Invites you to a seminar by:

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Simulating Molecular Interfaces: Materials Investigations in Adsorption and Catalysis

As the study of chemical processes, biological phenomena, and material science has reached the nanometer length scale, the physics of an interface has become an increasingly important topic. At this level, the measurements become less precise, the interpretation of the results are less intuitive, and sample uniformity becomes a challenge. These hindrances directly relate to our ability to study interfacial phenomena, since typical interfacial regions are defined in units of nanometers, commensurate with the dimensions of the molecules composing the interface. While experimental investigations are indispensable, simulations provide a complimentary approach to study these systems.

We are currently using molecular simulation methods and electronic structure calculations to investigate adsorption and reactions on surfaces and at interfaces. This presentation will demonstrate how these simulation approaches can be used to guide the synthesis of new materials and chemical processes, including:

- **Carbon nanotube-based electronic and magnetic materials**: here, we are using boron-doped carbon nanotubes as templates for stabilizing transition-metal nanoparticles and strings, guided by DFT calculations.

- **More robust and efficient fuel cells (PEM and SOFC)**: kinetic Monte Carlo approaches are being developed to capture the interfacial electrochemistry and charge transport through these materials.

- **Highly-fluorescent biological tags, based on metal nanoclusters**: DFT calculations are being used to predict the influence of stabilizing-ligands on the fluorescence of Au$_{3.5}$ metal clusters, which can be used for protein-level tracking, with minimal influence on biological functions.

An overview of these projects will be given, which will highlight our recent simulation progress, supported by experimental collaborations. Our ultimate goal is to use our simulation approaches to identify new targets for experimental synthesis.

**TUESDAY, FEBRUARY 28, 2012**

**INSTITUTE OF MATERIAL SCIENCE BUILDING, Room 20**

11:00 a.m.

*Refreshments will be served at 10:45 a.m.*
Bio

Prof. Turner completed his B.S. in Chemical Engineering from Auburn University and his Ph.D. in Chemical Engineering from NC State University with Prof. Keith Gubbins. He spent several years in industry with Monsanto, Birmingham Steel, and Trinity Consultants. He joined the University of Alabama as an assistant professor in 2003, he was soon appointed with the Reichhold-Shumaker Professorship, and he is now an Associate Professor. Over the past few years, he has been a visiting faculty fellow at NASA in Langley, VA and at the Naval Research Lab in Washington, D.C. His research deals with the computer simulation of chemical reactions and adsorption on surfaces and at interfaces. These simulations involve ab initio electronic structure calculations, as well as Monte Carlo and molecular dynamics simulations.

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