Simulations in graphene

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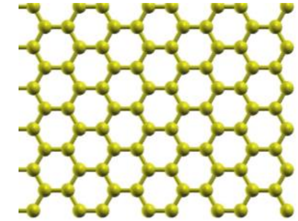
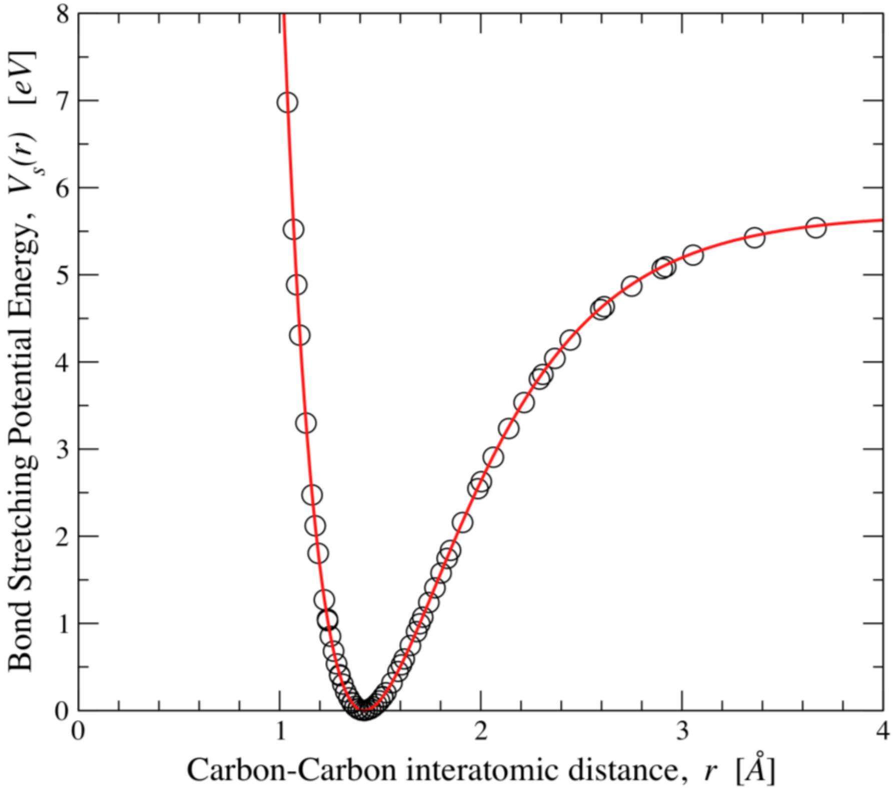
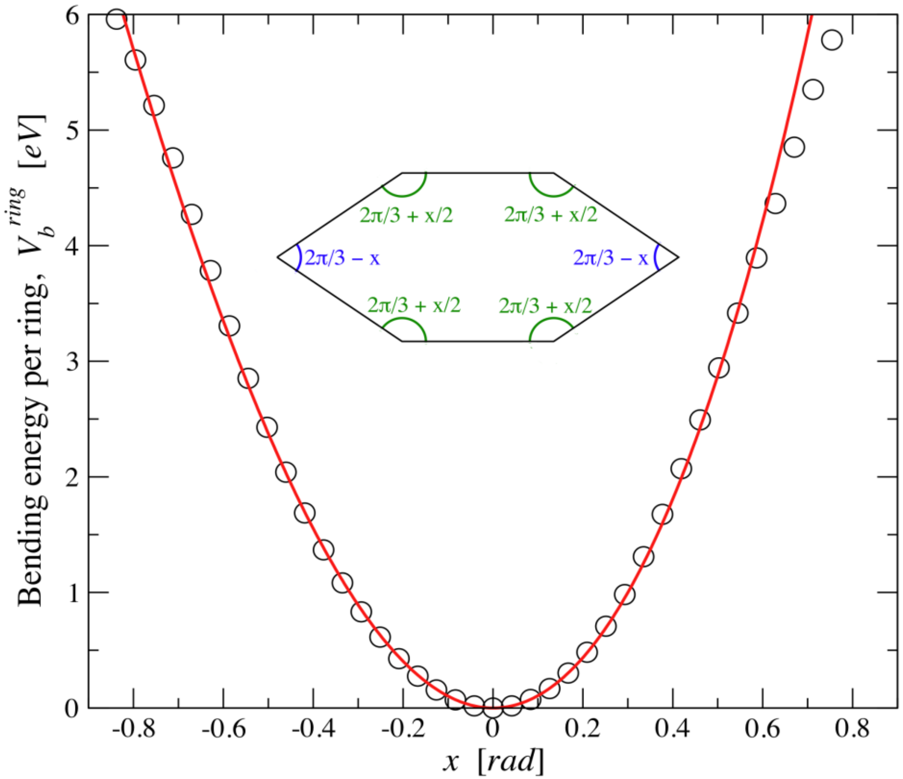
CRETE CENTER FOR
QUANTUM COMPLEXITY
AND NANOTECHNOLOGY

Atomistic simulations in graphene



In-plane bond stretching and angle bending interatomic potentials are derived using first principles methods (DFT) in appropriately deformed graphene configurations





Fitting with analytical expressions

$$V_s(r) = D\left(e^{-a(r-r_0)} - 1\right)^2$$

D = 5.7 eV, a=1.96 A^{-1}, r_0=1.42 A

$$V_b(\varphi) = \frac{k}{2}\left(\varphi - \frac{2\pi}{3}\right)^2 - \frac{k'}{3}\left(\varphi - \frac{2\pi}{3}\right)^3$$

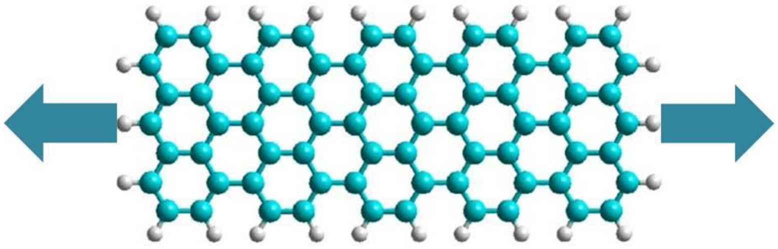
$$V_b^{ring} = \frac{3}{2}kx^2 + \frac{1}{2}k'x^3$$

k=7.0 eV/rad^2, k'=4 eV/rad^3

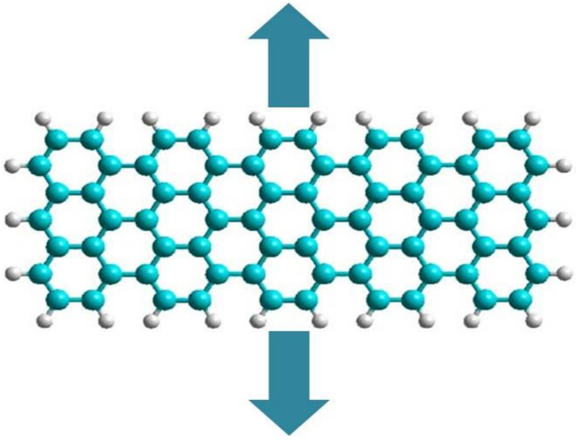
Kalosakas, Lathiotakis, Galiotis, Papagelis, *J. Appl. Phys.* **113**, 134307 (2013)

Mechanical response: Application of various loads

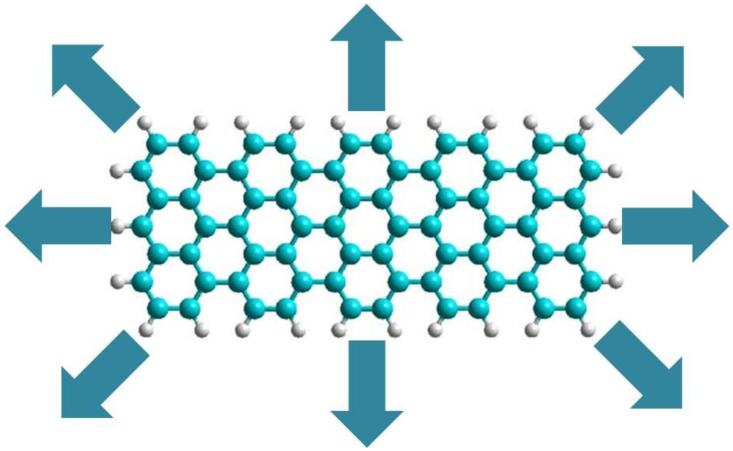
Uniaxial stress along the zigzag edge



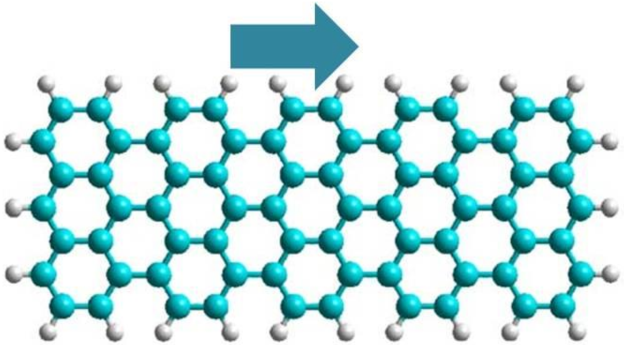
Uniaxial stress along the armchair edge



Hydrostatic pressure



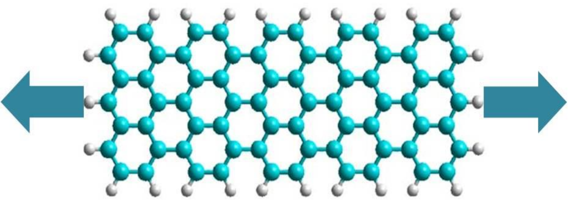
Shear stress along the armchair/zigzag edge



