

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Band gaps in armchair-edge graphene nanostrips¹ CARTER T. WHITE, DANIEL GUNLYCKE, Naval Research Laboratory, JOHN W. MINTMIRE, Oklahoma State University — First-principles calculations have shown that all graphene nanostrips terminated with hydrogen atoms exhibit band gaps at the Fermi level. In the case of armchair-edge nanostrips, the calculations contradict a first-nearest-neighbor tight-binding prediction that one third of these nanostrips should be metallic. At the one-electron level, at least two independent causes for the band gaps in these nanostrips have been suggested, namely lattice distortion and long-range interactions. In this presentation, we present theoretical calculations of arbitrary armchair-edge nanostrips. The model, which includes distortion of edge atoms and third-nearest-neighbor interactions, leads to band gaps and band structures which are in good agreement with those obtained from our first-principles calculations.

¹This work was supported by the NRC and ONR through NRL, and at OSU by the DOE EPSCoR program.

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Date submitted: 27 Nov 2007

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