**Notice and Invitation**

Defense of Master's Thesis

The Volgenau School of Engineering, George Mason University

**Aaron Lowenberger**

Bachelor of Science, Boston University, 2002

# THE STATIC AND DYNAMIC RESPONSE OF GRAPHENE CHEMICAL SENSORS: THE IMPACTS OF SURFACE DEFECTS

Friday, November 28, 2017, 11:00 AM – 12:00 PM

Engineering Building, Room 3507

Committee

Dr. Qiliang Li

Dr. Dimitris Ioannou

Dr. Patrick Vora

## Abstract

Chemical sensors are widely used in many technologies, with applications in medicine, industrial process monitoring, automotive and aerospace, military, and environmental protection. Due to the excellent electronic properties and unique two-dimensional (2D) structure, graphene has shown great promise as a highly sensitive, low noise sensor material. This research was to explore the static and dynamic response of graphene sensors upon exposure to different chemical vapors. Different graphene sensor configurations, including pristine graphene and graphene with four typical types of surface defects, were modeled in the presence and absence of five different chemicals. First-principle simulations were performed to study the electrostatic response of the different sensor configurations. The results were analyzed and compared with previously published experimental data, revealing the dominating defects present in the experimental sensors. In addition, the dynamic response of graphene sensors and the molecule-graphene interaction mechanism has been investigated by progressively changing the distance between the sensor and the vapor molecules. This study is very important for understanding the reaction mechanism between a 2D surface and chemical molecules, leading to high-performance chemical sensors.