Equilibrium under the application of a uniaxial force

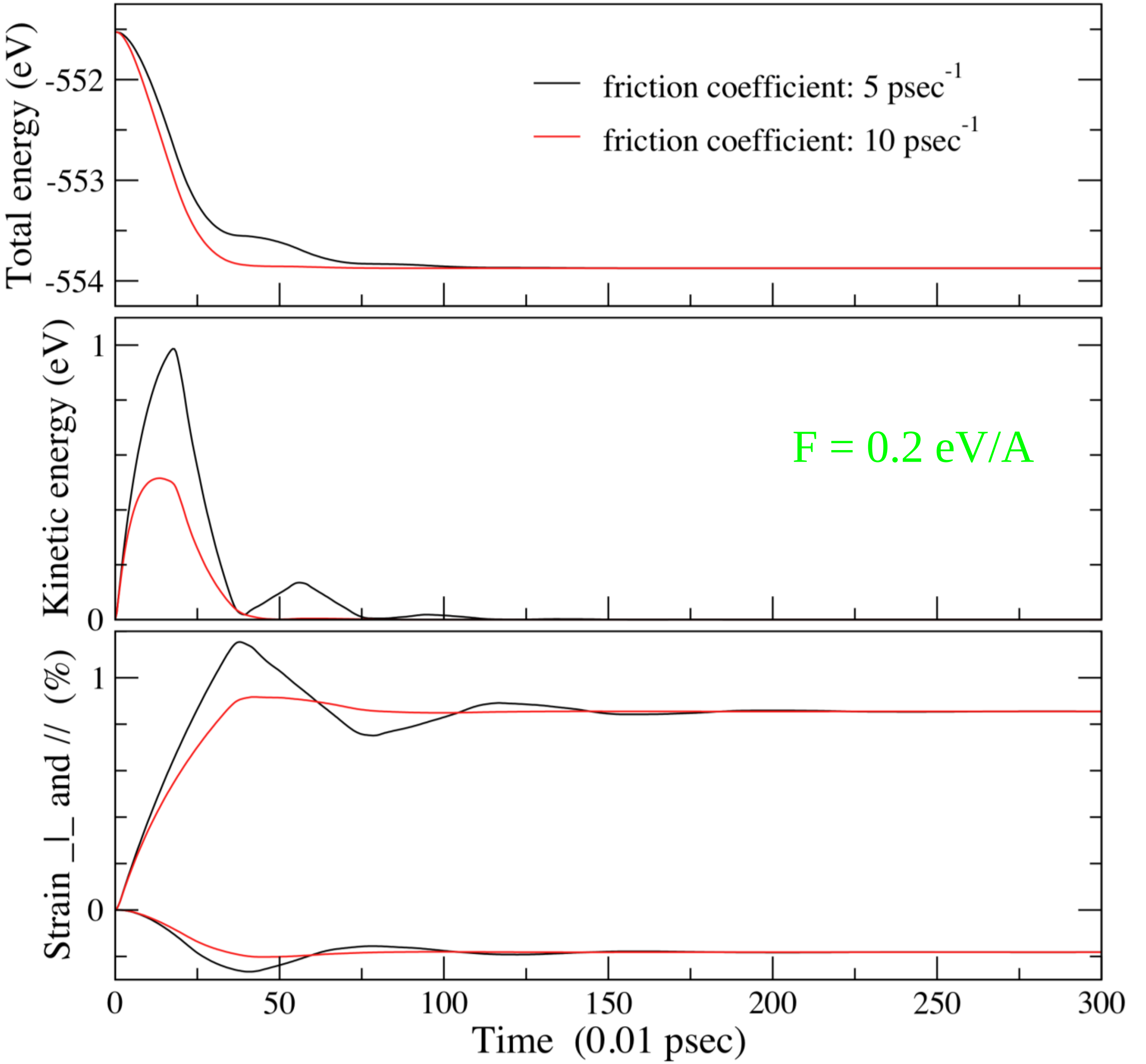
Start with the equilibrium structure of a graphene (without any force) containing 7482 or 17030 atoms

Apply a constant force at all atoms in the two edges

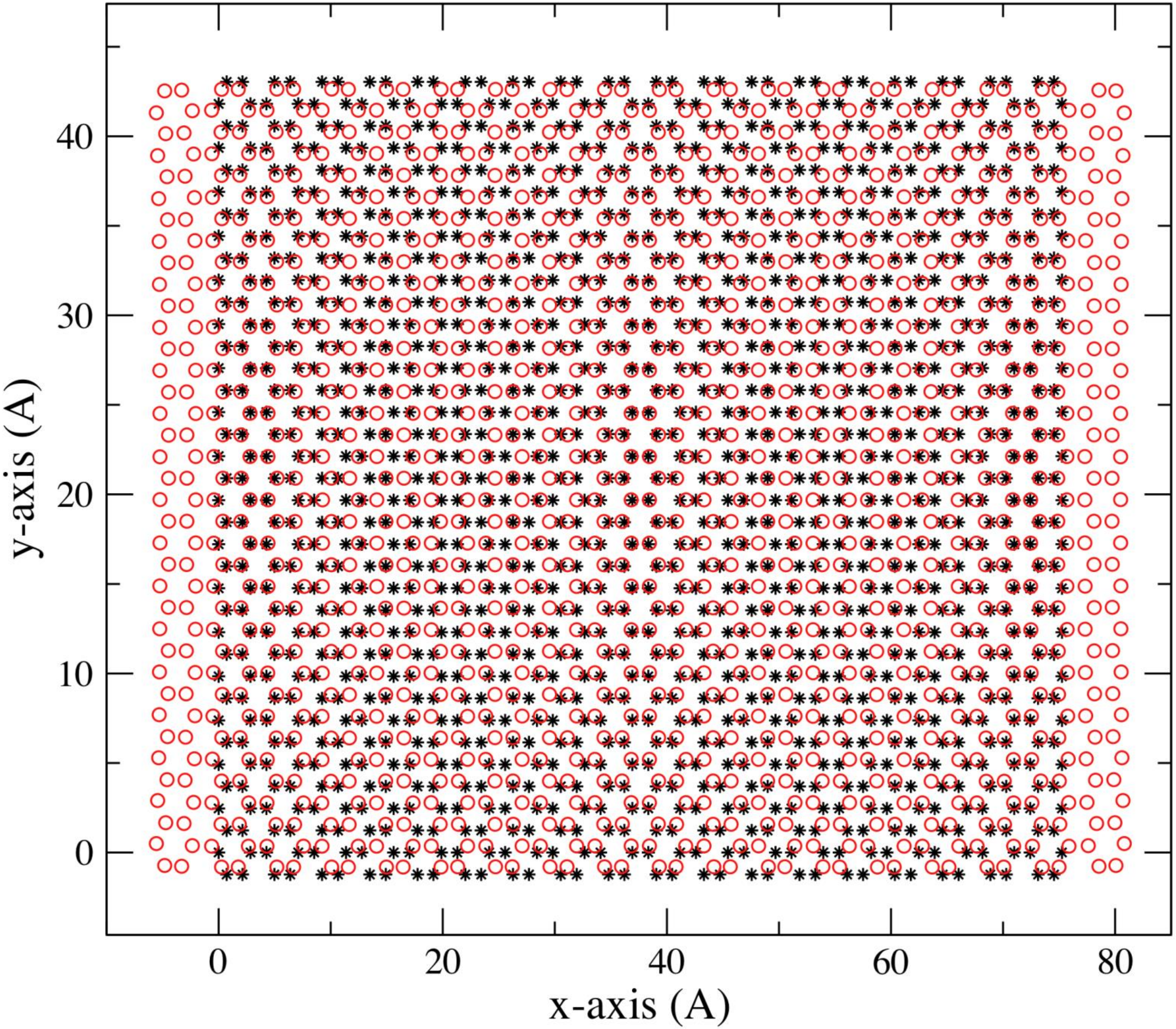


Follow with MD the evolution of the system, applying a friction term at each atom

