Announcing the Final Examination of Walter Malone for the degree of Doctor of Philosophy in Physics

Date: April 5th, 2019
Time: 9:30 a.m.
Room: PSB 445
Dissertation title: A theoretical investigation of small organic molecules on transition metal surfaces

Abstract:
With the ever growing number of proposed density functional theory (DFT) functionals it becomes necessary to thoroughly screen any new methods to determine their merit. Any new method should include a proper description of the van der Waals (vdW) interaction, which can prove vital to a correct description of a myriad of systems of technological importance. The first part of this dissertation explores the utility of several vdW-inclusive DFT functionals including optB86b-vdW, optB88-vdW, optPBE-vdW, revPBE-vdW, rPW86-vdW2, and SCAN+rVV10 by applying them to model systems of small organic molecules, pyridine (C_5H_5N) and thiophene (C_4H_4S), on transition metal surfaces. Overall, we find the optB88-vdW functional gives the best, most balanced description of both thiophene and pyridine on transition metal surfaces while revPBE-vdW, rPW86-vdW2, and SCAN+rVV10 perform especially poorly for these systems. In the second part of this dissertation we change our focus to potential applications of DFT. First we investigate the hydrodesulfurization (HDS) of thiophene. The removal of sulfur containing molecules from petrochemicals through HDS is an exceptionally important process economically and environmentally that could benefit from the discovery of more active catalysis. In this dissertation we manage to map the HDS rate of thiophene in realistic reaction conditions to the charge transfer to the thiophene molecule and adsorption energy of thiophene on bare transition metal surfaces in the hopes of predicting ever more active HDS catalysis. Finally we look at the adsorption of polythiophenes and 5,14-dihydro-5,7,12,14-tetraazapentacene (DHTAP) on Au(111) and Cu(110). Both of these molecules are candidates for use in molecular electronic devices, which are cheaper to produce and more flexible than their silicon counterparts. Overall, we find that polythiophenes may dissociate of Au, presenting an issue for their use in molecular electronic devices. DHTAP, in contrast, proves to be a suitable candidate for use in practical devices.

Outline of Studies:
Major: Physics

Educational Career:
M. S. University of Central Florida, Orlando, Florida, 2016
B. S. University of Portland, Portland, Oregon, 2014

Committee in Charge:
Dr. Abdelkader Kara (Chair)
Dr. Sergey Stolbov
Dr. William Kaden
Dr. Jayan Thomas (External Committee Member)

Approved for distribution by Dr. Abdelkader Kara, Committee Chair, on March 25, 2019.

The public is welcome to attend.