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Carbon Nucleation from ring seeds on Icosahedral Fe_{13}[1] ANTENEH TEFERA, MOGUS MOCHENA, Florida A&M University — Using ab initio molecular dynamics calculation, we computed the initial stages of carbon nanotube growth from ten – atom carbon rings on icosahedral Fe_{13}. The carbon ring interacts with Fe_{13} to form a zigzag structure due to a mismatch between the number of atoms on the ring and the atoms on the pentagonal ring of Fe_{13}, with formation energy of 2.2 ev. A mixture of carbon dimers and carbon atoms interact with the Fe_{13} + C_{10} structure to yield a tubular structure with the lowest energy. Another configuration of carbon atoms distributed in the vicinity hexagonal lattice sites interacts with Fe_{13} + C_{10} structure to form also a tubular structure that is almost degenerate in energy to the ground state. The results indicate that the icosahedral symmetry of the Fe_{13} with its magnetic moment almost intact is retained whenever the tubular structure is formed.

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