1) design and synthesis of organic and polymeric substrates and (2) investigation of interactions of SWNTs with organic and polymeric substrates.





- ELECTRONIC CONDUCTIVE NANOFIBERS WITH BIOSPECIFIC BINDING CAPACITIES:
- NEW MATERIALS FOR NANOSCALE BIOSENSORS





J.M.S.—PURE APPL. CHEM., A34(2), pp. 281–289 (1997)

**ALKALINE DEGRADATION OF RESORCINOL-FORMALDEHYDE RESINS: SOLID-STATE NMR, THERMAL ADSORPTION AND DESORPTION ANALYSIS, AND MOLECULAR MODELING**

LAWRENCE M. PRATT, ROSMARIE SZOSTAK, and ISHRAT M. KHAN\*

Department of Chemistry  
Clark Atlanta University  
Atlanta, Georgia 30314, USA

JANE BIBLER

Savannah River Technology Center  
Westinghouse Savannah River Company  
Aiken, South Carolina 29808, USA

**ABSTRACT**

Resorcinol-formaldehyde resins, used for alkali metal-cation exchange, were shown to degrade more rapidly in the metallated form compared to the protonated form. Solid-state  $^{13}\text{C}$  NMR showed additional peaks in the partially degraded resin corresponding to quinone and other carbonyl functionalities, which are absent in the undegraded resin. Semiempirical molecular orbital calculations were used in conjunction with the experimental data to elucidate the degradation mechanism.

281

Copyright © 1997 by Marcel Dekker, Inc.





- **Conclusions**
- ♦ Lots of Exciting Research at CAU
- ♦ Significant Expertise for Partnership to carry out Energy Related Research
- ♦ Education and Research is integrated
- ♦ Seeking to Develop Industrial Partnerships

