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Single-Wall Gold Nanotubes R. TUGRUL SENGER, Bilkent University, Turkey, SEFA DAG, Oak Ridge National Laboratory, USA, SALIM CIRACI, Bilkent University, Turkey — In recent ultra-high-vacuum transmission-electron-microscopy experiments evidence is found for the formation of suspended single-wall nanotubes (SWNTs) of gold. Similar to carbon nanotubes, the (n,m) notation defines the structure of the gold SWNTs. Experimentally, only the (5,3) tube has been observed to form among several other possible alternatives. Using first-principles calculations we demonstrate that gold atoms can form both freestanding and tip-suspended, chiral, single-wall nanotubes. Although freestanding, infinite (5,5) tube is found to be energetically the most favorable, the experimentally observed suspended (5,3) tube corresponds to a local minimum in the variation of wire-tension with the radius of the structure, which explains the experimental finding. Similarly, we predict the (4,3) tube as a favorable structure yet to be observed experimentally. Analysis of band structure, charge density, and quantum ballistic conductance suggests that the current on these nanotubes is less chiral than expected, and there is no direct correlation between the numbers of conduction channels and helical strands.
[1] R.T. Senger, S. Dag, and S. Ciraci, Phys. Rev. Lett. **93**, 196807 (2004).

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