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first-principles tight-binding study of band gaps in graphene ribbons DANIEL FINKENSTADT, Naval Research Laboratory, GARY PENNINGTON, University of Maryland, CHRIS ASHMAN, HPTi, MIKE MEHL, Naval Research Laboratory — Graphene has recently received much attention for the many interesting physical properties that it exhibits, including light Dirac fermion characteristics of its charge carriers and some experimental evidence of a minimum conductivity, even as the carrier concentration goes to zero. From a practical standpoint, the potential for large carrier mobility in graphene provides an attractive alternative to silicon-based devices, e.g. for field-effect transistors. Theoretical efforts towards designing these devices are focused on determining the geometry and chemistry needed to open up a semiconducting gap in the otherwise semi-metal band structure of a perfect, infinite graphene sheet. Such effects may allow gate control of the electronic conductance as found in semiconducting carbon nanotube devices. Here we use the NRL tight-binding method, which is fit to first-principles calculated data, to study the possibility of opening a gap in graphene by varying strip-width, edge shape with and without termination, and by allowing Peierl's distortion of the edges for narrow ribbons. We compare the tight-binding results with calculations based on the density functional theory.

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