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Ab Initio Investigation of the Structures of Fe-Doped Carbon Clusters CHRISTELLA LOVATO, CLIFTON BROWNRIGG, AJIT HIRA, Northern New Mexico College — We continue our interest in the theoretical study of carbon clusters to examine the effects of the doping of small carbon clusters (C_n, n = 2 - 15) with iron atoms. This work applies the hybrid ab initio methods of quantum chemistry to derive the different Fe_mC_n (m = 1-3) geometries. Of particular interest are linear, fan, and cyclic geometries. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Exploration of the singlet, triplet, quintet, and septet potential energy surfaces is performed. The type of bonding in terms of competition between sp^2 and sp^3 hybridization is examined, with a view to addressing the possibility of the stabilization of the doped carbon nano-particles in a diamond type structure. The potential for the existence of new pathways to the fabrication of nanotubes is explored.

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