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Theoretical Study of Stabilization of Fullerene-like Silicon Cages
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— We extend our work on fullerenes[1], by exploring the stabilization of fullerene-like silicon cages through intercalation of carbon atoms. *Ab initio* theoretical techniques are used to derive the physical and chemical properties of various $(Si_{60})_m C_n$systems (m = 1-3, n =1-10). The first phase of our investigation focuses on endohedral and exohedral complexes of a single $Si_{60}$with$C_n$clusters. Electron correlation effects are incorporated using both Many Body Perturbation Theory (MBPT) and Density Functional Theories (DFT). The second phase of the investigation examines the interactions of the fullerene-like silicon "super molecules" with the small carbon clusters. The properties discussed will include bondlengths, ground-state energies, optimum absorbate distances, dissociation channels, and dissociation energies are presented. Possibilities exist for applications in silicon-based electronics at the nano scale.

1. A. S. Hira and A. K. Ray, Phys. Rev. **A 52**, 141(1995); **A 54**, 2205(1996).

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