Announcing the Final Examination of Tyler Campbell for the degree of Doctor of Philosophy in Physics

Date: April 6, 2021
Time: 8:30 a.m.
Zoom Link:
https://ucf.zoom.us/j/97205324296?pwd=RmhSTW5IU1V1Q0RWNzJtSEVUUjBrUT09
Meeting ID: 972 0532 4296
Passcode: 619230

Dissertation title: Exploring New Materials as Promising Electrocatalysts for the Generation of a Clean and Renewable Energy Source

Abstract:

This work presents the research of myself, my advising professor, and our collaborators in first-principles studies of several catalytic materials for improving the efficiency and economics of hydrogen fuel cells, focusing on the oxygen reduction reaction (ORR) at the cathode, CO removal and the hydrogen oxidation reaction (HOR) at the anode, and the redox reactions used for water splitting through photocatalysis. We use a computational design approach to analyze the reaction thermodynamics, applying density functional theory (DFT) for most calculations. We find that, through a subversion of the linear scaling approximation for surface reactivity, an Au monolayer deposited on the early transition metals Nb and Ta is both stable under fuel cell operating conditions and reaches a higher onset potential for the ORR than the current expensive Pt-based cathodes. In a similar light, we find that Pd/Mo(110) and Pd/W(110) are both active toward the CO removal reaction and the HOR at the fuel cell anode through their interesting binding energy relations, in comparison to the Pt catalyst anode which suffers the problem of CO poisoning of active sites. We study the reaction thermodynamics of the two-dimensional structures C_2N and C_2N doped with P, whose band gaps are favorable with regards to solar light photocatalysis, but find that the redox reactions through several routes do not seem energetically favorable. We also study another candidate for photocatalytic water splitting, the wide-band gap semiconductor β-phase Ga_2O_3, assessing the effects of H- and Si-doping on the material's band structure through the GW method. We find, using DFT, that Si energetically prefers to substitute the Ga (I) atom and H prefers to bind to the O (2) atom. We find through GW analysis of the band gap that Si and H act as n-type dopants of β-Ga_2O_3.

Outline of Studies:
Major: Physics

Educational Career:
B. S. University of Central Florida, FL, 2015

Committee in Charge:
Dr. Sergey Stolbov (Chair)
Dr. William Kaden
Dr. Talat Rahman
Dr. Artem Masunov (External Committee Member)

Approved for distribution by Dr. Sergey Stolbov, Committee Chair, on March 17, 2021.

The public is welcome to attend remotely.