

Interlayer coupling in van der Waals heterostructures (KJM/MENA – BSc/MSc)

Two-dimensional (2D) materials can be isolated as individual layers and stacked into artificial van der Waals (vdW) heterostructures that pave the way for a greater range of functionality in materials and devices including flexible electronics and sensors. The adhesion characteristics between 2D materials are not only of fundamental interest for understanding the bonding and properties of heterostructures, but also for the development of fabrication pathways involving transfer by vdW pick-up. While the vdW interactions themselves are principally independent of temperature, thermally induced ripples in 2D materials can give rise to a temperature-dependence in adhesion that is not yet well understood between different types of materials such as graphene, h-BN and MoS₂. The adhesion characteristics will be studied by atomistic modelling and molecular dynamics simulations of vdW heterostructures at different temperatures.

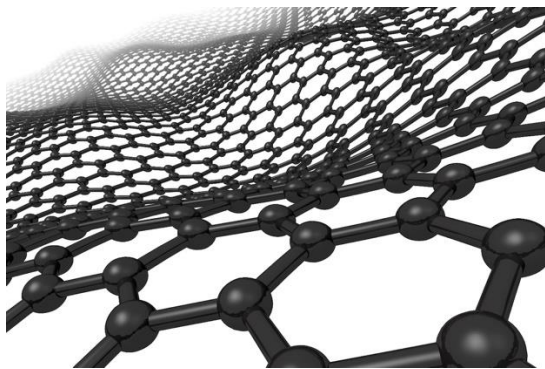


Figure 1: Thermally induced ripples in graphene (newatlas.com).