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First-Principles Simulations of Armchair-Edge Graphene Nanostrips. JUNWEN LI, JOHN W. MINTMIRE, Department of Physics, Oklahoma State University, Stillwater, OK 74078., DANIEL GUNLYCKE, CARTER T. WHITE, Chemistry Division, Naval Research Laboratory, Washington, DC 20375. — We have carried out a series of first-principles, local-density functional band structure calculations of finite-width graphene nanostrips with armchair edges. A simple nearest-neighbor tight-binding model predicts that the band structures of these materials should be directly related to those of zigzag single wall carbon nanotubes, with two-thirds of the structures being small gap semiconductors and one-third of the structures being zero gap systems. The band gap in the semiconducting strips would be expected to decrease monotonically with increasing strip width. In our first-principles results, we find that in addition to the zero gap systems becoming finite gap quasimetallic systems because of symmetry breaking (as in the single-walled nanotubes), we also find that the semiconducting strips split into two families with band gaps that deviate from the simple nearest-neighbor tight binding model. Within the framework of our computational results, we compare the band structures of graphene, single-walled nanotubes, graphene nanostrips, and other carbon nanostructures. This work was supported by the US Office of Naval Research and the DoD HPCMO CHSSI program, both directly and through the US Naval Research Laboratory.

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