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Calculating Young's modulus for a carbon nanotube FERAS ALZUBI, University of Central Florida, RONALD COSBY, Ball State University — Young's modulus for an armchair single-wall carbon nanotube was calculated using an atomistic approach and density functional theory (DFT). Atomic forces and total energies for strained carbon nanotube segments were computed using Atomistix's Virtual NanoLab (VNL) and ToolKit (ATK) software. For a maximum strain of one percent, elastic moduli were calculated using both force-strain and energy-strain data. The average values found for Young's modulus were in the range 1.2 to 3.9 TPa depending on the cross-sectional area taken for the carbon nanotube, consideration of Poisson's ratio, and the calculation method used. Three possible choices of cross-sectional area for the carbon nanotube are discussed and parameter and convergence tests for the DFT computations are described.

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