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Is a DNA-Wrapped Metallic Nanotube Still Metallic? S.E. SNYDER, S.V. ROTKIN, Department of Physics, Lehigh University, Bethlehem, PA, email: ses7@lehigh.edu — Modeling suggests that essential changes in electronic band structure can result from the helical wrapping of single-stranded DNA around a single-walled carbon nanotube (SWNT). The metal-to-semiconductor transition of a metallic nanotube is one of many possible changes. As SWNT/DNA hybrids become more popular, it is of great practical importance to determine how the charged backbone of single-stranded DNA may affect SWNT properties. As a first approximation, the change in band structure is modeled by considering the Coulomb interaction with a charged helical wrap. A range of models is developed to address a variety of wrappings of both metallic and semiconducting tubes. Parameters of the model include width, charge profile, and axial and angular displacement of the helix, periodicity along the helix, and, indirectly, chiral angle of the wrap. Band gap changes are shown to be fairly robust for axial and angular shifts of the helix. Trends of the band gap and strength of the potential perturbation with tube diameter and wrapping angle are explored. DNA is just one of several polymers which are presumed to helically wrap SWNTs and thereby disperse SWNTs in solution. Therefore, our study is relevant for electronics applications which require individual nanotubes dispersed via polymer wrapping.

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