Tuning the Poisson Ratio of Porous Graphene by Defects

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Introduction

Schwarzites, negative Gaussian curvature analogs of Fullerenes, are made up of sp2-hybridized carbon atoms. The negative Gaussian curvature of Schwarzites is due to the introduction of heptagonal and octagonal rings of carbon in the graphenic lattice. Schwarzites show a rich variety of physical and electronic properties, being semiconductors, insulators or metals, besides of having a high surface area.

$$\iint K dS = 4\pi(1-g) = 2\pi\chi$$

$$F - E + V = \chi$$

$$2N_4 + N_5 - N_7 - 2N_8 = 12(1-g)$$
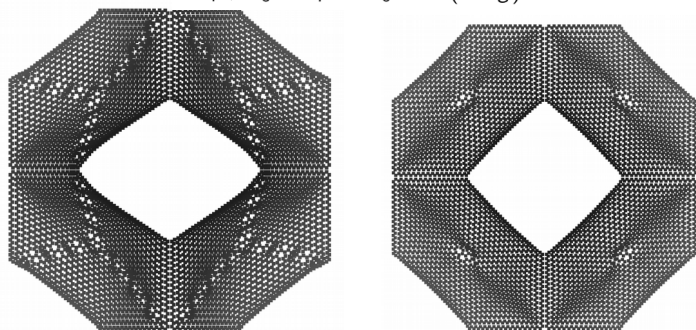
Methods:

Using molecular dynamics (MD) simulations we have studied the role that Stone-Thrower-Wales (STW) defects have on giant Schwarzites.
MD simulations were performed using the software package LAMMPS. The system was initially relaxed and consequent Deformations were performed on the system in order to obtain the matrix of elastic constants.
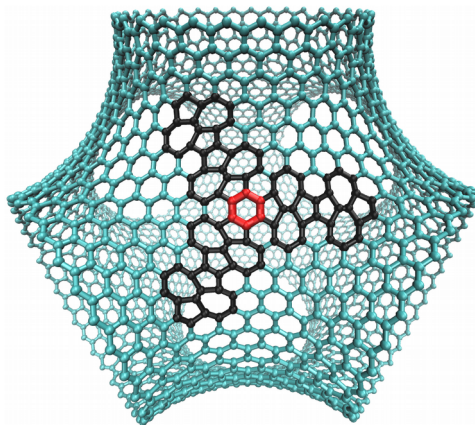For our calculations we used the AIREBO (2000) potential. Simulations were run in vacuum.
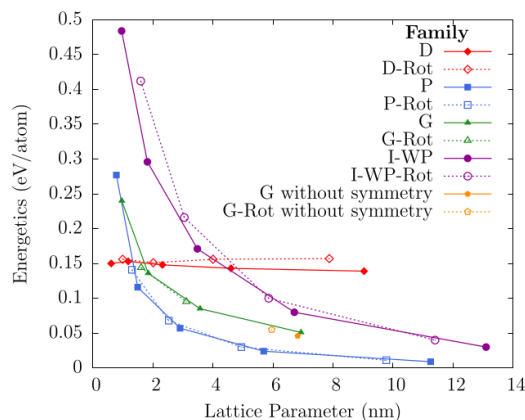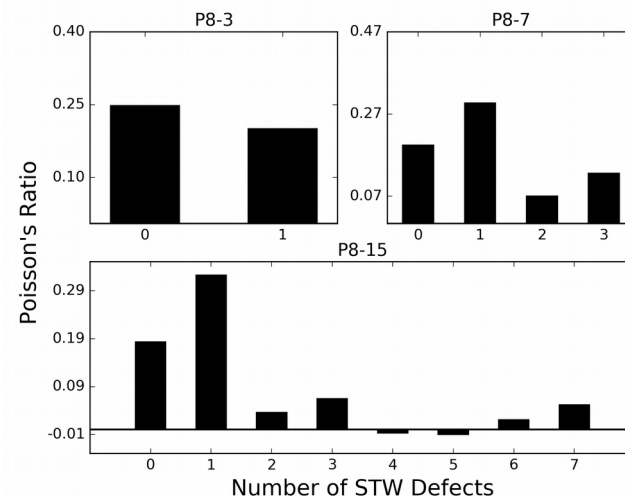

D.C. Miller et al. Carbon 96(2016) 1191-1199.

The primitive surface family is the most stable (energetically) structure from the possible Schwarzite families.

STW Defects

Results from TPMS with STW Defects

Introduction of STW defects decreases the lattice parameters. The Poisson ratio decreases up to a certain number of defects. If the local curvature of the structure increases too much the Poisson ratio Increases as well.

Poisson ration ~ Transverse strain / Axial strain

References:

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3. H. Terrones, A. Mackay, The geometry of hypothetical curved Graphite structures, Carbon 30 (8) (1992) 1251-1260.
4. S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995).