Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Is Orthorhombic C32 Actually a New Metastable Allotropic Form of Carbon? TAYLOR JUST, U. S. Naval Academy, MICHAEL MEHL, Naval Research Laboratory, DANIEL FINKENSTADT, U. S. Naval Academy, STEVEN RICHARDSON, Howard University — Carbon hybridizes in different geometries (sp, sp^2, and sp^3) forming a number of well-known allotropic forms such as: cubic diamond, graphite, C_{60}, graphene, hexagonal diamond, and amorphous carbon. With the advent of novel computational optimization tools many other candidate allotropic forms for carbon (e.g. monoclinic M-carbon, body-centered tetragonal C4 carbon (bct-C4), orthorhombic W-carbon, and Z-carbon) have been proposed which might be metastable at high pressures. In fact, the M-carbon structure has been experimentally seen with Raman spectroscopy. Recently, Zhang *et al.*[1] have reported the theoretical existence of a new allotropic form of carbon which they named: orthorhombic C32. In this work we have discovered that orthorhombic C32 is actually **not** a novel carbon allotropic form of carbon, but it is simply hexagonal diamond decorated with defect planes separated by arbitrary distances. We have used first-principles DFT calculations to compute the energies and phonon spectra for these structures and compared our results with an extensive library of other possible metastable allotropic forms of carbon from the literature.

[1]M. Zhang, H. Liu, Y. Du, X. Zhang, Y. Wang, and Q. Li, *Phys. Chem. Chem. Phys.* **15,** 14120 (2013).

Steven Richardson
Howard University

Date submitted: 15 Nov 2013 Electronic form version 1.4