

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Evolution of SiC nanoclusters from carbon fullerene: A density functional theoretic study. MUHAMMAD N. HUDA, National Renewable Energy Laboratory, Golden, CO-80401, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, TX-76019 — Formation of SiC fullerene type structures is still an unsolved issue as there is no experimental confirmation reported so far regarding their existence. However, theoretical research results are available in the literature where carbon fullerenes were taken as a base model for SiC fullerene type structures. In this presentation, we show by a systematic study on C₂₀ fullerene based SiC structures that this approach may not always reproduce the ground state structures; rather, the energetically favorable structure based on C₂₀ could be highly distorted and open structures. In general, Si atoms tend to cluster on the C₂₀ base structures. We observed a very systematic linear trend in the evolution of binding energies of SiC clusters from carbon fullerene and a detailed set of results on the electronic and geometric structures of these clusters will be presented.

Muhammad N. Huda
National Renewable Energy Laboratory, Golden, CO-80401

Date submitted: 02 Dec 2007

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