

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Silicon-carbon nano-structures to nano-tubes.¹ M.N. HUDA, LEONARD KLEINMAN, University of Texas at Austin, Austin, Texas 78712, A.K. RAY, University of Texas at Arlington, Arlington, Texas-76019 — There have been continuing efforts to stabilize silicon cage-type nano-structures or nano-tubes which can be used in similar ways as the carbon-based fullerene structures. This is due to the fact that the current semiconductor industries are based on silicon. Silicon carbide is the focus of scientific research due to its potential use even in extreme conditions, such as extreme high-temperature, high-power capabilities and high radiation conditions. In the present study, a set of novel silicon carbon nanostructures (Si_{2n}C_n) in tubular form have been studied which can be extended to form silicon carbide nano-tubes. Generalized gradient approximation to density functional theory has been used with an all electron basis set to study the stability of these structures. A frequency analysis has been performed to ensure that all the frequencies are real. A slight structural shift has been predicted between the hydrogen saturated and -unsaturated nano-tubes.

¹Work supported by the Welch Foundation, Houston, Texas (Grant Nos. F-0934 and Y-1525).

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Date submitted: 26 Nov 2005

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