Abstract Submitted
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First-principles Helical Elasticity in Carbon Nanotubes[1] H.M. LAWLER, University of Washington, J.W. MINTMIRE, Oklahoma State University, D.A. ARESHKIN, D. GUNLYCKE, C.T. WHITE, Naval Research Laboratory — As an application of a unique, one-dimensional first-principles method with screw-symmetric boundary conditions, we derive a helical elastic tensor, and with it express several fundamental physical quantities of extended quasi-one dimensional, helical systems, including torsional and longitduinal speeds of sound, radial-breathing frequencies, and Poisson's ratio. These quantities are then calculated for nearly every nanotube structure from 0.4 to 1.4 nm, and the results are interpreted through the in-plane elastic response of graphene.

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