

# Supporting Information

## Peculiar pressure effect on Poisson ratio of graphene as a strain damper

Qing Peng,<sup>\*,†</sup> Albert K. Dearden,<sup>‡</sup> Xiao-Jia Chen,<sup>¶</sup> Chen Huang,<sup>‡</sup> Xiaodong  
Wen,<sup>§</sup> and Suvaranu De<sup>†</sup>

*Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic  
Institute, Troy, NY 12180, U.S.A.*

*, Department of Scientific Computing, Florida State University, Tallahassee, FL, 32306,  
U.S.A., Center for High Pressure Science and Technology Advanced Research, Shanghai  
201203, China.*

*, and State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese  
Academy of Sciences, Taiyuan, 030001, China; Synfuels China Co. Ltd. Huairou, Beijing,  
China, 101407*

E-mail: qpeng.org@gmail.com

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\*To whom correspondence should be addressed

<sup>†</sup>Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, U.S.A.

<sup>‡</sup>Department of Scientific Computing, Florida State University, Tallahassee, FL, 32306, U.S.A.

<sup>¶</sup>Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China.

<sup>§</sup>State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, China; Synfuels China Co. Ltd. Huairou, Beijing, China, 101407

## Atomic structure

We optimized the equilibrium lattice constant for graphone. The total energy as a function of lattice spacing was obtained by specifying seven lattice constants varying from 2.50 Å to 2.56 Å, with full relaxations of all the atoms in the unit cells containing six carbon atoms and three hydrogen atoms. A least-square fit of the energies versus lattice constants with a fourth-order polynomial function yields the equilibrium lattice constant  $a=2.533$  Å. The parameters of the geometry of the ground state of graphone is summarized in Table S1 compared with graphene and graphane.<sup>S1</sup> To the authors' best knowledge, there is no experimental report of the structure parameters of graphone yet. Our results of the structural parameters agree with previous density functional theory calculations.<sup>S2-S4</sup>

Table S1: **Structural parameters.** The structural parameters of the ground state of graphone from density functional theory calculations, compared with those of graphane and graphene.<sup>S1</sup>

	Graphene	Graphone	Graphane
$a$ (Å)	2.468	2.533	2.540
C-C (Å)	1.424	1.483	1.537
C-H (Å)		1.167	1.110
C-C-C (°)	120	117.3	111.5
C-C-H (°)		99.5	107.4
$\Delta$ (Å)	0	0.244	0.459

## Ultimate stresses and strains

When strains were applied, all the atoms were fully relaxed. The elastic limit is defined by the ultimate stress that a material can withstand while being stretched. The ultimate strain is the corresponding strain of the ultimate stress, which is the maxima of a stress-strain curve. The ultimate strains for the armchair, zigzag, and biaxial deformations are summarized in Table S2.

Table S2: **Elastic limits** The ultimate strengths ( $\Sigma_u^a, \Sigma_u^z, \Sigma_u^b$ ) and ultimate strains ( $\eta_u^a, \eta_u^z, \eta_u^b$ ) under uniaxial strain (armchair and zigzag) and biaxial strains of graphone from density functional theory calculations, compared with those of graphane and graphene.<sup>S1</sup>

		Graphene	Graphone	Graphane
armchair	$\Sigma_u^a$ (N/m)	28.6	19.8	18.9
	$\eta_u^a$	0.19	0.16	0.17
zigzag	$\Sigma_u^z$ (N/m)	30.4	22.2	21.4
	$\eta_u^z$	0.23	0.21	0.25
biaxial	$\Sigma_u^b$ (N/m)	32.1	22.8	20.8
	$\eta_u^b$	0.23	0.22	0.23

## Elastic constants

The elastic constants were obtained using a two-step least-square fit of the stress-strain relationships<sup>S5</sup> and are summarized in Table S3, which provides an accurate continuum description of the elastic properties of graphone. They are suitable for incorporation into numerical methods such as the finite element techniques.

Table S3: **Elastic constants** Nonzero independent components for the second order elastic constants (SOECs), third order elastic constants (TOECs), fourth order elastic constants (FOECs), fifth order elastic constants (FFOECs), in-plane stiffness  $Y_s$ , and Poisson ratio  $\nu$  of graphone from density functional theory calculations, compared with graphane and graphene.<sup>S1</sup>

		Graphene	Graphone	Graphane
$Y_s$ (N/m)		340.8	251.7	246.7
$\nu$		0.178	0.119	0.078
SOECs	$C_{11}$ (N/m)	352.0	255.3	248.2
	$C_{12}$ (N/m)	62.6	30.4	19.4
TOECs	$C_{111}$ (N/m)	-3089.7	-1885.9	-2374.1
	$C_{112}$ (N/m)	-453.8	-350.9	-95.4
	$C_{222}$ (N/m)	-2928.1	-1855.1	-2162.8
FOECs	$C_{1111}$ (N/m)	21927	4824	19492
	$C_{1112}$ (N/m)	2731	4780	819
	$C_{1122}$ (N/m)	3888	1173	68
	$C_{2222}$ (N/m)	18779	8226	14823
FFOECs	$C_{11111}$ (N/m)	-118791	42518	-103183
	$C_{11112}$ (N/m)	-19173	-18271	816
	$C_{11122}$ (N/m)	-15863	-21132	-16099
	$C_{12222}$ (N/m)	-27463	20876	-10151
	$C_{22222}$ (N/m)	-134752	-113277	-134277

