

An Ab initio investigation of carbon nanotubes with square cross-section

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Resumo

The study of the mechanical properties of nanoscale systems presents new theoretical and experimental challenges. Of particular interest are the structures that do not exist at macroscale but can be formed at nanoscale, especially when significant stress/strain is present. Recently, Lagos et al [Nat. Nanotechnol. 4, 149 (2009)] reported the discovery of smallest metal (silver) nanotube which are formed spontaneously during the elongation of silver nanocontacts. Theoretical investigations suggested that the formation of these hollow structures requires a combination of minimum size and high stress regime. This unexpected discovery of a new family of nanotubes suggests that other "exotic" nanostructures may exist. In this work we have investigated a natural question that arrives from this discovery: "Could Carbon-based nanotube with square cross-section (CNTSC) exist?". In this way, we have carried out ab initio total energy calculation in the framework of density functional theory to study structural stability, and electronic properties of CNTSC tubes. Our results [J. Chem. Phys., in press] show that CNTSCs are at least metastable structures and present metallic properties and could be obtained from direct interconversion from CNT(2,2).