

Abstract Submitted
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A First Principles Study of Graphitic-Like Structures of SiC¹

MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville — Bulk SiC has many superior inherent properties. These outstanding properties are expected to be enhanced in SiC-based one-dimensional structures. Recently, SiC multiwall nanotubes were synthesized by two experimental groups. However, there is not yet any detailed study on their structures or properties. As a first step towards such studies, we have carried out structural optimization and the calculation of the energetics of SiC graphitic-like structures using the DFT-based VASP. We intentionally started with an initial configuration of buckled SiC graphitic-like sheet to model the possible effect of the dangling bonds associated with Si atoms. To our surprise, the configuration eventually relaxed to a regular flat graphitic-like form. Furthermore, we found that the energy of the relaxed graphitic-like sheet of SiC is only ~ 0.48 eV/atom higher than that of bulk β -SiC, indicating that the presence of carbon atoms in the network indeed has a stabilizing effect on the graphitic-like sheet of SiC. A detailed discussion on the structural and electronic properties of SiC graphitic-like structures will also be presented. This study is expected to pave the way for the understanding of structure and properties of SiC-based nanotubes.

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