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Biphenylene Based SiGe Nanoribbons:An ab-initio Study PRABATH WANAGURU, ASOK K. RAY, The University of Texas at Arlington — A study of four types of biphenylene based SiGe nanoribbons had been performed using the cluster approximation. Full geometry and spin optimizations were performed without any symmetry constraints using the hybrid functional B3LYP, an all electron 6-311G**//3-21G* basis set and the GAUSSIAN 09 suite of software. First phase of the calculations were carried out by keeping constant width (14 Å) and varying length (12-120 Å) for the nanoribbons. It is found that armchair type nanoribbons have higher saturation HOMO-LUMO gap (1.0 eV) compared to zig-zag like (0.2 eV) nanoribbons. Cohesive energy of the nanoribbons had increased with the length and saturated around 2.8 eV, for both armchair and zig-zag like types. In the second phase, we have doubled the width of nanoribbons and found that the HOMO-LUMO gap had decreased almost in half. Moving from smaller width to a larger width, ribbons were showing more of a sheet like character. We will present, in detail, cohesive energies, HOMO-LUMO gaps, density of states, and the bonding nature of Si and Ge atoms within the nanoribbons.

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