The system goes to a new equilibrium compatible to the applied forces

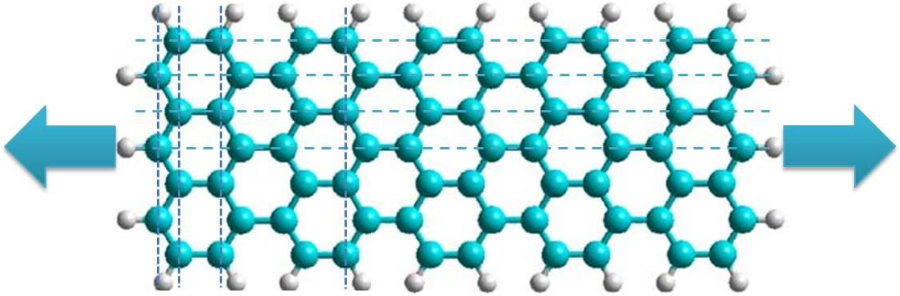


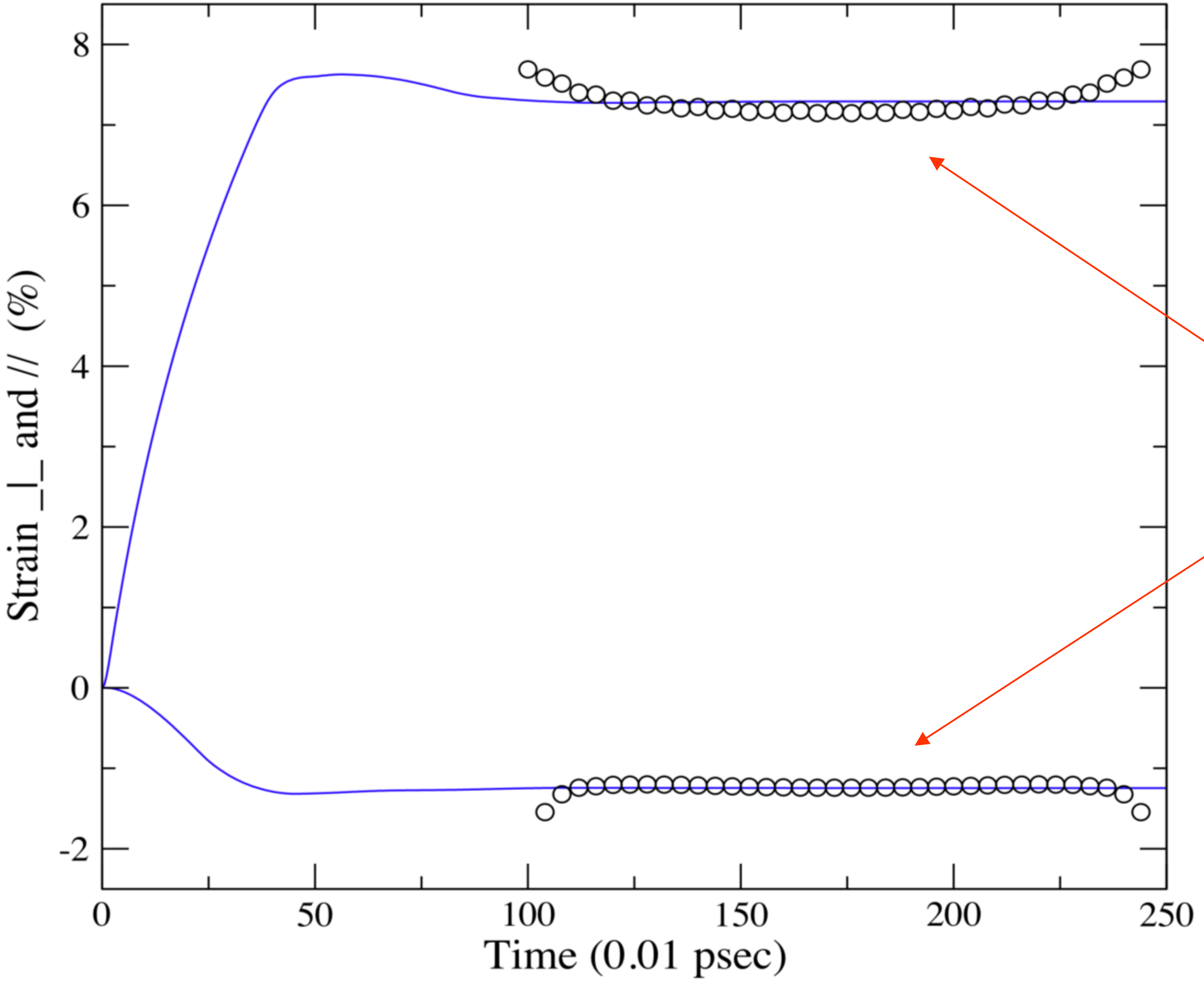
Equilibrium stretched structure



F = 2.4 eV/A

Strain distribution

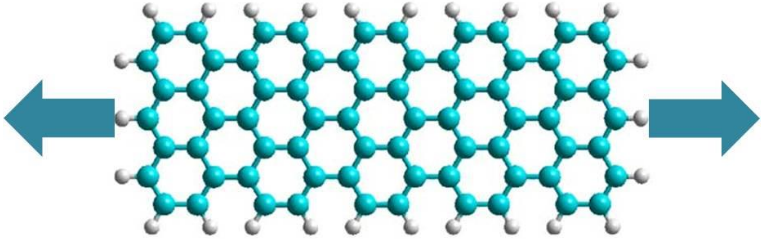


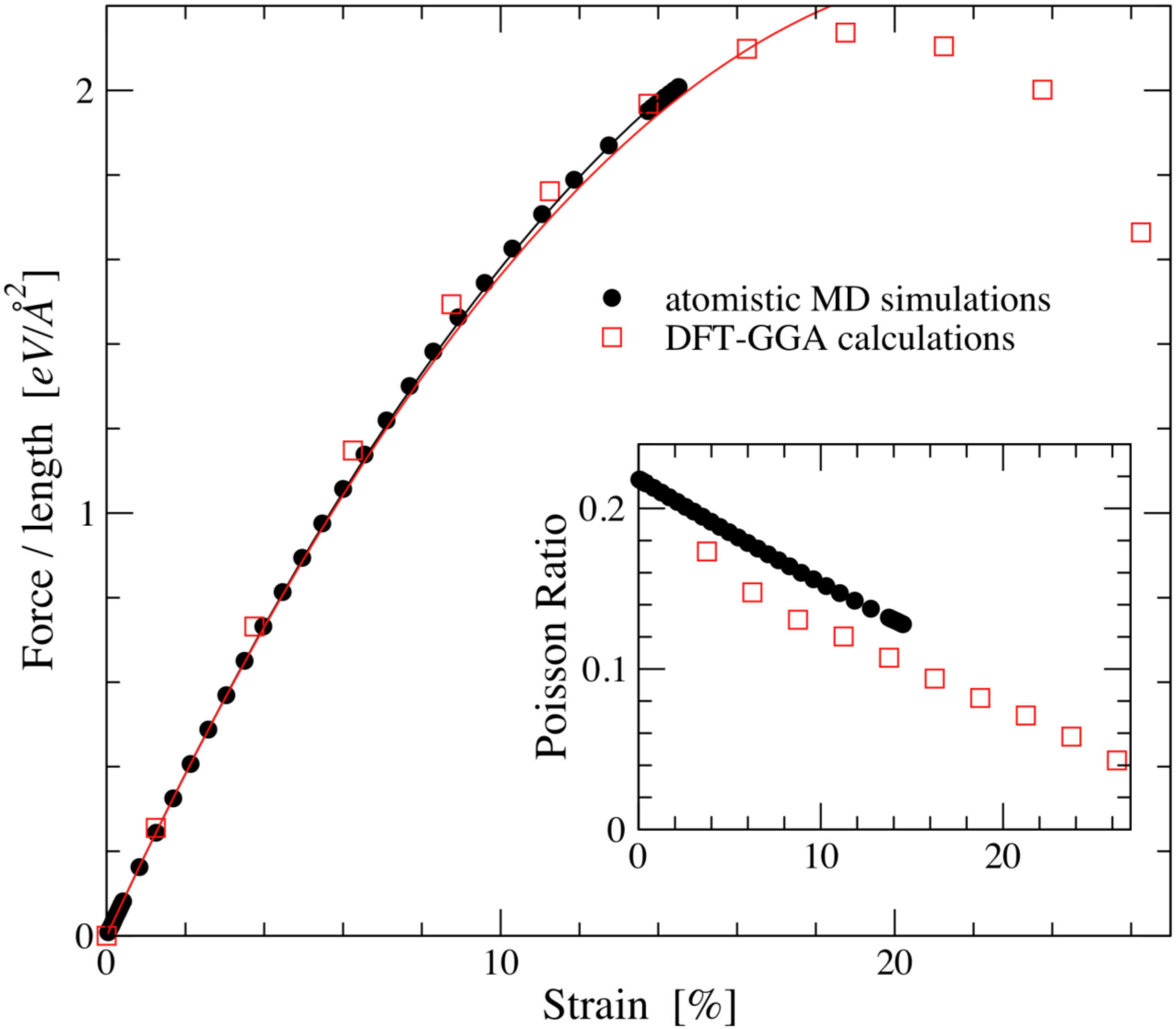


Distribution of strains along the horizontal/vertical lines of the graphene structure (at the end of the simulation)

F = 1.5 eV/A

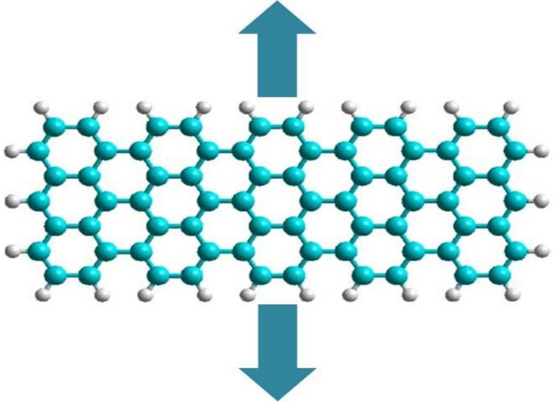
Graphene uniaxial stress response I

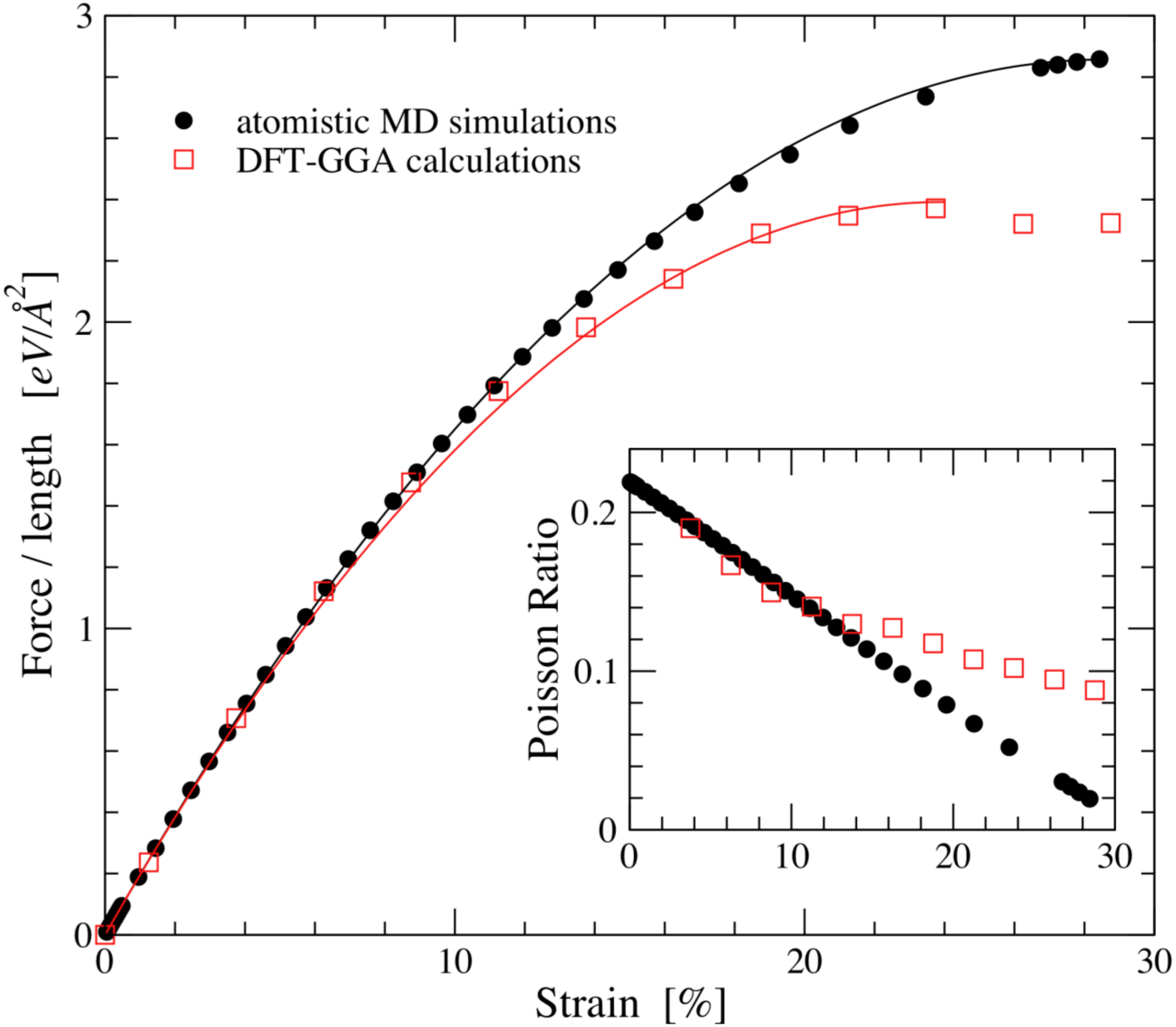




Young Modulus
E_{2D}=320 N/m

Graphene uniaxial stress response II





Young Modulus
E_{2D}=320 N/m

Comparison of calculated elastic constants with experimental and other theoretical results

2d Elastic constant: E_{2D} = 320 N/m
➔ effective Young modulus $E_{eff} = E_{2D}$/0.335nm = 0.96 TPa

Experimental estimate: E_{2D} = 340±50 N/m
➔ E_{eff} = 1.0±0.1 TPa — Lee et al., *Science* **321**, 385 (2008)

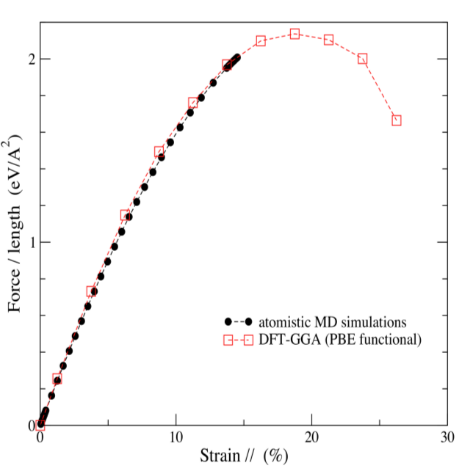
Other theoretical results:

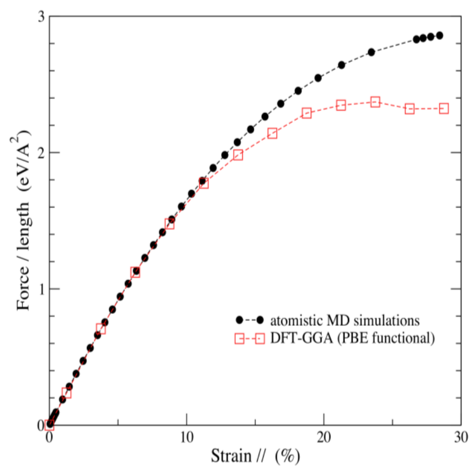
E_{eff} = 1.05 TPa (in both directions) — Liu, Ming, Li, *Phys. Rev. B* **76**, 064120 (2007)

