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What is the Goundstate Structure of Intermediate-sized Carbon Clusters? M. YU, I. CHAUDHURI, C.S. JAYANTHI, S.Y. WU, Univ. of Louisville — Recent study on the equilibrium structures of quantum dots of tetravalent semiconductors such as Si clusters revealed that the ground state structures of these clusters with diameters d<5 nm are icosahedrons comprising of tetrahedral building blocks rather than corresponding bulk-truncated clusters[1]. Among tetravalent semiconductors, carbon is the only element whose atoms could form sp, or sp^2 or sp^3 bonding configurations, leading to compact, fullerene, and bucky-diamond clusters[2]. It is then natural to raise the question as to what is the ground-state structure for the carbon cluster C_n for a given $n \geq 20$? We have recently initiated a preliminary study on the relative stability of carbon clusters C_n with $n$up to 700, using a molecular dynamics scheme based on a self-consistent and environment-dependent Hamiltonian developed at the U. of Louisville in the framework of the linear combination of atomic orbitals[3]. Our preliminary result indicates that in the range of n studied, the carbon fullerene clusters are still the most stable clusters, in contrast to the icosahedral cluster being the ground state structure for a series of discrete n values for the other tetravalent clusters. We will also discuss the other electronic properties of intermediate-sized carbon clusters. This work was supported by the U.S. DOE (DE-FG02-00ER4582). [1] Y. Zhao, *et al.,* Phys. Rev. Lett. **93**, 015502 (2004). [2] J. Y. Raty, *et al.,* Phys. Rev. Lett. **90**, 037401 (2003). [3] S.Y. Wu, *et. al.*, *Handbook of Materials Modeling* Vo.**l,** p.2935 (2005).

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