



## College of Science and Mathematics

### Department of Chemistry and Biochemistry

Fall 2017

The **Chemistry and Biochemistry Departmental Seminar Series** covers a broad range of fields in the Chemical and Biochemical Sciences. In past seminars, scientists from Academia, Government, and Industry have presented their most recent discoveries and contributions in their respective areas. This Seminar Series offers students and faculty the opportunity to interact directly with other leaders in their specializations and to gain a good overview of the entire range of fields in Chemistry and Biochemistry.

Seminars are held on Tuesdays in CL 1009 (Clendenin Building, Room 1009) on the Kennesaw Campus, 12:30 - 1:30pm, unless otherwise noted with special day/time/location information. All are invited to attend.

#### **Tuesday, September 26, 2017**

[Dr. Ron Hunter](#)

Scientist, The Coca-Cola Company

*An Act of Translation: Transferring Your Research Skills into Something Meaningful to Society*

This talk is for early-career professionals curious about how else their discipline-specific skills are transferrable to non-academic career paths, including areas of public policy and government research. Discussion will include how PhD-level skills can be used to impact society globally, as well as short-duration professional prospects and long-duration career opportunities.

View event on Facebook: <https://www.facebook.com/events/679543258914120/>

#### **Tuesday, October 17, 2017**

Kristin McKenna, David Fialho, and Martin Solano

[Center for Chemical Evolution](#), Georgia Institute of Technology

*What is research in graduate school really like? How do I get there?*

Join three graduate students from the Center for Chemical Evolution to learn about how they got where they are. Come ready with questions not just about the research presented, but also about how to pursue a path in science.

View event on Facebook: <https://www.facebook.com/events/1883411295008834/>

#### **Tuesday, October 24, 2017**

Dr. Emily Weikum

Medical Writer, [SciMentum](#)

*Allosteric Modulation of Nuclear Receptor Function*

Nuclear receptors are a family of ligand-regulated transcription factors that control specific gene programs across numerous biological processes. The assembly of distinct transcriptional complexes drives regulatory specificity, each complex attuned to a particular gene-, cell- and physiologic-context. These distinct complexes are influenced by allosteric effectors, such as DNA sequence and ligands, which modulate nuclear receptor function. These collective works utilize structural biology and biochemistry to examine these allosteric effectors of nuclear receptor function. We explore the

idea that different DNA sequences alter nuclear receptor structure. We show that the glucocorticoid receptor can interact directly with a sequence within inflammatory gene promoters. This finding represents a paradigm shift in our understanding of how the glucocorticoid receptor could repress transcription at these sites. We also structurally characterize the glucocorticoid receptor ligand-binding domain in complex with a widely used and potent clinical ligand. As there are only a few GR ligand binding domain structures reported, this work provided structural mechanisms driving this highly stabilizing ligand. Collectively, this work reviews the idea that these allosteric modifications drive different NR surfaces that are read by coregulator proteins, resulting in alternative transcriptional programs.

View event on Facebook: <https://www.facebook.com/events/357553048030963/>

**Tuesday, October 31, 2017**

[Dr. Christopher A. Baker](#)

Assistant Professor, Department of Chemistry, University of Tennessee, Knoxville

*Microfluidics and Nanoscale biosensors: small analytical tools to enable large biological insights*

Our group is developing novel bioanalytical technologies, like microfluidic instrumentation and nanoscale biosensors, to allow us to listen in on chemical communications that occur between the brain and body (i.e. neuroendocrine processes). Faster, more specific, and higher sensitivity measurements will elucidate the roles of peptide signaling in behavior and may shed new light on mechanisms of neurodevelopmental disorders like autism.

View event on Facebook: <https://www.facebook.com/events/137804866970462/>

**Tuesday, November 28, 2017**

[Dr. Olaseni Sode](#)

Assistant Professor, Department of Chemistry, Biochemistry and Physics, University of Tampa

*Exploring the electronic and vibrational structure of condensed phase CO<sub>2</sub> with ab initio methods*

A “first principles” many-body carbon dioxide potential energy function (*mbCO<sub>2</sub>*) is developed for CO<sub>2</sub> gas and condensed phase systems. The *mbCO<sub>2</sub>* potential was originally constructed as a dimer potential function with flexible-monomers calculated at the CCSD(T)-F12b/aug-cc-pVTZ level of theory. Recently, we have included three-body contributions, expressed as the sum of permutationally invariant polynomials and the Axilrod-Teller-Muto three-body function, and derived from a fit to over 15,000 CO<sub>2</sub> trimer configurations calculated at the CCSD(T)-F12a/aug-cc-pVDZ level. With the updated many-body potential, we revisit the optimization of CO<sub>2</sub> clusters as well as the energetic ordering of trimers. Anharmonic frequencies are determined using correlated vibrational structure methods and compared to experimental values with special attention directed at the intermolecular modes of vibration. Lastly, we extend our application of the *mbCO<sub>2</sub>* potential to the structure and thermodynamic properties of crystalline CO<sub>2</sub> in its low-temperature cubic and orthorhombic phases.

View event on Facebook: <https://www.facebook.com/events/540277579656374/>