ND*nano* Undergraduate Research Fellowship (NURF)
2014 Project Summary

1) Student name: Buchanan Bourdon
2) Faculty mentor name: Professors Alan Seabaugh and Susan Fullerton
3) Project title: Electrostatic Doping of 2D materials via Polymer Electrolytes: Using COMSOL to Simulate Ion-electron Transport

4) Briefly describe any new skills you acquired during your summer research:

This summer allowed me to continue my research from the past year by using COMSOL Multiphysics Software to simulate ion-electron transport. Over the summer, I learned how to properly couple multiple physics modules and simulate devices that qualitatively reproduced experimental results.

5. Briefly share a practical application/end use of your research:

To reduce power dissipation in electronics, we must reduce the operating voltages of the individual components, including memory. By using COMSOL Multiphysics software to model ion transport, we can gain insight on how to better develop low-voltage nanoionic memory devices that could lead to more efficient electronic devices.

Project Summary:

As electronic devices become smaller, the need for low-power components increases. Two-Dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), are promising because they allow us to approach the limits of vertical scaling when integrated into devices. However, new doping strategies are required for 2D materials because traditional strategies, such as substitutional doping, will destroy the electrical properties of the materials. One strategy is electrostatic doping using ions. In our lab, we use ion doping to modulate the electrical conductivity of a graphene channel for the development of a new, 2D memory device, and to create p-n junctions for tunneling in 2D field-effect transistors (FETs). The goal of this summer's research was to use COMSOL Multiphysics Software to model ion-electron transport to better understand the underlying fundamental physics of electrostatic doping, and inform the experimental approach.

To simulate the formation of the electrostatic double-layer required to increase the current through the graphene, we modeled a 100 x 100 nm parallel-plate device consisting of graphene / polymer electrolyte / graphene, where the polymer electrolyte was polyethylene oxide (PEO) and $LiClO_4$. Using materials properties derived from experiment, including dielectric constants and ion diffusion coefficients, we described ion transport by coupling the Nernst-Planck equation with Poisson's equation. We determined that in the 100 x 100 nm parallel-plate model, with an applied electric field of 1 mV/nm, the ions establish an electrostatic double-layer in 0.5 s, and relax to equilibrium in 1 s at room temperature. We studied dynamic p and n-type doping by sweeping the gate voltage (V_G) between -150 to 150 mV and monitoring the cation

(Li^+) and anion (ClO_4^-) charge carrier density at the graphene surface. From experiment, we know that if the V_G is modulated by 0.2 V/s, the ions will not have sufficient time to reach equilibrium, giving rise to a large hysteresis in the current-voltage (I_d-V_G) data (Fig. 1). This result is qualitatively captured by the COMSOL simulations (Fig. 2). When the sweep rate is decreased from 1 V/s to 0.01 V/s, the ions have sufficient time to reach steady-state and exhibit no hysteresis (Fig. 2).

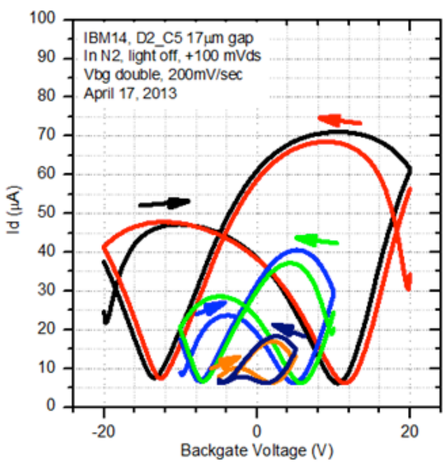

Figure 1

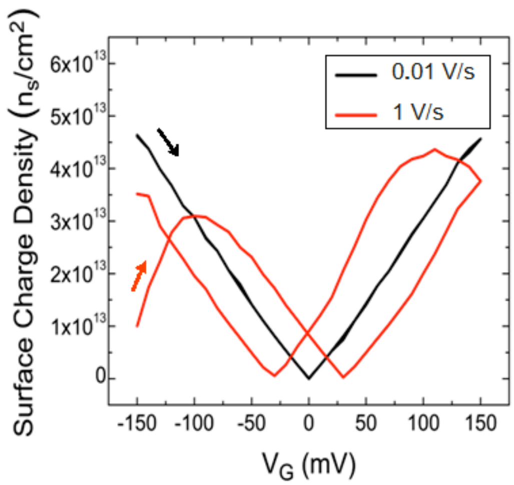

Figure 2

Publications (papers/posters/presentations):

I presented a poster at the 2014 Summer Undergraduate Research Symposium. The poster was titled "Electrostatic Doping of 2D materials via Polymer Electrolytes: Using COMSOL to Simulate Ion-electron Transport" and was coauthored by Huilong Xu, Alan Seabaugh, and Susan Fullerton.

I was a co-author on an abstract submitted to the 2014 International Electron Devices Meeting (IEDM) on 6/24/14.

Title: "A new approach for 2D crystal memory utilizing nanometer-thick ion conductors"

Authors: Fullerton, Susan K. (Notre Dame), Lu, Hao (Notre Dame), Bourdon, Buchanan (Notre Dame), Kinder, Erich W. (Notre Dame), Li, Huamin (Notre Dame), O'Neill, Katie (Notre Dame), Nahas, Joseph J. (Notre Dame), Sabnis, Sushant A. (Notre Dame), Xu, Huilong (Notre Dame), Wang, Weihua (UT/Dallas), Gong, Cheng (UT/Dallas), Kim, Hanchul (UT/Dallas), Kwak, Iljo (UC/San Diego), Park, Jun Hong (UC/San Diego), Park, Sang Wook (UC/San Diego), Sardashti, Kasra (UC/San Diego), Furuyama, Taniyuki (Tohoku Univ.), Kobayashi, Nagao (Tohoku Univ.), Cho, Kyeongjiae (UT/Dallas), Kummel, Andrew (UC/San Diego), Seabaugh, Alan C. (Notre Dame).