Announcing the Final Examination of Didarul Alam for the degree of Doctor of Philosophy in Physics

Date: August 29, 2023

Time: 1:00 p.m.

Link: https://ucf.zoom.us/j/93023743014?pwd=emhaZDlhLzFmT1hzT2ZzKzZzcWR4UT09 **Dissertation Title:** Probing Electron Correlations with First-Principles Calculations of The High-Harmonic Spectrum in Solids.

Abstract:

High harmonic generation (HHG) is an extreme non-linear phenomenon where strong laser-field pulses interact with a medium to produce coherent and high-frequency harmonics of the incident light. Since its first observation in solids in 2011, pioneering theoretical studies have already been done and led to the understanding of some of the details of the microscopic mechanism behind this phenomenon in materials, like the role of intra- and inter-band transitions, the contribution of the transition dipole moments to the even and odd harmonic peaks, effects of broken symmetry, etc. However, the role of electron correlation effects in the HHG in strongly correlated materials was much less understood. In this thesis, on the examples of semiconductor ZnO, perovskites BaTiO₃ and BiFeO₃ and transition-metal oxide VO₂ I studied the role of these effects in the high-harmonic (HH) spectra of solids by using time-dependent densityfunctional theory approach with the exchange-correlation kernel obtained with dynamical mean-field theory. As I demonstrate, correlation effects significantly modify the HH spectrum of all systems, in particular through the ultrafast modification of the electronic spectrum in ZnO. In the case of BaTiO₃, correlation effects generate "super-harmonics" - periodic enhancements and suppressions of specific harmonic orders that depend on the correlation strength. In the case of BiFeO₃, the effects of memory in HHG were also analyzed and it was found that they lead to a further extension of the harmonic cutoff. In my final part, I analyzed the HH spectrum of VO_2 , including the case of strongly nonlinear response, and found that the obtained spectrum with correlation-induced higher harmonics is in good agreement with experimental data. Obtained results shed more light on the role of electron correlations in the HH spectrum and the ultrafast dynamics in complex materials and may have applications in modern ultrafast optical and electronic technologies.

Outline of Studies:

Major: Physics

Educational Career:

M.S. University of Central Florida, 2022 M.S. University of Dhaka, 2016 B.S. University of Dhaka, 2014

Committee in Charge:

Dr. Volodymyr Turkowski (Chair) Dr. Michael Chini (Co-Chair) Dr. Luca Argenti Dr. Jayan Thomas (External Committee Member)

Approved for distribution by Volodymyr Turkowski, Committee Chair, on August 07, 2023.

The public is welcome to attend remotely.