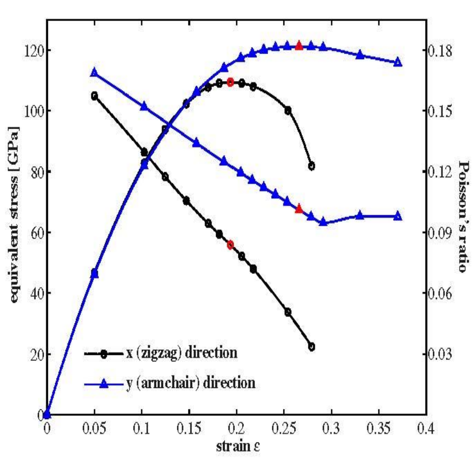
E_{eff} = 1.05-1.06 TPa — Zakharchenko, Katsnelson, Fasolino, *Phys. Rev. Lett.* **102**, 046808 (2009)

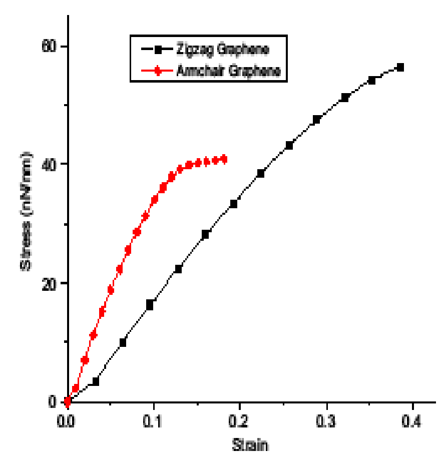
E_{eff} = 1.1 TPa (0.6 TPa in the other direction) — Gao, Hao, *Physica E* **41**, 1561 (2009)

Values of E_{eff} in the range 0.5 – 3.5 TPa have been reported in the literature









Comparison of calculated intrinsic strength with experimental and other theoretical results

2d Intrinsic strength: σ_{2D} = 39-45 N/m (32-34 N/m in the other direction)

➔ effective intrinsic strength $\sigma_{eff} = \sigma_{2D}/0.335\text{nm}$ = 120-130 GPa (100 GPa)

Experimental estimate: $\sigma_{2D} = 42 \pm 4$ N/m

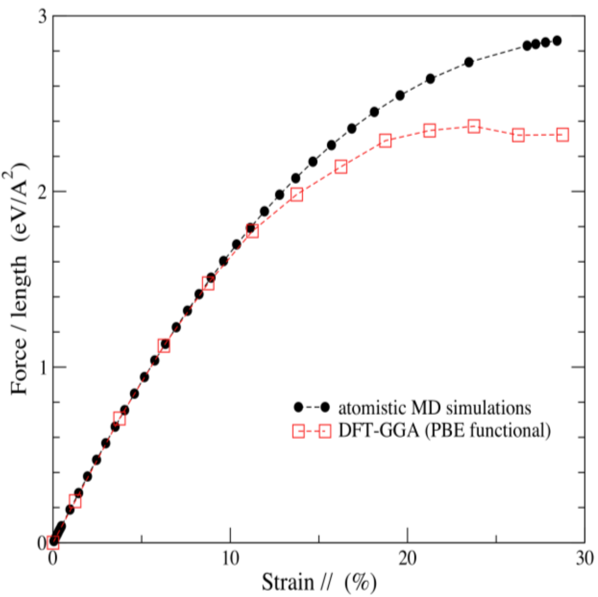
➔ $\sigma_{eff} = 130 \pm 20$ GPa

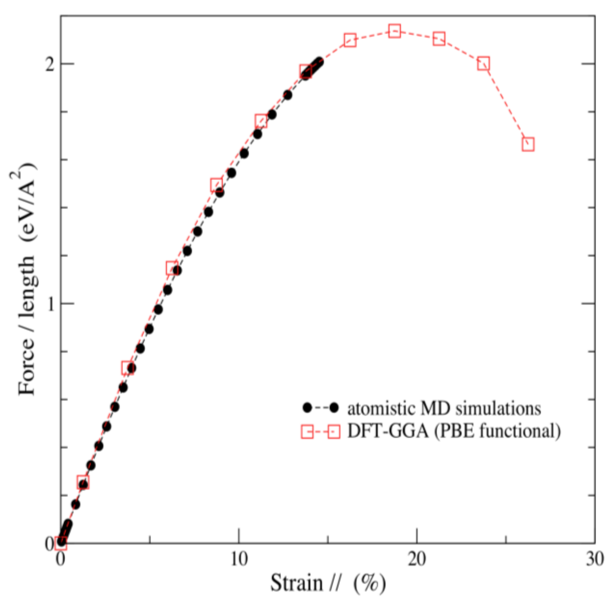
Lee et al., *Science* **321**, 385 (2008)

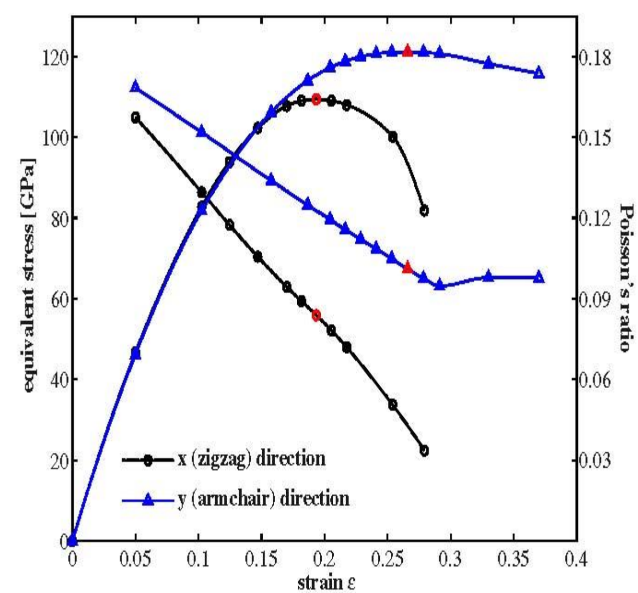
Other theoretical results:

σ_{eff} = 121 GPa (110 GPa in the other direction)

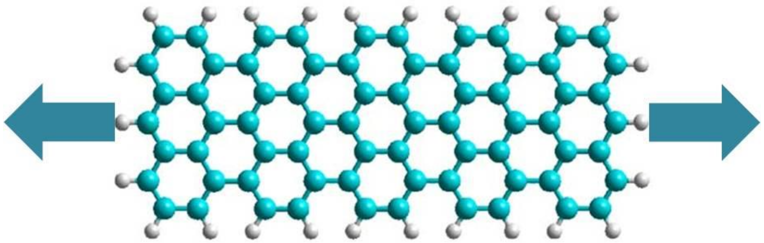
Liu, Ming, Li, *Phys. Rev. B* **76**, 064120 (2007)

