Strain-induced band gap changes in carbon nanotubes

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First-principles density-functional calculations of the strain-induced band gap changes in moderate-gap single-walled (n,0) carbon nanotubes (SWNTs) are presented. It is confirmed that (n,0) SWNTs fall into two classes depending upon n mod 3 = 1 or 2. Under strain, the two families of semiconducting SWNTs are distinguished by equal and opposite energy shifts for these gaps. For (10,0) and (20,0) tubes, the potential surface and band gap changes are explored up to approximately ±6% strain or compression. For each strain value, full internal geometry relaxation is allowed. The calculated band gap changes are ±(115±10) meV per 1% strain, positive for the mod 1 and negative for the mod 2 family, about 10% larger than the tight-binding result of ±97 meV and twice as large as the shift predicted from a tight-binding model that includes internal sublattice relaxation.