

Abstract Submitted
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Symmetry Breaking and Low-energy Vibrations in Amorphous Graphene YUTING LI, DAVID DRABOLD, Department of Physics and Astronomy, Ohio University, CONDENSED MATTER AND SURFACE SCIENCE TEAM — Crystalline graphene is one of the hottest topics in condensed matter science. Recent experiments revealed the existence of amorphous graphene introduced by electron radiation. Here we explore computationally the electronic, structural and vibrational properties of amorphous graphene using the Wooten-Weaire-Winer models due to Kumar and Thorpe. These models are flat and contain both even and odd-member rings. A density functional study shows the odd-member rings changes the electronic structure near the Fermi level. And carbon pentagons induce local curvature, thus breaking the planar symmetry in analogous with fullerenes [1]. Systematically exploring the inherent structures shows the puckered states are more stable and occupy deeper basins on the potential energy landscape. The vibrational modes and spectra provide evidence that one might detect the presence of amorphous graphene from a vibrational signature. We also discuss the imaginary modes indicating the evolution from flat to puckered states and very low energy conformational fluctuations reminiscent of floppy modes [2].

[1] Y. Li, F. Inam, A. Kumar, M. Thorpe, and D. A. Drabold, Phys. Status Solidi B 248, 2082 (2011)

[2] Y. Li, D. A. Drabold, Phys. Status Solidi B. doi: 10.1002/pssb.201248481(2012).

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