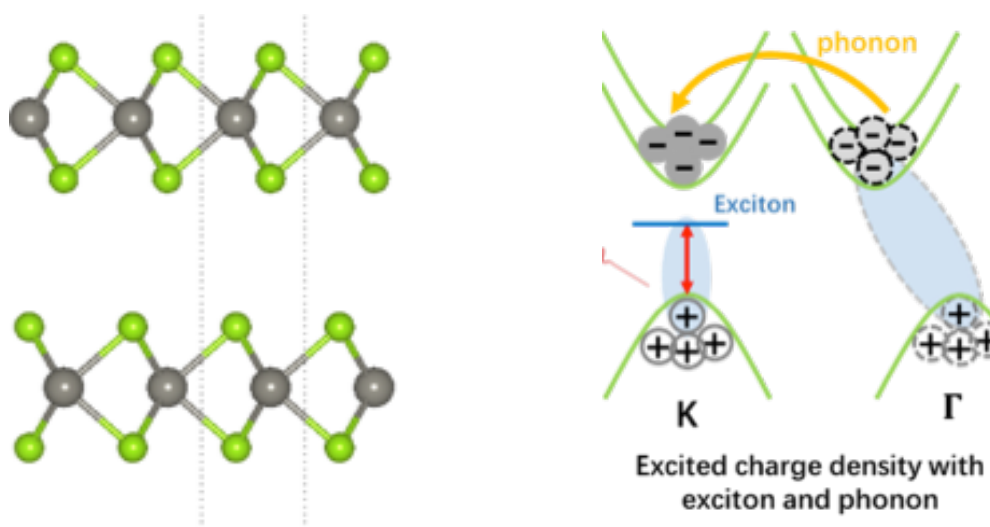




Ultrafast charge and spin dynamics in functional materials: insights from beyond DFT methods

Prof. Dr. Talat S Rahman

Department of Physics, University of Central Florida



Intra- and inter-layer excitons play a dominant role in the ultrafast dynamics and photoemissive properties of transition metal dichalcogenides (TMDs). In this talk, I will present our analysis of the emissive properties of these two types of excitons in bilayer WSe_2 using time-dependent density-functional theory, in the density-matrix representation, combined with many-body theory. I will show that intra- and inter-layer coupling between excitons and charges leads to inter-layer migration of excitons that is reflected in the emission spectrum. While momentum direct (bright) intra- and inter-layer excitons have the largest binding energy the indirect (dark) excitons also contribute to the emission spectrum. We also find phonons to significantly enhance the number of excited excitons by transforming them from intra- to intravalley states with longer decay times. Nonlinear effects such as high harmonic generation will also be discussed. Extension to spin dynamics will be discussed time permitting.