Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Building Physical Carbon Nanoparticles from Small-World Networks: Density Functional Theory Calculations JEREMY A. YANCEY, M.A. NOVOTNY, Mississippi State University Dept of Physics and Astronomy, HPCC Center for Computational Sciences, STEVEN R. GWALTNEY, Mississippi State University Dept of Chemistry, HPCC Center for Computational Sciences — We have performed B3LYP/6-31G* Density Functional Theory calculations on carbon cluster nanoparticles built with (pseudo) small-world network topologies to determine whether they are stable and can exist in nature. Such particles may have novel material properties due to their (pseudo) small-world nature [1]. We have embedded a ring of carbons with one or more small-world connections made with and without additional carbon atoms. No carbon is allowed to make more than four bonds. The energy per atom of these (pseudo) small-world carbon systems is compared with benchmark carbon clusters including monocyclic rings, linear rods, graphene fragments, and various fullerenes from C_{20} to C_{60}. The energy per atom and vibrational frequency calculation results for these materials indicate that there are pure-carbon small-world nanomaterials that are reasonable for real world synthesis. We present both NMR and IR spectra for these nanoparticles. [1] M.A. Novotny, *et al*, J. Appl. Phys, **97**, 10B309 (2005).

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Date submitted: 20 Nov 2007 Electronic form version 1.4