Abstract Submitted
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A Theoretical Analysis of the Effect of the Hydrogenation of Graphene to Graphane on Its Mechanical Properties[1] Q. PENG, CHAO LIANG, WEI JI, SUVRANU DE, Rensselaer Polytechnic Institute — We investigated the mechanical properties of graphene and graphane using first-principles calculations based on density-functional theory. A conventional unitcell containing a hexagonal ring made of carbon atoms was chosen to capture the finite wave vector "soft modes", which affect the the fourth and fifth elastic constants considerably. Graphane has about 2/3 ultimate strengths in all three tested deformation modes – *armchair*, *zigzag*, and *biaxial*– compared to graphene. However, graphane has larger ultimate strains in *zigzag* deformation, and smaller in *armchair* deformation. We obtained the second, third, fourth, and fifth order elastic constants for a rigorous continuum description of the elastic response. Graphane has a relatively low in-plane stiffness of 240 N/m which is about 2/3 of that of graphene, and a very small Poisson ratio of 0.078, 44% of that of graphene. The pressure dependence of the second order elastic constants were predicted from the third order elastic constants. The Poisson's ratio monotonically decreases with increasing pressure.

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