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Interwall interactions and electrical conductance in telescoping carbon nanotubes YONG-JU KANG, Department of Physics, KAIST, YONG-HOON KIM, University of Seoul, KEE JOO CHANG, Department of Physics, KAIST — Telescopically aligned carbon nanotubes, where the inner core shells are pulled out from the house shells with larger diameters in multi-walled nanotubes, are good systems to interwall interactions and their effect on electron conduction. In several tight-binding calculations, there exists some controversy in the quantum conductance of telescoping nanotubes. In this work, using the non-equilibrium matrix Green function approach within the first principles local-density-functional approximation, we study the quantum transport behavior of the (5,5)/(10,10) telescoping nanotube. Varying the hybridized double wall region, we investigate the effect of interwall interactions on the electron transport and compare the results with those obtained from tight-binding calculations. Although individual tubes have two conducting channels at the Fermi level, only one channel gives rise to electrical conduction with antiresonance dips in transmission, while the other channel is suppressed. Thus, the maximum conductance is close to G_0, in contrast to single π-orbital tight-binding calculations, which showed the maximum conductance close to $2G_0$. Our first-principles calculations indicate that the tight-binding model significantly overestimates the interwall coupling between the inner and outer shells.

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