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A Hybrid Density Functional Study of Zigzag SiC Nanotubes.[1]
KAZI ALAM, ASOK RAY — Using *ab initio* hybrid density functional theory based calculations, we report here the electronic and geometric structure properties of *three* different types of single-walled zigzag silicon carbide nanotubes from (3,0) to (11,0). Our calculations show type 1 structures to be most stable, with the cohesive energies of the newly proposed type 3 nanotubes intermediate between type 1 and type 2. For all nanotubes, Si atoms moved outward after relaxation making two concentric cylinders of Si and C atoms. The HOMO-LUMO ("band") gaps for type 1 and type 2 nanotubes show an oscillatory pattern as the tube diameter increases but for type 3, the gap decreases monotonically with increasing tube diameter. All the tubes studied here appear to have triplet ground states except for type 1 (3, 0). It is expected that these tubes with significant surface reconstructions, varieties of band gaps, and magnetic properties would have interesting and important applications in the field of band gap engineering and molecular electronics.

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