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Novel Silicon-Carbon Nanostructures: A DFT Study on the Stability of $Si_{60}C_{2n}$ (n= 3, 10, 12) Clusters.[1] A. SRINIVASAN, University of Texas at Arlington, M.N. HUDA, University of Texas at Austin, A.K. RAY, University of Texas at Arlington — In this work, we extend our previous work on $Si_{60}C_{2n}$ (n=1, 2) clusters by the addition of six, twenty and twenty-four carbon atoms on the surfaces of the Si_{60} cages by substitution and inside the cage at various symmetry orientations [1]. The theoretical formalism used is the generalized gradient approximation to density functional theory and full geometry and spin optimizations have been performed using the Gaussian 03 software. For the silicon atom, the Hay-Wadt pseudo-potential with the associated basis set is used for the core and the valence electrons, respectively. For the carbon atom, the Dunning/Huzinaga double zeta basis set is employed. Different electronic properties of these nanostructures will be discussed in detail. The binding energy per atom for these nanostructures increases with the number of carbon atoms, with the structures having carbon atoms on the surface being more stable. The stability of the nanostructures depends on the orientation of the carbon atoms, as well as on the natures of Si-C and C-C bondings. [1] A. Srinivasan, M. N. Huda and A. K. Ray, Phys. Rev. A, in press; A. Srinivasan and A. K. Ray, J. Nanosci. and Nanotech., in press.

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