Abstract:
Two-dimensional (2D) van der Waals (vdW) heterostructures have attracted great attention in the past five years. By stacking different 2D materials to bond via the vdW force, these artificial heterostructures provide interesting and new material phase space for exploration. In this talk I shall focus on one aspect of the 2D vdW materials: the Moiré pattern. In visual arts, Moiré pattern is an optical perception of a new pattern formed on top of two similar stacking patterns. In 2D vdW heterostructures, the Moiré pattern is a physical superlattice which brings about novel electronic properties. To theoretically predict the physical properties of the Moiré superlattice, systems containing more than ten thousand atoms often need to be analyzed by first principles. In this talk I shall begin by briefly discussing how one may break the “size limit” so that very large first principles simulations within the density functional theory can be carried out. Afterward, I shall present and discuss some of the calculated novel properties of the Moiré superlattice: the emergence of a secondary Dirac cone, the suppression of the carrier mobility, and the formation of multiple helical valley currents, on various 2D vdW heterostructure materials. Some of these properties can well be the basis of interesting applications.