## Calculations with other exchange-correlation functionals

To test the accuracy of our calculations, we repeat all calculations with three other exchange-correlation functionals, as revised revised Perdew-Burke-Ernzerhof (revPBE),<sup>S6</sup> Perdew-Burke-Ernzerhof revised for solids (PBEsol),<sup>S7</sup> and revised Tao-Perdew-Staroverov-Scuseria (revTPSS).<sup>S8</sup> The results of Poisson ratio of graphone as a function of in-plane pressure are shown in Fig. S1. For comparison, we plot the Poisson ratio from these three functionals together with our original PBE functionals in the following figure. The scale of the y-axis is changed to [0,0.15] for a clear view (original is [0,0.5]). As shown in Fig. S1, all these calculations reveal that the Poisson ratio of graphone increases with an increasing in-plane pressure.

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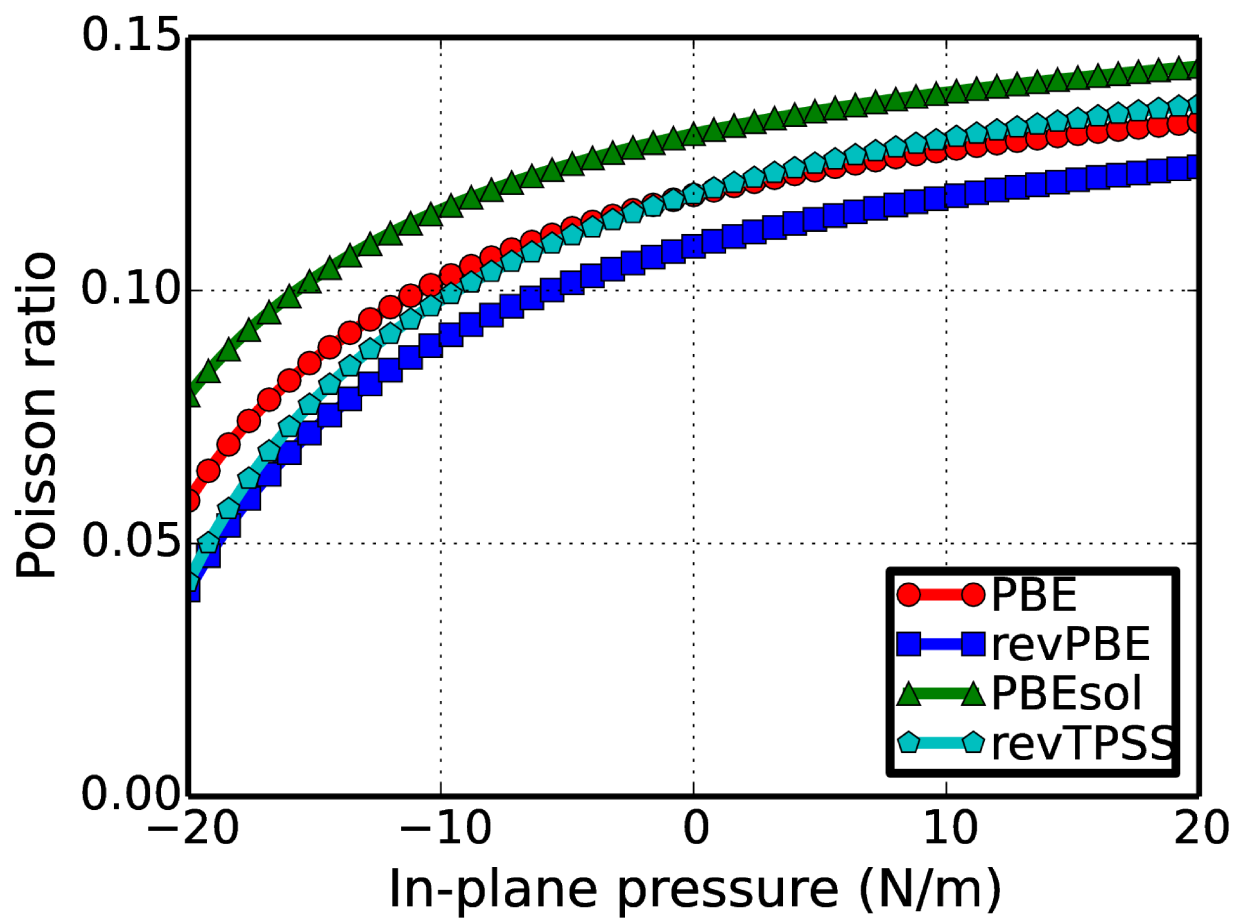


Figure S1: **Poisson ratio from different exchange-correlation functionals** The Poisson ratio as a function of the pressure is predicted from calculations with four exchange-correlation functionals.