Undergraduate Research Seminar
Wednesday, October 1st, 2014 5:30 p.m.
Leigh 309

Kyle Chesney

"Computational and Electrochemical Analysis of Benzidine Derivatives"

We have carried out computational and experimental studies on the effects of modifying the structure of N,N,N',N'-tetramethyl-[1,1'-biphenyl]-4,4'-diamine (benzidine) – via introduction of functional groups in various positions as well as incorporation of a heteroatom linking the aromatic rings – to evaluate the usefulness of these variants with regards to their application as a suitable cathode material for grid-level electrical energy storage. Specifically, we performed computational analysis via density functional theory (DFT) methods to elucidate the electronic properties, as well as nuclear independent chemical shifts (NICS) to probe the stability of the molecules throughout their various oxidation states; we have discovered that the heteroatom series exhibited desirable electronic properties while maintaining a low molecular weight, and furthermore, a furan derivative exhibited the best combination of stability and high redox potential. Electrochemical analysis, via cyclic voltammetry (CV), confirmed that a dimethyl flourene variant exhibited 2 reversible redox couples at high potentials, well in line with our predicted values. Ongoing and future work will focus on experimental examination of the properties of 2 other molecules which have been down-selected via computational studies, namely the previously mentioned furan derivative as well as a thiophene derivative.

Kevin Montes

"Improving Nuclear Spin Polarization of 129Xe Gas."

In the majority of nuclear magnetic resonance experiments, proton spin is detected. This method is useful because of the high abundance of hydrogen nuclei in most experiments, and the high nuclear-spin polarization achieved with it at standard magnetic field strengths. However, since the development of hyperpolarized gas NMR methods, noble gas atoms like 3He and 129Xe have become useful in situations where protons are less abundant (i.e. in the lungs) and where their nuclear spin polarizations can be used to obtain more detailed magnetic resonance images. These noble gases can be hyperpolarized, or have their nuclear spin polarizations increased by orders of magnitude, through a process called spin-exchange optical pumping (SEOP). During this process, a mixture of alkali metal atoms, buffer gas, and noble gas atoms to be hyperpolarized is heated and pumped through a cell in a uniform magnetic field. Circularly polarized light is used to excite the atoms and transfer the alkali metal atoms' angular momentum to the noble gas.

Since the SEOP process is dependent upon several variables, it has been difficult to maximize the polarization of 129Xe for NMR experiments. My project aimed at producing simulations of the temperature and flow conditions inside the hyperpolarization optical cell in order to guide the optimization of the SEOP process. I designed three different cell geometries and a model to mimic the gas mixture used in the lab. Then, I compared the results of the physics simulations run on each design to determine the most effective cell geometry.

Lauren McCarthy

“Stochastic Impact Ionization in Nanostructured Semiconductors”

The Gunn Effect and impact ionization are two well-studied effects in bulk semiconductors. Devices that make use of the Gunn Effect, for example, form an important group of microwave emitters that have numerous applications. Despite their importance, these processes as applied to nanostructured systems are not yet fully understood. The device in this study, a GaAs/AlGaAs heterostructure with a nanoconstriction, has been designed to exhibit strong nonlinearities in its current-voltage characteristics caused by the Gunn Effect and impact ionization. Devices such as these have the potential to become a new class of sensors and emitters, specifically in the THz range. We cannot move forward with these studies, however, until we fully understand these mechanisms. To clarify the role of the impact ionization mechanism in the device, we studied the time dependent current response to an applied bias. At certain applied biases, the current response becomes bi-stable and over time can spontaneously jump in magnitude signifying that the sample has undergone impact ionization, which is followed by Gunn oscillations. This jump in current appears to be stochastic, in other words, it occurs randomly in time. By studying the time dependent current response of this device, we can learn about the mechanisms of these fundamental processes that will enable the rational design of a new class of semiconductor sensors and emitters.