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Structural stability of clean and passivated nanodiamonds having ledge, step, or corner features

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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 nanoscale diamond structures with clean or hydrogenated surfaces that possess certain simple features including ledges, steps, and corners. Computational studies using Density Functional Theory (DFT) with the Car-Parrinello Molecular Dynamics (CPMD) code, consuming~2,284,108.97 CPU-hours of runtime on the IBM Blue Gene/P supercomputer (23 TFlops), confirm that fully hydrogenated nanodiamonds 1-2 nm in size possessing ledges with various combinations of convex or concave edgelines where any two of the three principal diamond faces meet will maintain stable sp 3 hybridization.

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Keywords

Carbon, Corner, Cuboid, DFT, Diamond, DMS, Ledge, Mechanosynthesis, Nanocarbon, Nanodiamond, Nanopart, Nanotechnology, Octahedron, Reconstruction, Stability, Step