Abstract Submitted
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Edge Phonons of Graphene from Tight-Binding.[1] DANIEL FINKENSTADT, U.S. Naval Academy, Physics Department, N. BERNSTEIN, D. GUNLYCKE, M.J. MEHL, U.S. Naval Research Laboratory, Washington, DC — Edge-states in graphene can affect the band-gap and carrier group velocities in narrow (< 5 nm) graphene nanoribbons. As a first, tight-binding approximation from simple nearest-neighbor hopping, it is shown that armchair nanoribbons have large band-gaps compared to zigzag nanoribbons, which are metallic, unless certain crucial effects are included in the calculation, e.g. magnetic- , quasiparticle- , charge-self-consistent- and/or relaxation- based degeneracy lifting. All of these effects open a small band gap, and the interplay between relaxation and electronic-structure may be examined by calculating the edge phonons of graphene. To this end, we expand on our previous, all-neighbor tight-binding Hamiltonian [*Phys. Rev. B* **76**, 121405(R) (2007)] and include charge self-consistency at the edge of a zigzag nanoribbon. By allowing charge transfer and structural-relaxation at zigzag edges, we are able to remove imaginary phonons and verify the opening of a small band-gap in zigzag ribbons, which is characterized by the phonon density-of-states and normal modes of carbon-hydrogen edge bonds. These calculations are relevant to ribbons cut along non-ideal directions, as well, and we will discuss edge-disorder.

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