

Abstract Submitted
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Thinnest Insulating and Semiconducting Nanotubes of SiO_x (x = 1 and 2) ABHISHEK SINGH, VIJAY KUMAR, Dr. Vijay Kumar Foundation, 45 Bazaar Street, K. K. Nagar (West), Chennai 600078, India, Institute for Materials Research, Tohoku University, Sendai 9, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University, Sendai 980-8578, Japan — While carbon nanotubes have been extensively studied, nanotubes of inorganic materials are of much interest due to their novel properties. Among these silica nanotubes are of special interest because of their hydrophilic nature, easy colloidal suspension formation, and surface functionalization. Here we show from *ab initio* total energy calculations using ultrasoft pseudopotential plane wave method that nanotubes of SiO_x (x = 1 and 2) can be formed with different diameters and lengths. The optimizations have been performed using conjugate gradient technique within the generalized gradient approximation for the exchange-correlation energy. We have studied finite and infinite nanotubes of SiO_x in triangular, square, pentagonal and hexagonal crosssection. Further we show that for both stoichiometries, the pentagonal nanotubes are energetically most favorable. The bonding nature in these nanotubes is predominantly covalent. The band structure of infinite SiO nanotube shows it to be semiconducting. However, SiO₂ nanotubes are insulating. These are the thinnest possible nanotubes of SiO_x. These nanotubes along could be the ideal circuit element for the nano-electronics.

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