CENTER FOR FUNCTIONAL NANOSCALE MATERIALS (NSF CREST HRD-1137751)

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The Center for Functional Nanoscale Materials seeks to address the dual goals of increasing the capacity of Clark Atlanta University to train talented minority scientists in the area of the physical sciences and of advancing human understanding of nanoscale materials science.

Introduction:

Goals set in 2006 for the NSF CREST Center for Functional Nanoscale Materials:

- **Build up capacity to graduate 5-7 domestic Minority-American PhDs by 2015-2016 in the area of nanoscience**
- **Improve the precollege pipeline into careers in science and technology.**
- **Conduct beneficial and innovative research for the benefit of the Nation and all humanity.**
- **Develop individuals with tools and skills to take up leadership roles in STEM research and education.**

These goals have required significant improvement of research support services at Clark Atlanta

Examples of Research projects

Project 1: Self-Assembly of Hairy Nanoparticles with Hard Polystyrene Cores and Soft Polydimethylsiloxane Shells

Hairy core-shell nanoparticles have emerged as a unique class of polymeric nanocomposites. Hairy nanoparticles with hard polystyrene (PS) cores and soft polydimethylsiloxane (PDMS) shells have been synthesized by living anionic polymerization via a "one-pot synthesis" approach. The size and composition of both core and shell components can be controlled. The synthetic approach produces an entirely new class of hairy nanoparticles. Differential scanning calorimetry thermograms of the core-shell nanoparticles show two distinct transition temperatures corresponding to a glass transition temperature (T_g) of PS segment and a melting transition temperature (T_m) of PDMS segment, indicating the formation of a phase separated system. The synthesized hairy nanoparticles showed different morphologies dependent on the content of PDMS due to the fusion of particles. Solvents play a crucial role in the fusion of particles. Diethyl ether can reduce the fusion of particles and generate almost uniform particles. The hairy nanoparticles can self-assemble into hierarchical suprastructures. The hairy nanoparticles may have potential applications in emerging industries such as high-density microelectronic materials and lithography.

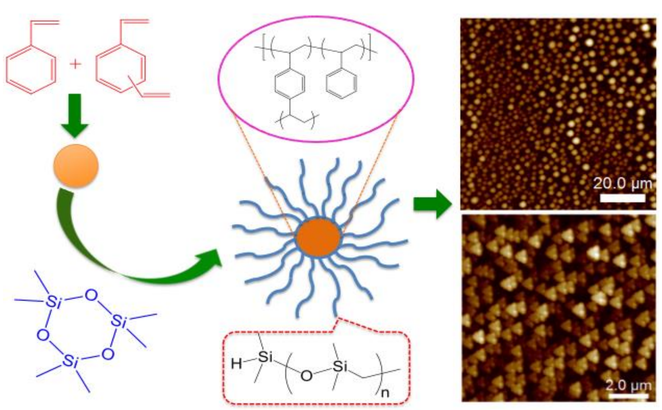
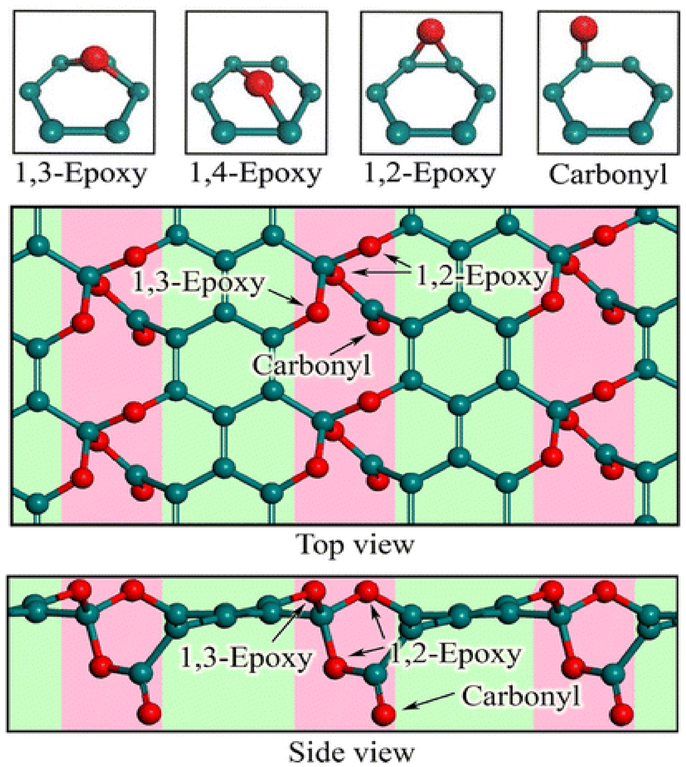


Figure. Atomic Force Microscope (AFM) images showing the controlled self-assembly of nanostructured building blocks (hairy nanoparticles or HNPs) into higher ordered suprastructures.

