Polarized excitons and optical activity in single-wall carbon nanotubes

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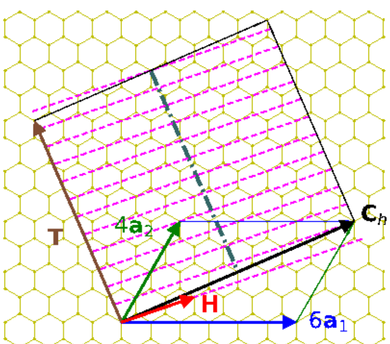
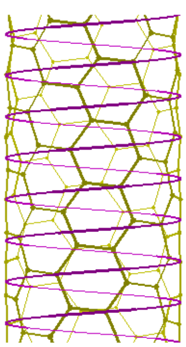
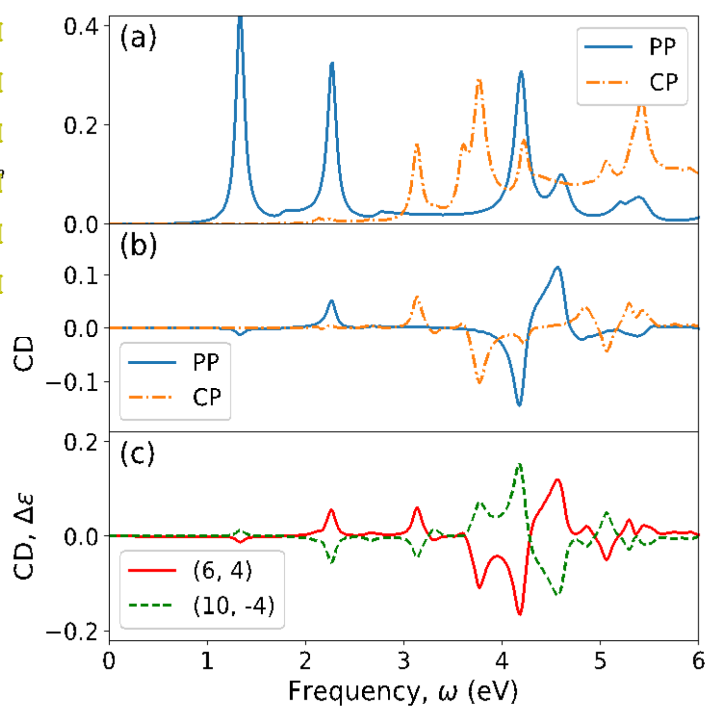
The polarized transitions and optical activity of single-wall carbon nanotubes (SWNTs) are stud- ied theoretically by Pariser-Parr-Pople (PPP) Hamiltonian and excitonic theory. Based on the in- trinsic helical and rotational symmetries, the single-electron energy and properties of a SWNT with arbitrary chirality can be characterized by a helical band structure, which can be solved analytically without considering Coulomb interaction. The dipole-moment matrix elements, magnetic-moment matrix elements, and the selection rules can also be found under the scheme. With the Coulomb interaction included, the absorption and circular dichroism (CD) spectra of SWNTs are calculated by Hartree-Fock approximation and singly-excited configuration interaction. The features of parallel-polarized and cross-polarized excitons in the spectra are then studied. The results are well comparable with the reported experimental spectra. The effects of electron-hole asymmetry and axial magnetic field interaction on the polarized excitons are also discussed. It is found that, the selection rule of cross-polarized transition not only reflects the intrinsic symmetries of SWNTs but also indicates the handedness of the exciton absorption, thus it can be used to analyze the Faraday rotation in the CD spectrum.







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