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Mesoscopic Band Gap Engineering in SWNTs: How the Symmetry Affects Electronic Properties

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We discuss mechanisms to control the band gap in carbon single-wall nanotubes (SWNTs) of certain symmetry. One can apply external perturbation, such as electric field, mechanical deformation or a combination of two above, to a pristine semiconductor/metal SWNT. Band structure, e.g., band gap and density of states (DoS) at the Fermi level, will reflect the perturbation. The SWNT symmetry and its doping level determine whether the external perturbation will open the gap (in a metallic NT), increase or decrease the gap (in semiconductor NT). When the perturbation is not uniform along the SNWT a possibility for creating molecular heterojunctions and heterostructures opens. The perturbations considered in the talk range from local electrostatic potentials (that change the electronic structure in a small region) to periodic potentials (that superimpose a periodic perturbation on the lattice potential of the SWNT) to uniform mechanical deformation and polarization. It is important to take into account long-range Coulomb interactions between charge carriers in SWNT because the screening changes the picture for the band gap/DoS modulation.

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