

Abstract Submitted  
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**Ab Initio Simulations of Nano-Diamond Surface Reconstruction**

WILLIAM MATTSON, RADHAKRISHNAN BALU, US Army Research Laboratory — We have simulated with in the Density Functional Theory (DFT) spherically cut nano-diamonds from bulk diamond at ambient conditions. The 2.6 nanometer diameter sphere is then allowed to relax at 250K and surface reconstruction is observed. Four hemispherical fullerene like regions form on the surface and while the interior maintains the diamond structure, it undergoes compression equivalent to over 30GPa in the bulk. Results of dynamic shearing will be presented.

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