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Broken Optical Symmetry in DNA-SWNT Hybrids: Spectroscopic Signaling of the Helical Wrap[1]

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Functionalizing single-stranded DNA on a single-wall carbon nanotube (SWNT) has allowed isolating individual tubes, making them soluble, and separating SWNTs according to their chirality. Such strong technological impact motivated our study of the optical properties of the DNA-SWNT hybrids, commonly used now for the solution-based fabrication and experiments. The helicity of the DNA wrap may interfere with the intrinsic Hamiltonian of the SWNT and result in bandstructure modulation. Our modeling predicts a symmetry lowering in the hybrid due to the Coulomb potential of the regular helical wrap of the ionized backbone of the ssDNA, followed by the qualitative changes in the cross- or circularly polarized SWNT absorption spectrum (with no or little change in the parallel polarization). In particular, we predict the appearance of a new peak in the cross-polarized absorption of the ssDNA-SWNT at a frequency lower than that of all allowed transitions in the bare tube. Such effect can be used for optical identification of the wrap at sufficient ssDNA coverage. Wrap signaling happens also via another optical effect, a strong circular dichroism even in the complex with an achiral SWNT, and even at the frequencies where ss-DNA has no absorption features at all. Symmetry of the wrap is central to determine such a circular dichroism of the hybrid. Having in mind that the exact geometry of a DNA wrap for an arbitrary tube is not precisely known yet, we put forward a general model capable of tracking optical effects, varying the parameters of the wrap and/or tube diameter. For various ssDNA backbone helical angles and for various tubes we predict different absorption spectra, though a general qualitative feature of the helical symmetry breaking, the appearance of new van Hove singularities and circular dichroism, must be present.

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