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Electronic Band Structures of Graphene Nanomeshes WILLIAM OSWALD, ZHIGANG WU, Department of Physics, Colorado School of Mines — Owing to its many remarkable properties, graphene is very promising for electronic and opto-electronic applications for size miniaturization and improving performance; however, bulk graphene is a semi-metal with zero band gap, and many methods have been proposed to open up a sizable band gap. In this work, we carry out first-principles calculations based on the density functional theory (DFT) to investigate electronic band structures of graphene nanomeshes (GNMs), the defected graphene containing a high-density array of nanoholes, studying the bandgap opening mechanism and evaluating band gap as functions of structural parameters, including hole size, hole shape, hole-hole distance, and hole arrangement. Our results suggest that while the band gap opening is a result of quantum confinement at nanomesh necks, the size of band gap depends strongly on the detailed GNM structures. For the simplest hexagonal holes, two thirds of GNMs remain semi-metallic and the rest one third are semiconductors.

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