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A hybrid density functional study of double walled armchair SiC nanotubes[1] KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas Arlington — As a continuation of our studies of single walled SiC nanotubes,[2] we report here a systematic study of double walled armchair type1 SiC nanotubes using the finite cluster approximation. The geometries of smaller armchair SiC nanotubes inside bigger armchair nanotubes have been spin optimized using the hybrid functional B3LYP (Becke's three-parameter exchange functional and the Lee-Yang-Parr exchange-correlation functional) and the Los Alamos National Laboratory double-ζ basis set as implemented in the GAUSSIAN 03 suite of programs. The results have been compared with published experimental and theoretical results in the literature on single walled and multi walled SiC nanotubes. A detailed study of binding energies, Mulliken charges, density of states and HOMO-LUMO gaps has been performed for type 1 SiC nanotube from (n,n)@(n+3,n+3) to (n,n)@(n+5,n+5) (n=3-7). Results on radial buckling and optimized diameter will also be reported to study and compare inter wall interactions between the two coaxial SiC nanotubes. Possibilities of work on other types of SiC nanotubes currently underway in our group will also be discussed.

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[2]K. Alam and A. K. Ray, Nanotechnology, **18**, 495706 (2007); Physical Review B, **77**, 035436 (2008).

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