Ordering and properties of pure and binary two dimensional honeycomb films

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Abstract:

There has been a great deal of interest in two dimensional systems with honeycomb symmetry such as graphene, hexagonal boron nitride (hBN) and molybdenum disulfide. The interest arises from their extraordinary electronic and mechanical properties and the potential for a myriad of electronic device applications.

In this talk I will discuss the development of continuum phase field crystal and related amplitude expansions for modelling these systems and the use of these models to predict the strain induced Moire patterns that form when the films are grown on 111 surfaces and to provide initial conditions for molecular dynamics and density functional calculations. The combined continuum and atomistic approaches are used to calibrate the continuum models and provide predictions for grain boundary and triple junction energies, of misorientation on Moire patterns and the influence of microstructure on thermal conductivity.