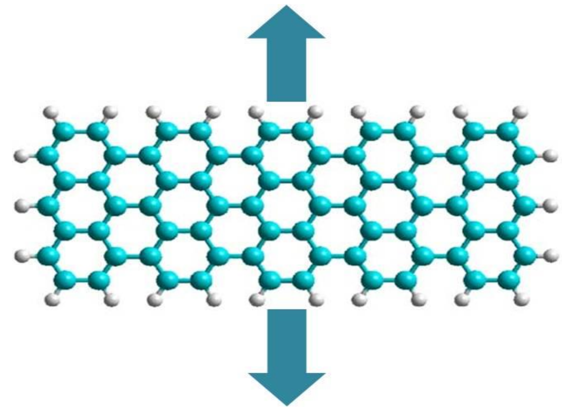


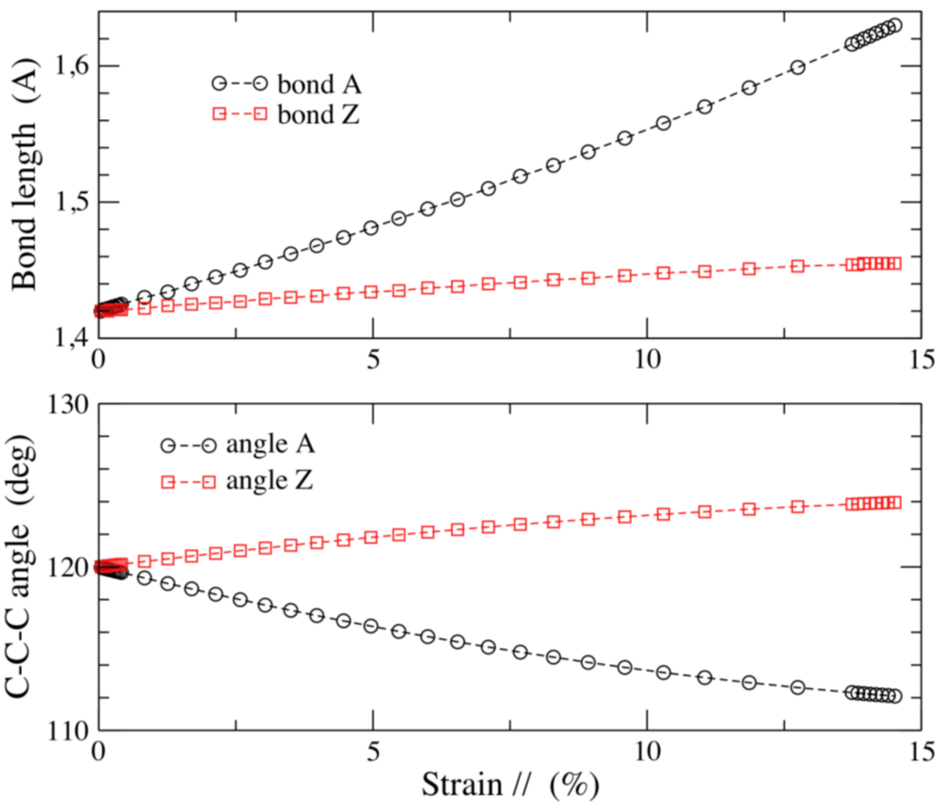


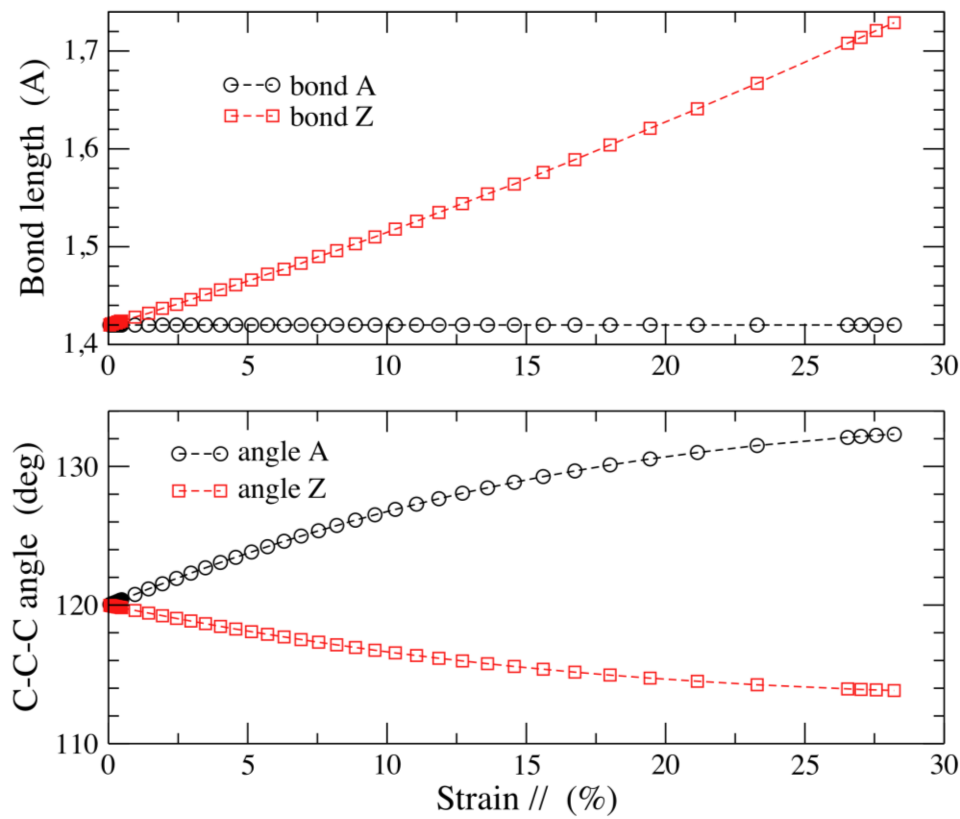


Deformations of bond lengths and angles

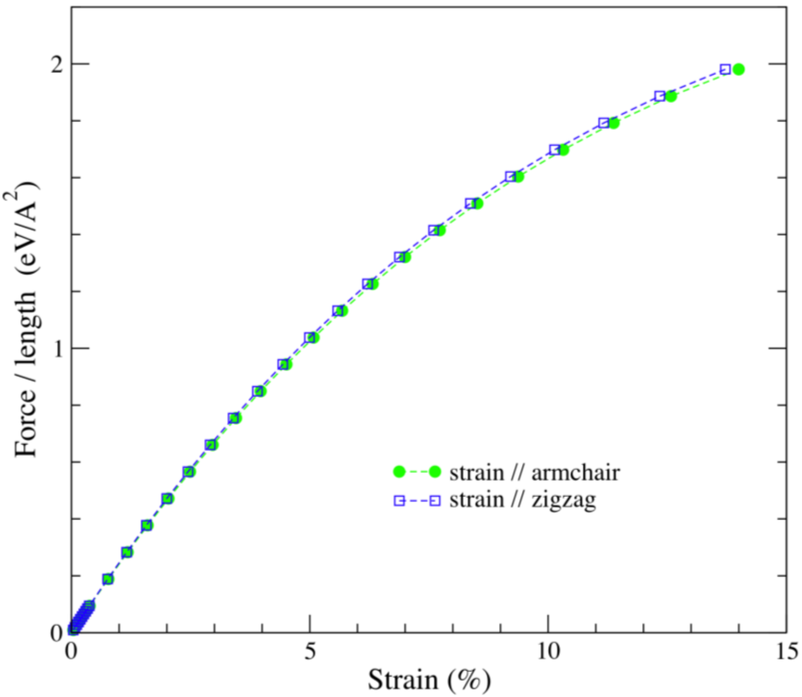


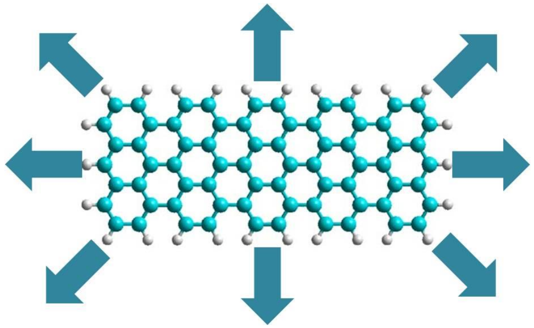


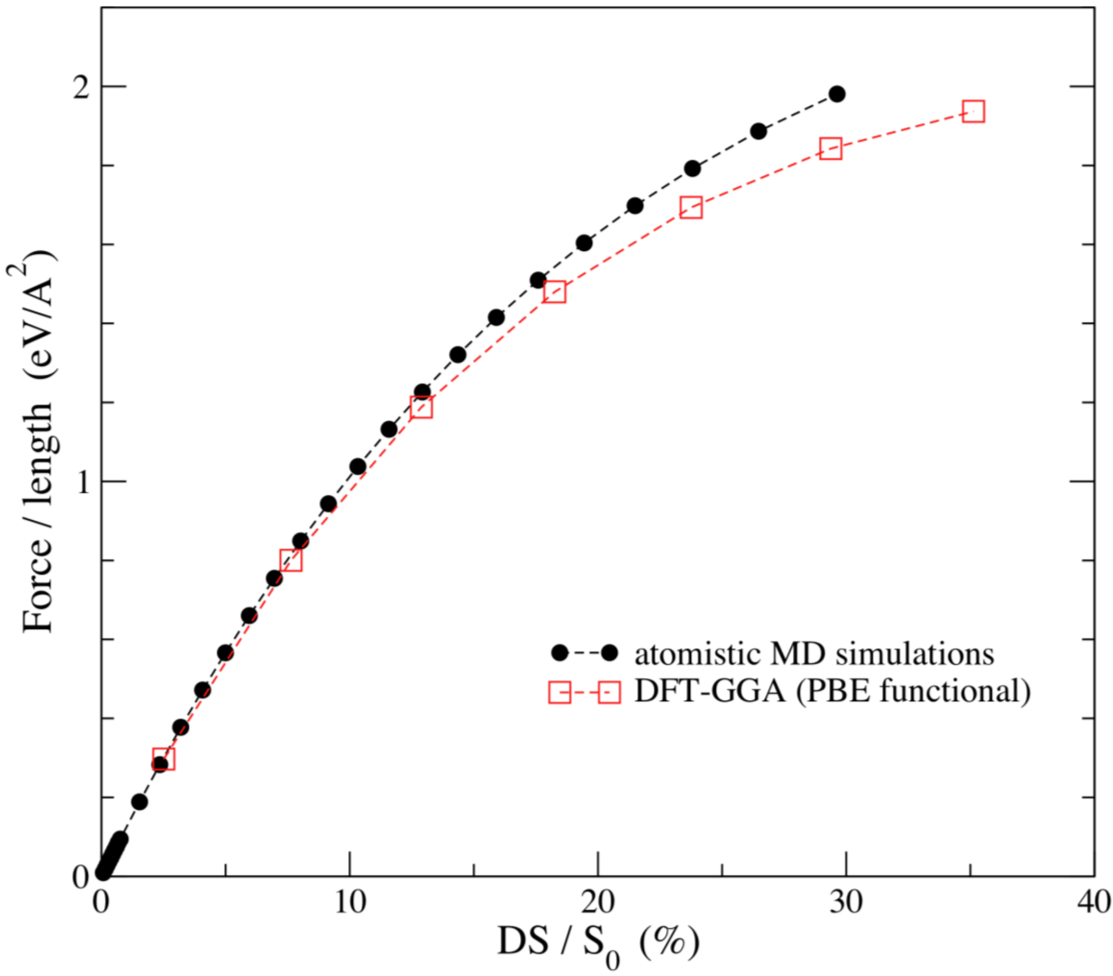




Graphene hydrostatic response



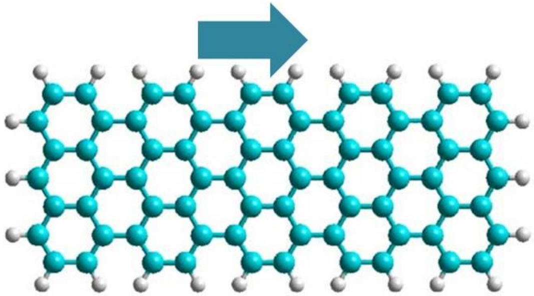


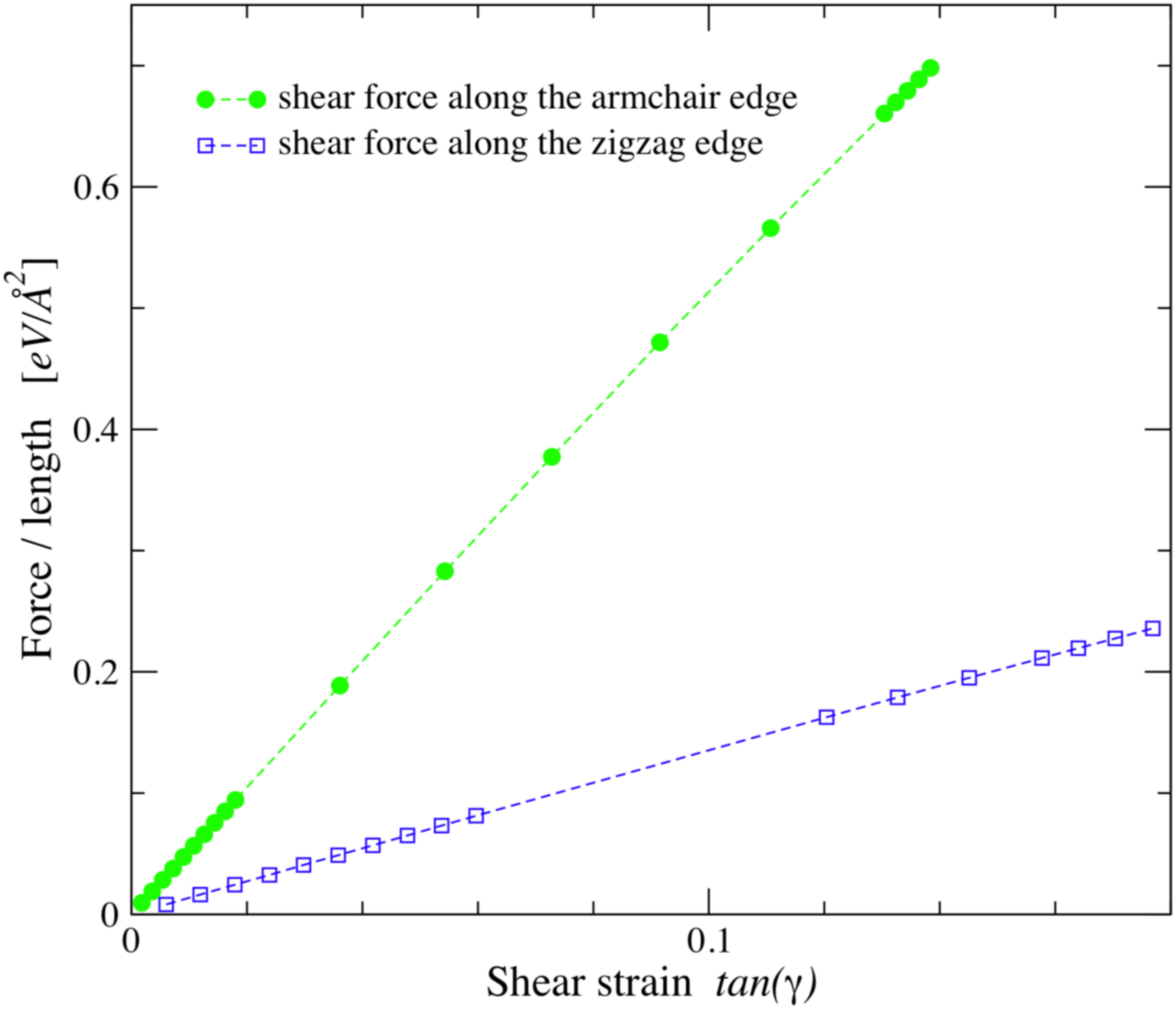


Bulk Modulus

B_{2D}=200 N/m

Graphene shear stress response



