

Abstract Submitted
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Band-gap engineering in graphene systems for electronic applications SUJATA PAUL, MARCO BUONGIORNO-NARDELLI, NC State University — Ultrathin graphite films including monolayers, bilayers and graphene nanoribbons are intensely studied for the development of future electronic and optoelectronic devices. In this work we will present first principles electronic/phonon structure calculations to elucidate the role of geometry and interactions (electric field, edge functionalization, gating etc.) in the determination of the electronic properties of a wide variety of graphene systems (multi-layers, ribbons etc.). One preliminary objective of this task is to explore ways to accurately control the band gap through the careful design of the active graphitic systems. The coupling between electron and lattice dynamics will be analyzed via the evaluation of the electron-phonon coupling parameters and phonon dispersions calculations. We will discuss the growth of graphene layers on a preferred substrate e.g. SiC and Si. We will identify possible graphene-substrate geometries through first principles calculations and investigate the role of interfacial bonding in the modification and engineering of the band gap.

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