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Conductance and elastic modulus of a strained carbon nanotube FERAS ALZUBI, University of Central Florida, RONALD COSBY, Ball State University — A first principles atomistic calculation of the electrical conductance for a strained, single-wall metallic carbon nanotube segment containing forty eight atoms and placed between copper electrodes is reported. Density functional theory and a non-equilibrium Green's function technique, encoded in a commercial software package, are used to calculate the electronic structure and current-voltage characteristics for small strains. A monotonic decrease in conductance with strain is predicted. Using force-strain data, a modified Young's modulus is computed for isolated, stretched nanotube segments containing up to 192 atoms. The computational methods, parameters, Poisson ratios, area selections, and results are described.

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