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Novel Silicon-Carbon Nanostructures: Electronic structure study on the stability of Si60C2n Clusters. A. SRINIVASAN, M.N. HUDA, A.K. RAY, The University of Texas at Arlington — The formalism of generalized gradient approximation to density functional theory has been used to study the electronic and geometric structures of $Si_{60}C_{2n}$fullerene-like nanostructures. In our previous work, we have shown that the additions of carbon atoms increase the stability of smaller silicon cages [1]. In this talk, we will present our results on the addition of two and four carbon atoms on the surface of the Si_{60} cages by substitution as also inside the cage at various symmetry orientations. Full geometry optimizations have been performed using the Hay-Wadt basis set without any symmetry constraints using the Gaussian 03 suite of programs [2]. Binding energies, ionization potentials, electron affinities and the "band" gaps of the stable silicon-carbon fullerene like nanostructures will be presented and discussed in detail. In general, we find that the optimized silicon-carbon fullerene-like cages have increased stability compared to the bare Si_{60}cage. Possibilities of adding larger carbon clusters to the Si_{60}structure will also be discussed. *Work supported, in part, by the Welch Foundation, Houston, Texas (Grant No. Y-1525). [1] M. N. Huda and A. K. Ray, Phys. Rev. A **69**, 011201(R) (2004); Eur. Phys. J. D **31**, 63 (2004). [2] *Gaussian 03*, M. J. Frisch *et al.* Gaussian Inc., Pittsburgh, PA.

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