Announcing the Final Examination of Mahtab Ahmad Khan for the Degree of Doctor of Philosophy in Physics

Date: Tuesday, November 21, 2017
Time: 10:00 a.m.
Room: PS 160/161

Dissertation title:
Electronic, optical and magnetic properties of Graphene and single-layer Transition metal dichalcogenides in the presence of defects.

Abstract:
Two-dimensional (2D) materials, such as graphene and single-layer (SL) transition metal dichalcogenides (TMDCs), have attracted a lot of attention due to their fascinating electronic and optical properties. Graphene was the first 2D material that has successfully been exfoliated from bulk graphite in 2004. The discovery of graphene has opened up new horizons in the field of condensed matter physics and material sciences. Especially, charge carriers interacting with the honeycomb lattice of carbon atoms of graphene appear as massless Dirac fermions. Massless quasiparticles with linear dispersion are also observed in surface states of 3D topological insulators and quantum Hall edge states. My first project deals with the two-dimensional Hong-Ou-Mandel (HOM) type interference experiment for massless Dirac fermions in graphene and 3D topological insulators. Since massless Dirac fermions exhibit linear dispersion, similar to photons in vacuum, they can be used to observe the HOM interference intensity pattern as a function of the delay time between two massless Dirac fermions. We show that while the Coulomb interaction leads to a significant change in the angle dependence of the tunneling of two identical massless Dirac fermions incident from opposite sides of a potential barrier, it does not affect the HOM interference pattern. We apply our formalism to develop a massless Dirac fermion beam splitter (BS) for controlling the transmission and reflection coefficients. We calculate the resulting time-resolved correlation function for two identical massless Dirac fermions scattering off the BS.
My further projects deal with single-layer (SL) transition metal dichalcogenides (TMDCs), such as MoS2, WS2, MoSe2 and WSe2, which have recently emerged as a new family of two-dimensional (2D) with great interest, not only from the fundamental point of view, but also because of their potential application to ultrathin electronic and optoelectronic devices. SL TMDCs are direct bandgap semiconductors, which can be used to produce smaller and more energy-efficient devices, such as transistors and integrated circuits. Moreover, the band gap lies in the visible region, which makes them highly responsive when exposed to visible light, a property with potential applications in optical detection. In contrast to graphene, SL TMDCs exhibit large intrinsic spin-orbit coupling (SOC), originating from the d orbitals of transition metal atoms. The presence of considerably high SOC (up to few hundred meV) [5–7] makes them candidate materials for exploring spin physics and spintronic applications. Wafer-scale production of SL TMDCs is required for industrial applications. It has been shown that artificially grown samples of SL TMDCs through various experimental techniques, such as physical vapor deposition (PVD), chemical vapor deposition (CVD), and molecular beam epitaxy (MBE), are not perfect, instead certain type of imperfections such as point defects are always found to be present in the grown samples. Defects compromise the crystallinity of the sample, which results in reduced carrier mobility and deteriorated optical efficiency. However, defects are not always unwanted; in fact, defects can play an important role in tailoring electronic, optical, and magnetic properties of materials. Using Density functional theory we investigate the impact of point defects on the electronic, optical, and magnetic properties of SL TMDCs. First, we show that certain vacancy defects lead to localized defect states, which in turn give rise to sharp transitions in in-plane and out-of-plane optical susceptibilities of SL TMDCs. Secondly, we show that a naturally occurring antisite defect Mo_S in PVD grown MoS2 is magnetic in nature with a magnetic moment of $2\mu_B$, which can be tuned by shifting the position of the Fermi level either by gate voltage or by chemical doping. Thirdly, we argue that the antisite defect Se_W in WSe_2 leads to long lived localized

excited states, which can explain the observed single quantum emitters in CVD grown WSe2 samples, with potential application to quantum cryptography.

Outline of Studies:
Major: Physics

Educational Career:
M. Phil. Quaid-i-Azam University, Pakistan 2008
B. S. University of the Punjab, Pkaistan 2004

Committee in Charge:
Dr. Michael N. Leuenberger (Chair)
Dr. Eduardo Mucciolo
Dr. Hari Saha
Dr. Laurene Tetard (External Committee Member)

Approved for distribution by Dr. Michael N. Leuenberger, Committee Chair, on March 13, 2017.

The public is welcome to attend.