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电场对(4, 0)Zigzag模型单壁碳纳米管的影响

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摘要：

The structural and electronic properties of a (4, 0) zigzag single-walled carbon nanotube (SWCNT) under parallel and transverse electric fields with strengths of 0-1.4×10-2 a.u. were studied using the density functional theory (DFT) B3LYP/6-31G* method. Results show tha the SWCNT are dependent on the external electric field. The applied external electric field strongly affects the molecular dipole moments. The induced dipole moments increase linearly with increase in the electrical field intensities. This study shows that the application of p transverse electric fields results in changes in the occupied and virtual molecular orbitals (MOs) but the energy gap between the highest occupied MO (HOMO) and the lowest unoccupied MO (LUMO) of this SWCNT is less sensitive to the electric field strength. The electronic and length of the SWCNT show small changes over the entire range of the applied electric field strengths. The natural bond orbital (NBO) electric charges on the atoms of the SWCNT show that increase in the external electric field strength increases the separation of the ce and negative electric charges of the carbon nanotube.

关键词： Single-walled carbon nanotube Parallel and perpendicular electric field Dipole moment Density functional theory B3LYP

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