Announcing the Final Examination of John Janisch for the degree of Doctor of Philosophy in Physics

Date: March 10, 2026
Time: 12:00 p.m.
Room: PSB 445 (
https://ucf.zoom.us/j/7117301350?pwd=aUhYUGE3UjE2dXVOajVya0EvdEwyUT09)
Dissertation title: Development and application of robust DFT-based machine learned interatomic potentials for simulating and understanding dynamics on solid surfaces and at liquid-solid interfaces.

Abstract:
Machine learning has become an increasingly powerful tool for many aspects of society and everyday life. The application of machine learning to the scientific community, specifically the design of materials at an electronic structure level, is still a rapidly evolving branch of research. Reliable development and production of these machine learning applications is of great importance if physics researchers want to harness the speed and efficiency improvements that machine learning has to offer. This thesis demonstrates some uses of machine learning for physics applications and shows the complexity of some electrocatalysis problems that could be aided by machine learning.

The first subject of this thesis focuses on applications of machine learning to problems inaccessible to typical ab initio methods such as density functional theory (DFT). It is shown that machine learned interatomic potential (MLIP) may explain phenomena in extended systems that are inaccessible with DFT. The DFT-based MLIP that we developed for defect-laden single-layer hexagonal boron nitride simulate grain boundary motion in qualitative agreement with observation, and that developed for the Si(001) surface provides for the first time rationale for the observed temperature dependent metallization of this surface.

The second subject of this thesis covers the study of electrocatalytic environments during chemical reactions. Utilizing grand canonical DFT the electrochemical environment can be studied at different electrode potentials, allowing DFT to more accurately represent the conditions present in experiments. Looking at the carbon dioxide reduction to carbon monoxide on a gold electrode and a molecular catalyst, cobalt phthalocyanine, the effects of alkali and ammonium-based cations are probed. These ab initio simulations reveal that ammonium-based cations improve adsorption and protonation of carbon dioxide, the rate-limiting steps on metal and molecular catalysts, respectively. Finally, there is a discussion and comparison of implicit solvation models for the modeling of electrocatalytic environments with DFT.

Outline of Studies:
Major: Physics

Educational Career:
B. S. Michigan Technological University, 2020

Committee in Charge:
Dr. Talat Rahman (Chair)
Dr. Sergey Stolbov
Dr. Patrick Schelling
Dr. Xiaofeng Feng
Dr. Titel Jurca (External Committee Member)

Approved for distribution by Dr. Talat Rahman, Committee Chair, on March 3, 2026.

The public is welcome to attend.

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