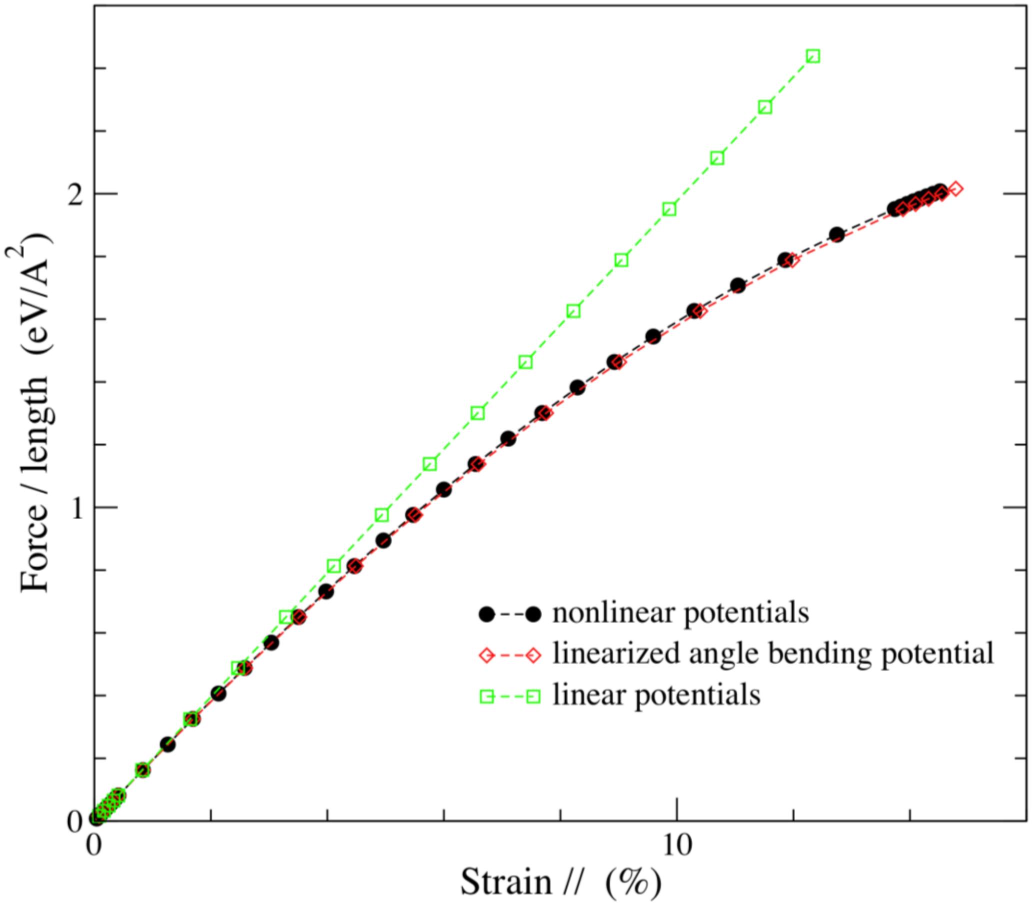


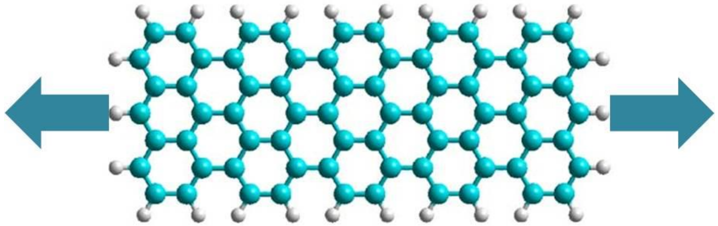
Shear modulus

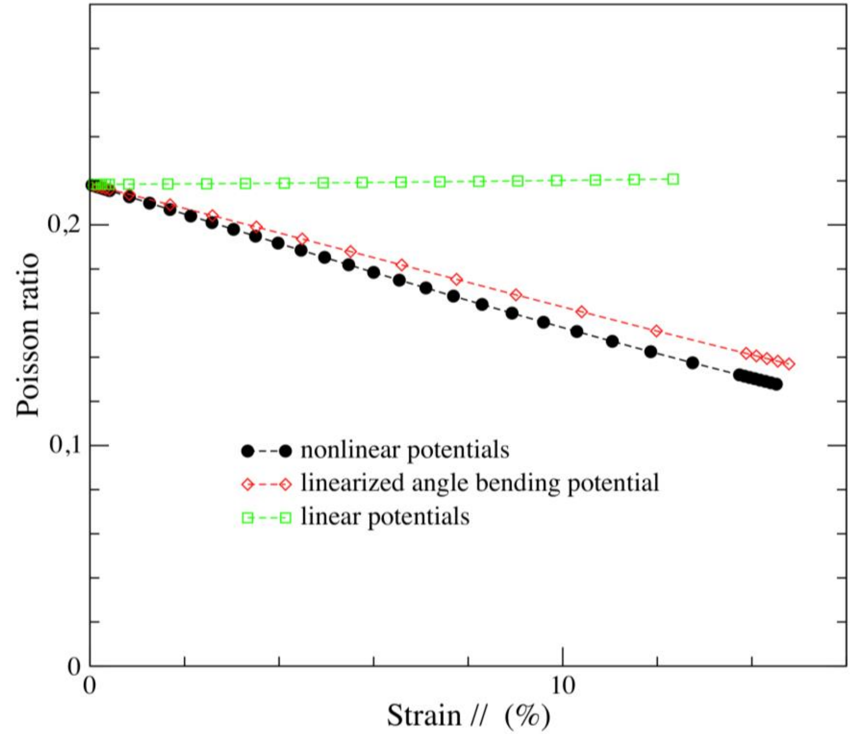
G^{a}_{2D}=84 N/m

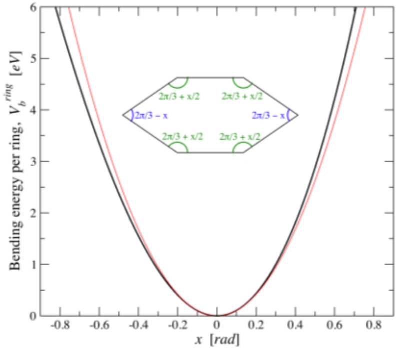
G^{z}_{2D}=22 N/m

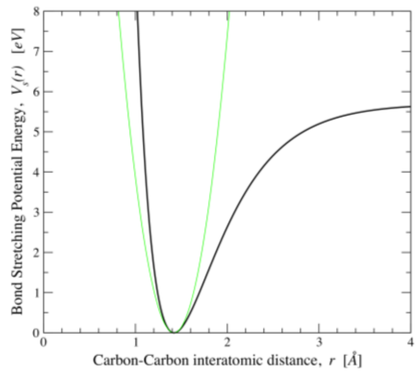
Comparison with linearized force fields





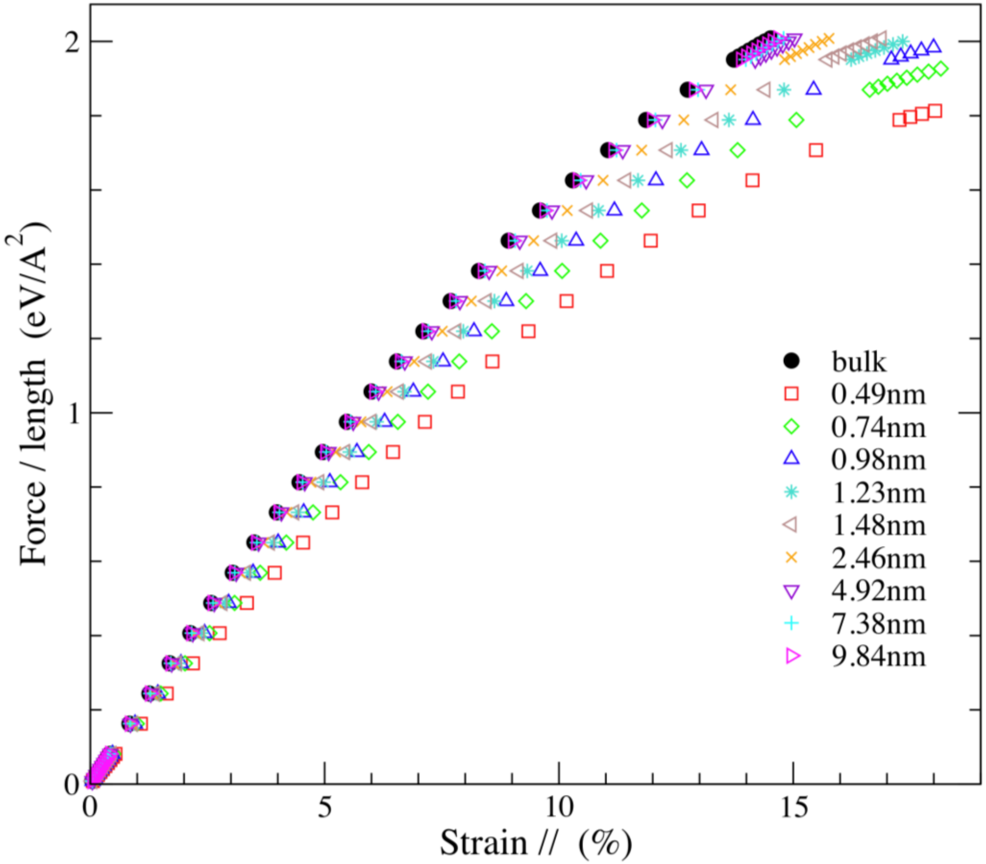


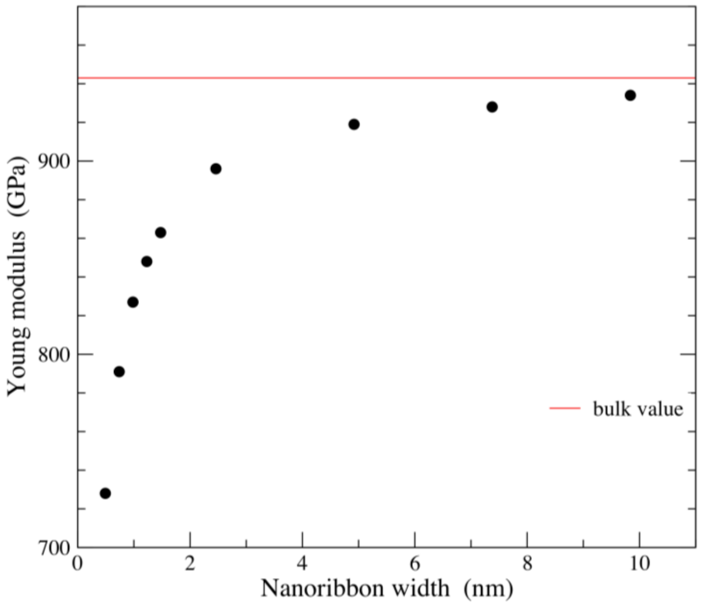




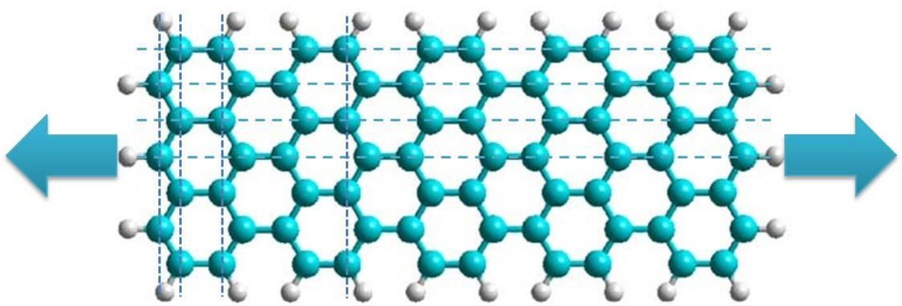
Kalosakas, Lathiotakis, Galiotis, Papagelis,
J. Appl. Phys. **113**, 134307 (2013)

