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A Nanocluster Based Study of Silicon Carbide Nanocones: Existence and Stability[1] KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A systematic study of silicon carbide nanocones of different disclination angles and different tip geometries using the finite cluster approximation is presented. The geometries of the nanocones have been spin optimized using the hybrid functional B3LYP (Becke's three-parameter exchange functional and the Lee-Yang-Parr correlation functional) and the all electron 3-21G* basis set. The study indicates that the binding energy per atom or the cohesive energy of the nanocones depends not only on the size of the nanocones but also on the disclination angle of the nanocones. The electronic properties of nanocones depend on disclination angles, size of the nanocone clusters and the edge structure of the nanocones. Given similar cluster size, silicon carbide appears to favor tubular structures over two dimensional graphene-like structures. For relatively smaller clusters the B.E./atom oscillates in all cases except in nanocones of disclination angle 300°. This indicates the greater stability of nanocones of some particular size as compared with its neighboring sizes. A study of binding energies, NBO charge, density of states and HOMO-LUMO gaps has been performed for all nanocones from disclination angles of 60° to 300°.

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