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Small World Carbon Nanomaterials: Density Functional Theory Simulations[1] JEREMY YANCEY, MARK NOVOTNY, Dept. of Physics and Astronomy, Mississippi State University, STEVEN GWALTNEY, Dept. of Chemistry, Mississippi State University — The possible existence of small, pure carbon molecules based on physical small-world networks is addressed using density functional theory calculations. A ring of atoms with one or more small-world connections between pairs of non-nearest-neighbor sites was chosen for the network topology. The small-world connections are made with and without additional carbon atoms placed along the link. The energy per atom of these small-world carbon systems is compared with benchmark carbon clusters such as the C_{20} ring, bowl, and cage isomers, the C_{60} Buckyball, monocyclic pure carbon rings ranging from C_4 to C_{60}, bare linear carbon chains ranging from C_2 to C_{48}, fullerenes ranging from C_{20} to C_{60}, and various all-carbon graphitic fragments. The energy per atom results for these materials provides an indication that some of these pure-carbon small-world nanomaterials are reasonable for real world synthesis.

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