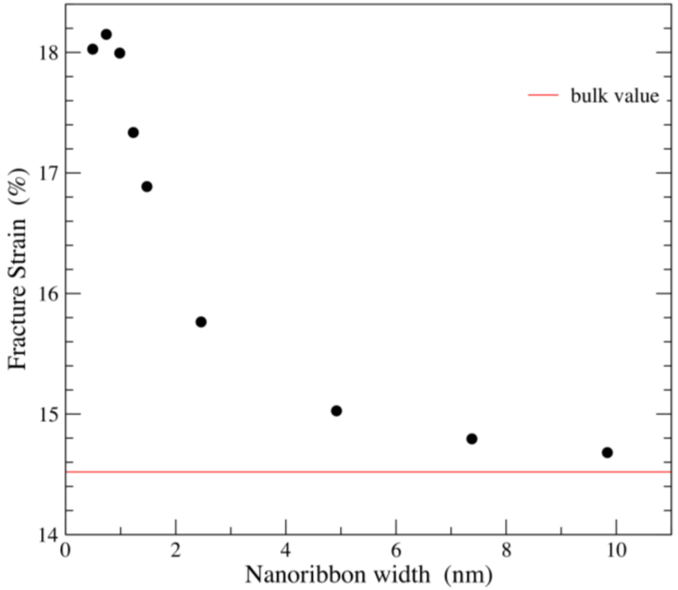
Graphene nanoribbons





Nanoribbons consisted of 5-60 layers

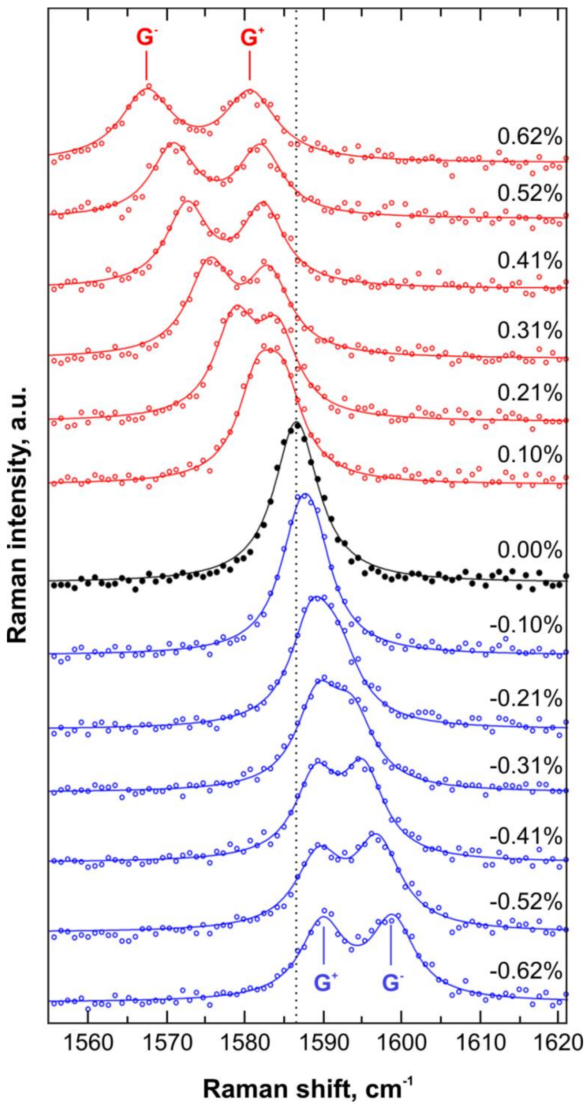




Current projects

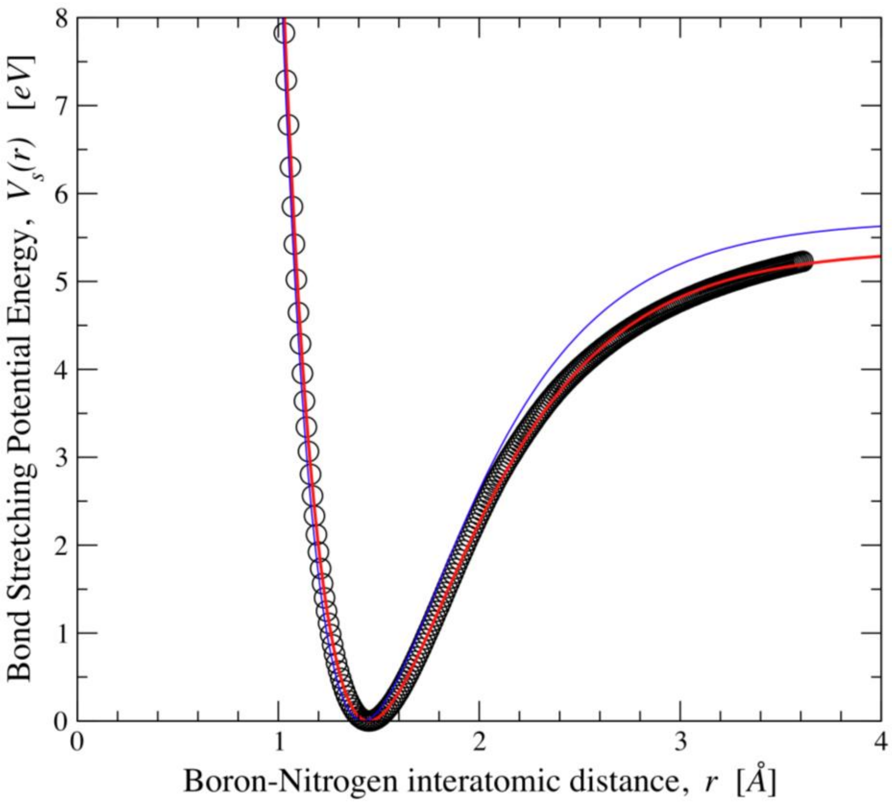
- Effect of defects (vacancies, line defects, etc.) in the elastic properties of graphene.

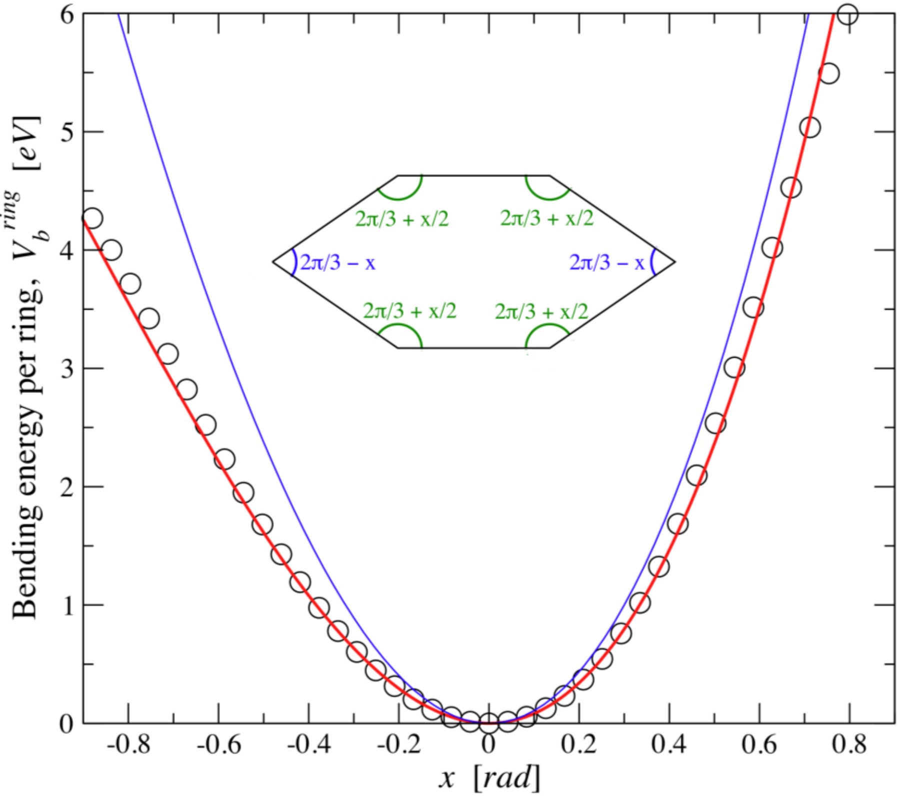
- Phonon Dispersion obtained from MD through the velocity autocorrelation function.
  Dynamic response under strain.
  Raman G-band splitting.



