

Spring 2019 Colloquium

Department of Physics & Astronomy, TAMU-Commerce

Feb 7, Thursday, 4-5 PM in Science Building 127

(coffee and cookies will be served at 3:50 PM)

Computational Condensed Matter Physics

Surface and Interface Properties of van der Waals materials

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Dr. Santosh KC earned his B.S. (2003) degree in Physics from Tribhuvan University, NEPAL, and M.S. (2011) and Ph.D. (2014) in Materials Science from University of Texas at Dallas. His research focus was on the computational study of materials for semiconductor devices and energy storage applications. Then, he worked at the Materials Science & Technology Division, Oak Ridge National Laboratory till June 2018. Currently, Dr. KC works as a post-doctoral research associate at the Materials Department, University of California, Santa Barbara. His

overall research focuses on computational Materials Science and Condensed Matter Physics using quantum mechanical computations.

Abstract

Recently, there has been significant research activities on two dimensional (2D) materials after the experimental realization of graphene. Layered transitional metal dichalcogenides (TMDs) have emerged as the potential alternative channel materials for ultra-thin and low power nanoelectronics and opto-electronics devices. Highly tunable and unique electronic properties of TMDs made them promising novel materials for various other applications as well. However, to realize the superior performance of devices based on TMDs, the physical and chemical properties like their defect chemistries and stabilities under various chemical environments need to be understood. To facilitate the experimental efforts, it is important to examine the atomic level insights on the properties of TMDs. In this talk, I will present our research on the defect structures, oxidation, and corresponding electronic properties of TMDs as well as its interfaces, such as semiconductor-dielectric interface and semiconductor-metal contact. Moreover, the impact of various interfacial defects on electronic properties will be discussed, which in fact helps to simulate the realistic interfacial phenomenon and optimize the properties of the semiconducting devices. In addition, I will discuss some efforts in predicting atomic and magnetic properties of 2D magnetic materials and illuminating the importance of van der Waals interaction.