Hairy Nanoparticles with Hard Polystyrene Cores and Soft Polydimethylsiloxane Shells: One-Pot Synthesis by Living Anionic Polymerization and Characterization *Macromol. Chem. Phys.*, (2016), DOI: 10.1002/macp.201600314

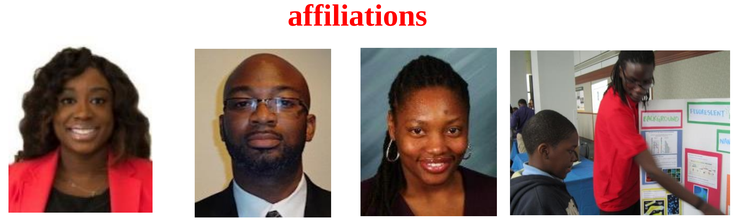
Project 2: Epoxy-Carbonyl Conformation of Graphene Oxides

The structural, electronic, and vibrational properties of graphene oxide are studied by employing a particle swarm optimization search along with density functional theory calculations. A novel low-energy semiconducting configuration for the C2O phase of graphene oxide that consists of a combination of 1,2 and 1,3-epoxides as well as carbonyl functional groups running along the armchair direction. A detailed analysis of the corrugation and bonding reveals the unique features of the new conformation in conformity with experimental observations. The findings shed light on structural and electronic characteristics that are essential for future improvement of nanodevices.



Epoxy-Carbonyl Conformation of Graphene Oxides *J. Phys. Chem. C*, 2016, 120 (39), pp 22739–22743; **DOI:** 10.1021/acs.jpcc.6b07648

Few of our recent PhD Graduates with current affiliations



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Jereme Doss, PhD
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Project 3: Complex Three-dimensional Lanthanide Metal–organic Frameworks with Variable Coordination Spheres Based on Pyrazine-2,3,5,6-tetracarboxylate

Metal–organic frameworks {[Ln4IJpztc)3IJH2O)11]·10IJH2O)}n (Ln = GdIJ1), TbIJ2); pztc = pyrazine-2,3,5,6- tetracarboxylate) containing variable coordination spheres and with a complex and unusual three dimensional structure, were synthesized by the reaction of H4pztc with the respective LnIJIII) salt in water under hydrothermal conditions. The compounds were characterized by single crystal X-ray crystallography, elemental and thermal analysis, and FTIR spectroscopy. The asymmetric units in these compounds have four symmetry-independent LnIJIII) ions and these are octa- and nona-coordinate centers, with irregular coordination polyhedra from ijLnIJpztc)2IJH2O)6], ijLnIJpztc)2IJH2O)4], LnIJpztc)3IJH2O)3], ijLnIJpztc)3IJH2O)], and ijLnIJpztc)4] cluster units. The fully deprotonated ligand, pztc, coordinates to the Ln3+ ions through seven or through ten of its atoms (i.e., the maximum coordination number for this ligand). The three-dimensional open framework contains irregular channels along the [001] crystallographic direction. The channels are approximately 12 Å wide at their largest dimension and contain strongly hydrogen bonded water molecules of crystallization which further stabilize the structure. The solvent accessible volume is 20% of the total volume. The structures exhibit magnetic behavior that is characteristic of the respective isolated paramagnetic lanthanide ions.

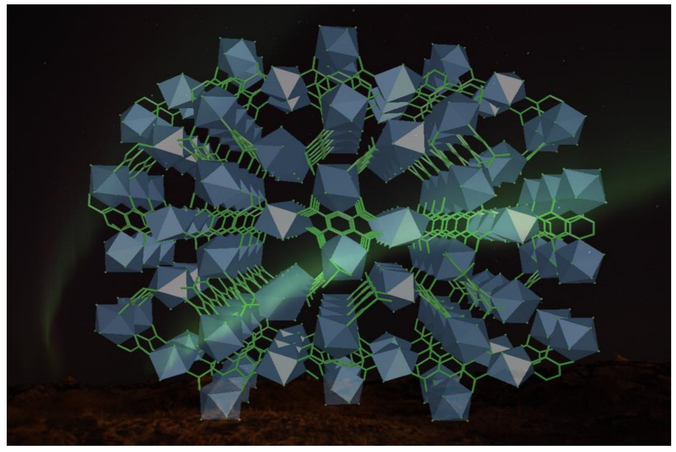

Figure: Complex three-dimensional lanthanide metal–organic frameworks with variable coordination spheres based on pyrazine-2,3,5,6-tetracarboxylate

Complex three-dimensional lanthanide metal– organic frameworks with variable coordination spheres based on pyrazine-2,3,5,6-tetracarboxylate, CrystEngComm, 2015, 17, DOI: 10.1039/c4ce02564d

Conclusion:

Since CFNM was established in 2006, we have been successful in developing an ecosystem which has the capacity and supportive environment to work with not only doctoral students but also MS students.

A total number of doctoral degree awarded by the NSF CREST CFNM is twenty-seven (27).

Furthermore, during the same period the NSF CREST CFNM has also awarded thirteen (13) MS degree.

During the just completed academic year (2015-2016), five students earned the doctoral degrees.

The Center has become a major producer of PhD scientists from groups underrepresented in the science and technology areas.

Funding