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Edge states and optical transition energies in carbon nanoribbons[1] JIE JIANG, WENCHANG LU, JERRY BERNHOLC, Center for High Performance Simulation and Department of Physics, North Carolina State University, Raleigh, NC 27695-7518 — The local density of states (LDOS) of edge states and optical transition energies in carbon nanoribbons are investigated with density-functional calculations. The LDOS in either magnetic or non magnetic phases show peaks both below and above the Fermi level. The peaks in the two phases are localized in different energy ranges. Moreover, the LDOS in the two phases have the same decay shapes. The defects at zigzag edges are found to destroy spin-polarization in edge states. They also tend to increase the decay length in edge states by mixing defect and edge states. Thus, the LDOS measured by scanning tunneling spectroscopy shows different features depending on the edge quality. We also find that the optical transition energies E_{ii} are not affected by the spin-polarization. However, edge effects tend to increase E_{ii} values by 1.25/W, where W is the ribbon width. Therefore, the ratios of E_{ii} in nanoribbons for different i are changed from those observed in single-wall carbon nanotubes.

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