Carbon Based Electronics: A Computational Study

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Abstract

Due to their exceptional electronic, opto-electronic, and mechanical properties,carbon-related materials such as fullerenes, carbon nanotubes (CNTs), and graphene nano-ribbons (GNRs) have been studied extensively in recent years. Computer-aided design tools are needed to explore the physics of CNT- and GNR-based devices and to optimize their performance. Carrier transport in these devices can be described by the non-equilibrium Green's functiontechnique and band-structure by a tight-binding model. The numerical implementation of these models and methods to reduce computation time and memory requirement are discussed. Simulation studies of CNT-FETs, CNT-based photodetectors, and GNR-based heterostructures are presented.