Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Systematic Enumeration of sp^3 Nanothreads and Computational Study of their Properties ENSHI XU, PAUL E. LAMMERT, Department of Physics, Pennsylvania State University, VINCENT H. CRESPI, Department of Physics, Material Science and Engineering and Chemistry, Pennsylvania State University — A novel 1D allotrope of carbon arise from slow decompression of solid benzene in high-pressure (GPa) cells, wherein columns of benzene, guided by "topochemical" constraint as six-valent 1D super-atoms, rehybridize into a crystal of sp^3 nanothreads. We exhaustively enumerate the allowed hexavalent bonding topologies and discovered several new low-energy allotropes not previously described. The intermediate conformational nature of these systems – stiffer than a polymer, more reconfigurable than a nanowire or nanotube – allows the translational repeat unit for interatomic connectivity ("topological unit cell") to deviate from the crystallographic unit cell. A topological unit of 12 carbons accommodates thirty-seven distinct chemically stable nanothreads, fourteen of which are within 80 meV/carbon of the most stable member. Careful optimization of aperiodic helicity reveals the most stable structures to be chiral; several are stiffer (per carbon atom) than bulk diamond. They have the large gaps of saturated hydrocarbons, but reasonable routes exist towards producing semiconducting variants. We generalize Euler's rules for ring counting to cover these systems, and propose a naming convention that can be generalized to handle a broad range of pregenitor molecules.

Enshi Xu
Department of Physics, Pennsylvania State University

Date submitted: 14 Nov 2014 Electronic form version 1.4