**Topics of Two-Dimensional Materials and Their Heterostructures**

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It has become possible in recent years to fabricate and manipulate two-dimensional nanomaterials in the laboratory that are as thin as one to few atomic layers. The reduced dimensionality gives rise to unique physical and chemical properties that differ from those of traditional bulk materials, and intriguing physical properties have been found in these few-layer systems. Computational studies have played a central role in understanding and predicting these novel properties. In this talk, I will focus on a few representative systems, including graphene systems and monolayers of transition metal dichalcogenides that exhibit properties ranging from charge density waves [1] to the quantum spin-Hall effect [2]. The hybrid system of boron nitride and graphene (*h*-BNC) at low BN doping serves as an ideal platform for band-gap engineering and valleytronic applications. The calculations find a linear dependence of the band gap on the BN concentration at low doping, arising from an induced effective on-site energy difference at the two C sublattices as they are substituted by B and N dopants alternately. In addition, our calculations show that the Moiré patterns in van der Waals heterostructures will modify the local band gap, interlayer interaction, and structural parameters [3-5]. I will also discuss one-dimensional topological insulators manifested in graphene nanoribbons, in which localized spin states may exist at the end or near the junctions. A symmetry protected topological classification is formulated for any type of termination with -quantized Berry phase when summed over all occupied bands.

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