

Abstract Submitted
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A Hybrid Density Functional Study of Capped Silicon Carbide Nanotubes¹ KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A systematic study of fullerene hemisphere capped finite SiC nanotubes of type 1 using cluster approximation is presented. Nanotubes (3,3) and (5,0) are capped by C₂₀-fullerene hemisphere(C₁₀) and (5,5) and (9,0) are capped by C₆₀-fullerene hemisphere (C₃₀). Geometries of the tubes have been spin optimized using the functional B3LYP, 3-21G* basis set and the GAUSSIAN 03 software. The study indicates that fullerene capping of a SiC nanotube changes the electronic and geometric structure properties of SiC nanotubes. For example, the binding energy per atom for infinite nanotube (5,5) is 4.993eV whereas the same nanotube with C- and Si-caps has the binding energy per atom of 5.989eV and 4.812eV, respectively. C-capped nanotubes are energetically more preferable compared to Si-capped. The HOMO-LUMO gaps of the capped nanotubes are significantly lower compared to those of infinite nanotubes.

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