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Electronic structure of single-walled carbon nanotubes inside helical DNA wraps STACY SNYDER, SLAVA ROTKIN, Lehigh University — Single stranded DNA can helically wrap a single-walled carbon nanotube (SWNT) leading to changes in electronic structure, which is the subject of our study. Other charged polymers may produce band gap modulation similar to that observed for DNA-SWNT complexes. For these hybrids we assume a regular helical wrap, the potential of which breaks the symmetry of the pristine SWNT. Band structure changes are modeled quantum mechanically using the tight binding method together with self-consistent electrostatics. Gap modulation and band structure symmetry-lowering effects may result in variation of the optical spectra, especially for (slightly forbidden) transverse optical transitions. The effect of environmental screening of charges is investigated. Self-consistent electrostatic calculations yield cohesion energy between a charged, regular wrap and a SWNT of the order of tenths of eV per DNA base [1]. [1] Snyder, S. E., and Rotkin, S. V., Polarization Component of Cohesion Energy in Single-Wall Carbon Nanotube-DNA Complexes, JETP Letters 84, 348 (2006).

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