Announcing the Final Examination of **Md Afjal Khan Pathan** for the degree of Doctor of Philosophy in Physics

Date: June 03, 2021
Time: 10:00 a.m.
Zoom Link: https://ucf.zoom.us/j/91988103709?pwd=S1FTUGJRbGxFWUtuTVdCd1phVStBQT09
Meeting ID: 919 8810 3709
Passcode: 149404
Dissertation title: Understanding the Mechanism of Surface Chemical Reactions by Tracking Unstable Intermediate Species

Abstract:
The detection of intermediate species formed during surface chemical reactions is essential because it can provide critical information about the reaction mechanisms at surfaces and interfaces. Therefore, the overarching goal of this research was to understand the mechanisms of surface catalytic, photocatalytic, and photoinduced reactions by monitoring the intermediate species formed during these reactions.

To understand the initial steps of the carbon monoxide hydrogenation reaction on two-dimensional (2D) MoS_2 and TaS_2 materials, temperature programmed desorption and reaction are employed. Large-area 2D-MoS_2 and 2D-TaS_2 were prepared on a Cu(111) substrate under ultra-high vacuum conditions via physical vapor deposition. The highly crystalline surfaces of both 2D-MoS_2 and 2D-TaS_2 exhibit poor catalytic properties. However, when defects are created at the surface of 2D-MoS_2 and 2D-TaS_2, the catalytic activity of these materials dramatically increases. The CO hydrogenation reaction on both surfaces proceeds through the dissociative adsorption of H_2 and the formation of HCO. HCO is directly detected from TaS_2, but not from MoS_2, because of the ability of MoS_2 to break the CO bond of HCO monomers and dimmers, which leads to the detection of C_2H_2.

To study the mechanisms of photoinduced and photocatalytic reactions, a technique based on time-of-flight mass spectrometry in conjunction with femtosecond pump-probe spectroscopy is employed. In one example, the photoinduced reaction of CD_3I on an amorphous cerium oxide surface is studied with time, mass, and energy resolution to understand the effect of surface morphology on the reaction dynamics. In a different example, photocatalytic water (D_2O) splitting in the presence of CH_3I on a TiO_2(110) surface is studied. In this case, rich details about the reaction mechanism are obtained through the detection of intermediates such as D, OD, DO_2, CH_3, and I, and final products such as CH_3D and CH_3OD. This type of research could open new avenues for understanding a variety of heterogeneous chemical reactions.

Outline of Studies:
Major: Physics

Educational Career:
M. S. in Physics, University of Dhaka, Bangladesh, 2012
B. S. in Physics, University of Dhaka, Bangladesh, 2010

Committee in Charge:
Dr. Mihai E. Vaida (Chair)
Dr. Talat S. Rahman (Vice Chair)
Dr. William Kaden
Dr. Titel Jurca (External Committee Member)

Approved for distribution by Dr. Mihai E. Vaida, Committee Chair, on May 21, 2021.
The public is welcome to attend remotely.