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Structural stability of clean, passivated, and partially dehydrogenated cuboid and octahedral nanodiamonds up to 2 nanometers in size

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Abstract

The use of precisely applied mechanical forces to induce site-specific chemical transformations is called positional mechanosynthesis, and diamond is an important early target for achieving mechanosynthesis experimentally. The next major experimental milestone may be the mechanosynthetic fabrication of atomically precise 3D structures, creating readily accessible diamond-based nanomechanical components engineered to form desired architectures possessing superlative mechanical strength, stiffness, and strength-to-weight ratio. To help motivate this future experimental work, the present paper addresses the basic stability of the simplest nanoscale diamond structures-cubes and octahedra-possessing clean, hydrogenated, or partially hydrogenated surfaces. Computational studies using Density Functional Theory (DFT) with the Car-Parrinello Molecular Dynamics (CPMD) code, consuming ~1,466,852.53 CPU-hours of runtime on the IBM Blue Gene/P supercomputer (23 TFlops), confirmed that fully hydrogenated nanodiamonds up to 2 nm (~900-1800 atoms) in size having only C(111) faces (octahedrons) or only C(110) and C(100) faces (cuboids) maintain stable sp 3 hybridization. Fully dehydrogenated cuboid nanodiamonds above 1 nm retain the diamond lattice pattern, but smaller dehydrogenated cuboids and dehydrogenated octahedron nanodiamonds up to 2 nm reconstruct to bucky-diamond or onion-like carbon (OLC). At least three adjacent passivating H atoms may be removed, even from the most graphitization-prone C(111) face, without reconstruction of the underlying diamond lattice. Copyright © 2011 American Scientific Publishers.

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Keywords

Bucky-Diamond, Carbon, Cuboid, Dehydrogenation, DFT, Diamond, Dimerization, DMS, Fullerene, Hydrogen, Mechanosynthesis, Nanodiamond, Nanotechnology, Octahedron, OLC, Reconstruction, Stability