ABSRACT

Title of thesis: WETTING OF GRAPHENE

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Graphene, a most remarkable 2-D material, has attracted immense attention for its highly non-trivial physical properties making it ideal for a myriad of applications from electronics to biology. Fundamental to several of these applications is the interaction of graphene with water necessitating an understanding of wetting of graphene. Here, molecular dynamics simulations have been employed to understand two fundamental issues of graphene wetting: (a) dynamics of graphene wetting and (b) wetting of graphene nanostructures. The first problem unravels that wetting dynamics of graphene nanodrops is exactly similar to that of standard non 2-D (or non-layered) solids – this is an extremely important finding, given the significant difference in the wetting statics of graphene with respect to standard solids stemming from graphene wetting translucency effect. This same effect, as we show in our second problem, interplays with the roughness effect introduced by nanostructures to trigger graphene superhydrophobicity following a hitherto unknown route.