

Announcing the Final Examination of Bushra Ashraf for the degree of Doctor of Philosophy in Physics

Date: March 12, 2026

Time: 1:30 P.M.

Room: BA2 0208 (<https://ucf.zoom.us/j/95215731633?from=addon>)

Dissertation title: FIRST-PRINCIPLES INSIGHTS INTO ELECTRONIC AND MAGNETIC STRUCTURE AT HYBRID INTERFACES AND LOW-DIMENSIONAL MATERIALS AND REACTIONS ON SURFACES

Abstract:

Low-dimensional materials and transition metal surfaces/interfaces provide complementary platforms for understanding how dimensionality, symmetry, spin-orbit coupling (SOC), and interfacial charge transfer/hybridization jointly control electronic structure, emergent magnetism, and surface reactivity. Using first-principles modeling with experimental comparisons, this work aims to establish interfacial structure-property relationships across low-dimensional systems. Strained Pd adlayers on 2H-MoS<sub>2</sub>(0001) provide a controlled platform to separate strain-driven exchange from interface-induced quenching in an itinerant d-electron metal. Although expansive strain promotes magnetism in free-standing Pd, strong Pd-MoS<sub>2</sub> hybridization and charge transfer suppress the monolayer moment and leave a narrow thickness window where magnetism re-emerges in the bilayer. Spin-orbit coupling further reshapes the ground state by driving thickness-dependent magnetic anisotropy and reorientation, showing that the combined effects of strain, symmetry breaking, and interfacial coupling set magnetism. In an analogous interface-chemistry context, molecular interaction with Pt(111) demonstrates how charge redistribution and local bonding control molecular reactivity: N-methylaniline (NMA) switches from low-coverage activation to high-coverage stabilization, and under hydrocarbon coadsorption, ethylidyne acts as an active partner that enables methyl transfer to form N, N-dimethylaniline while stabilizing key intermediates. In the quasi-one-dimensional transition-metal trichalcogenide HfSe<sub>3</sub>, DFT calculations show maintenance of an indirect band gap as thickness increases from monolayer to bulk and reveal SOC-driven valence-band splitting near the Brillouin-zone center. Direction-resolved dispersions quantify pronounced transport anisotropy: carriers are light ( $\sim 0.27 m_e$ ) along the chain direction (in the direction of Hf-atoms) and significantly heavier ( $\sim 1.17 m_e$ ) perpendicular to the chains, consistent with polarization-dependent nano-ARPES results. Orbital- and symmetry-resolved analysis further shows that the lowest-energy optical transition is symmetry suppressed, while the optically allowed onset arises from higher-lying states, explaining the separation between electronic and optical gaps. Overall, this work shows that interfaces are active design elements and that symmetry-aware modeling provides practical levers for tuning electronic, magnetic, and chemical behavior in low-dimensional materials and transition-metal surfaces.

Outline of Studies:

Major: Physics

Educational Career:

B.S. Physics, Quid-e-Azam University, Islamabad, Pakistan

M.Phil. Physics, Quid-e-Azam University, Islamabad, Pakistan

M.S. Physics, University of Central Florida, Orlando, Florida, USA

Committee in Charge:

Dr. Talat S. Rahman (Chair)

Dr. William Kaden

Dr. Sergey Stolbov

Dr. Duy Le

Dr. Fudong Liu (External Committee Member)

Approved for distribution by Dr. Talat S. Rahman, Committee Chair, on February 24, 2026.

The public is welcome to attend.