

COMPUTER MODELLING OF THE OPTICAL  
ABSORPTION SPECTRUM OF SINGLE-WALLED  
CARBON NANOTUBE BUNDLES

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S u m m a r y

The computer modelling of the optical absorption of single-walled carbon nanotube (SWCNT) bundles in the approximation of normal distributions of nanotube radii and chiral angles is carried out. The electronic and optical properties of SWCNT bundles are investigated with the use of the Su—Schrieffer—Heeger (SSH) theory under linear electron-phonon coupling. The localized states demonstrate the nonlinear aspects of excited states in SWCNTs. It is found that SWCNTs with different radii have a strong oscillatory dependence of the optical absorption on the incident light energy. A decrease in lengths and the uncapping of nanotube's ends shift the peaks of the optical absorption spectrum to the region of relatively high energies and suppress their height.