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Influence of strain on the work functions of carbon nanotubes investigated by the first-principles method WAN-SHENG SU, National Center for High-performance Computing, Tainan 744, Taiwan, HAN HU, Department of Physics, National Chung Cheng University, Chia-Yi 621, Taiwan — The responses of work functions to uniaxial strain for infinite-length single-walled armchair (AC) [(2,2) and (7,7)], and zigzag (ZZ) [(3,0) and (12,0)] carbon nanotubes (CNTs) are investigated based on density functional theory. It is found that as the strain is increased, the work function of ZZ (3,0) tubes decreases monotonically from 6.2 to 5.7 eV, whereas that of AC (2,2) tubes varies between 4.6 and 4.8 eV in a somewhat complicated manner. As for ZZ (12,0) and AC (7,7) tubes with large diameters, the work functions of ZZ (12,0) change almost linearly from 4.3 to 4.7eV, while for AC (7,7) the work function values grow monotonically from 4.2 to 4.6 eV. Finally, the changes of the energy band give a qualitative understanding of how work function is affected by the uniaxial strain.

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