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Anomalous dependence of band gaps of binary nanotubes on diameters[1] KAPIL ADHIKARI, MUHAMMAD HUDA, ASOK RAY, Department of Physics, University of Texas at Arlington — Using cluster approximation, AlN, BN, GaN, SiGe, SiC, and GeC armchair type 1 nanotubes have been spin optimized using the hybrid functional B3LYP, a double ζ basis set and the GAUSSIAN 03 software. The electronic structures of group III nitride and group IV-IV nanotubes indicate that the band gap increases with tube diameter contrary to behavior expected from quantum size effects. A detailed study indicates that, in a class of binary nanotubes with partial ionic contributions in the bonds, for example, AlN, BN, GaN, GeC, and SiC, ionicity of the bonds decreases as diameter decreases due to increased sp^3 contribution. This causes the band gap to increase with diameter. But in nanotubes with covalent bonding, for example SiGe, the gap decreases with diameter. A general trend for a class of binary nanotubes is established.

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