Frank, Tsoukleri, Parthenios, Papagelis, et al., *ACS Nano* **4**, 3131 (2010)

- Force fields and mechanical properties of Boron-Nitride





$$V_s(r) = D\left(e^{-a(r-r_0)} - 1\right)^2$$

$$V_b(\varphi) = \frac{k}{2}\left(\varphi - \frac{2\pi}{3}\right)^2 - \frac{k'}{3}\left(\varphi - \frac{2\pi}{3}\right)^3$$

$$V_b^{ring} = \frac{3}{2}kx^2 + \frac{1}{2}k'x^3$$

Young Modulus E_{2D}=260 N/m

➔ $E_{eff} = E_{2D}/0.33\text{nm} = 0.79$ TPa (~80% of graphene)

Summary

- Analytical empirical potentials (bond stretching and angle bending) have been provided for atomistic MD simulations of graphene in 2D.
- The mechanical response of graphene is examined using atomistic MD simulations and DFT calculations
- Various kinds of loads have been investigated (uniaxial stresses, hydrostatic pressure, shear stresses)
- The obtained elastic parameters are in good agreement with experimental as well as other theoretical results

Collaborators

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Theoretical and Physical Chemistry Institute, NHRF, Greece

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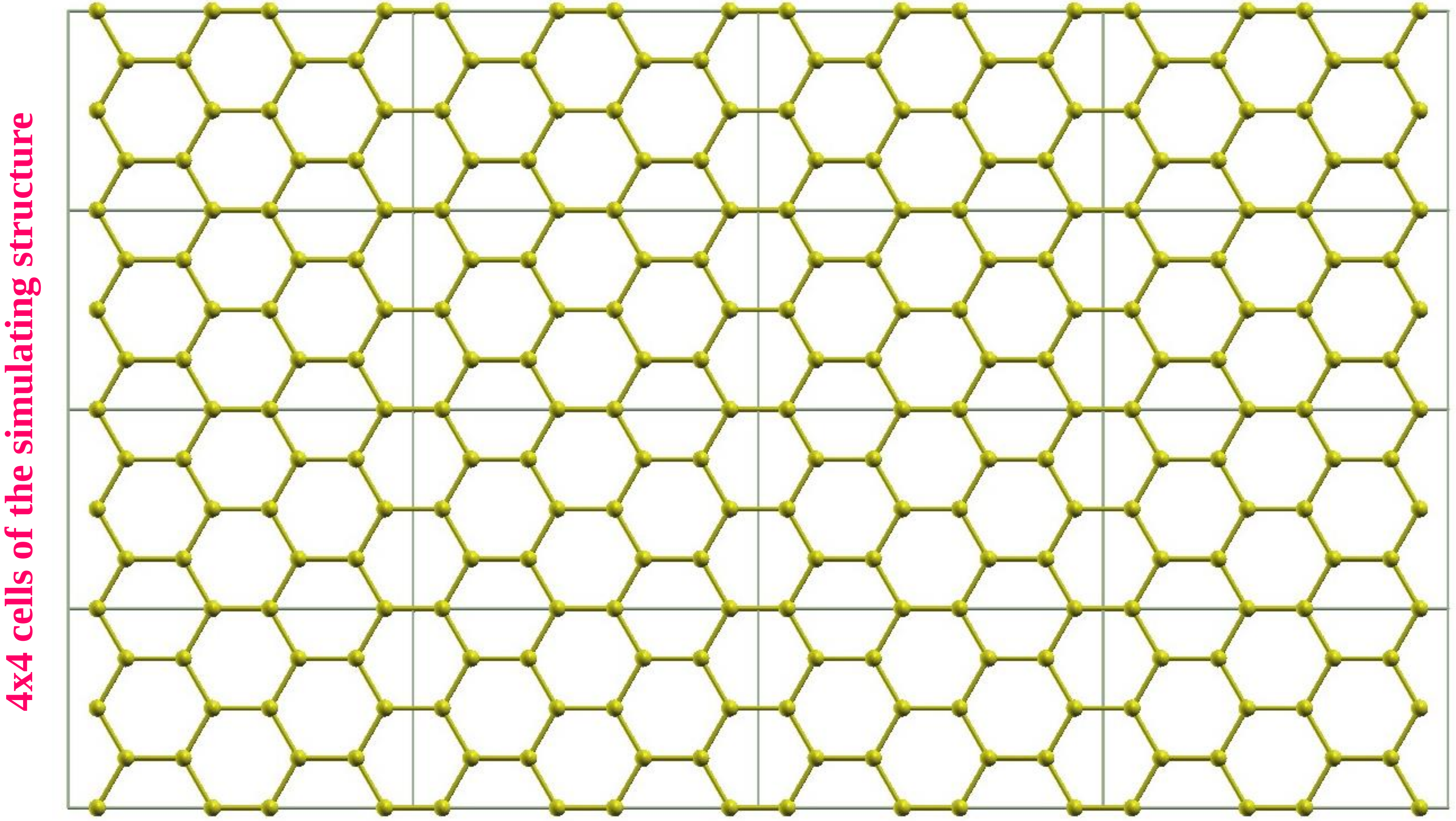
European Union
European Social Fund

OPERATIONAL PROGRAMME
EDUCATION AND LIFELONG LEARNING
investing in knowledge society
MINISTRY OF EDUCATION & RELIGIOUS AFFAIRS, CULTURE & SPORTS
MANAGING AUTHORITY
Co-financed by Greece and the European Union

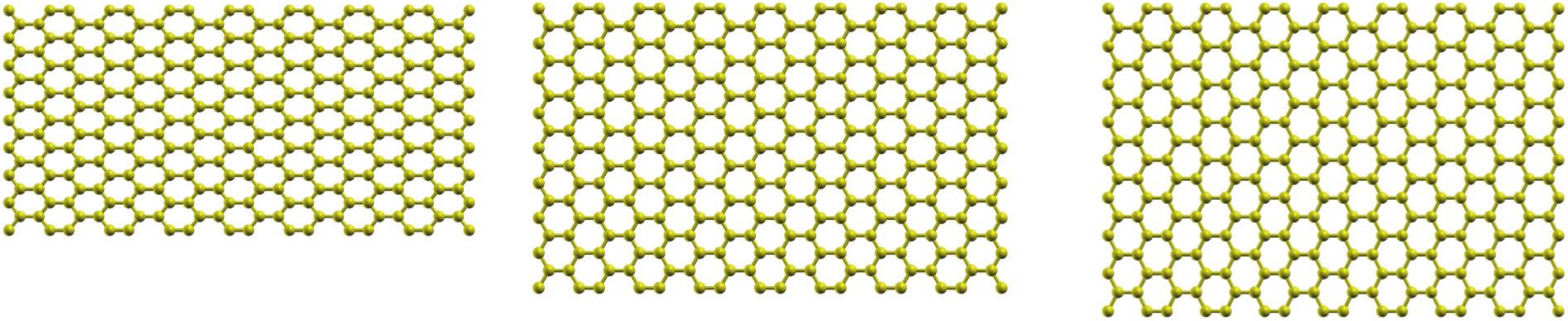
NSRF
2007-2013
programme for development
EUROPEAN SOCIAL FUND

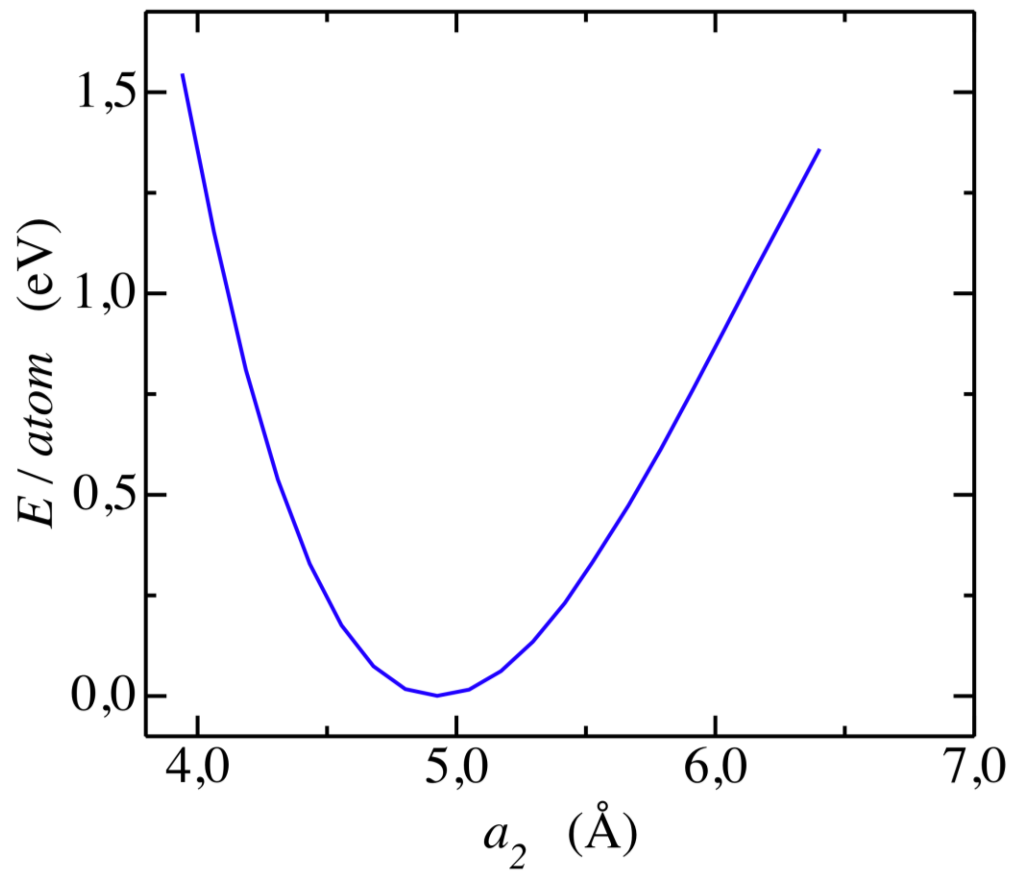
DFT calculations

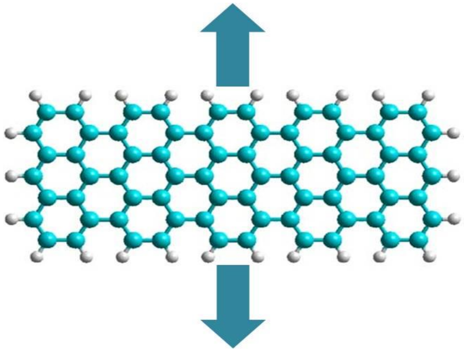
Generalized Gradient Approximation with PBE functionals (satisfactory description for solids)



Calculations are performed on one cell (dimensions a_1x a_2), using periodic boundary conditions.
A *fixed strain* is applied on the y direction and the energy of the equilibrated structure is found.

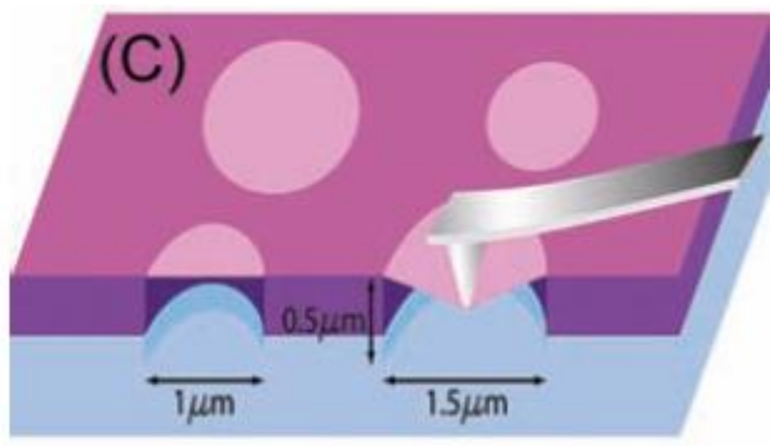




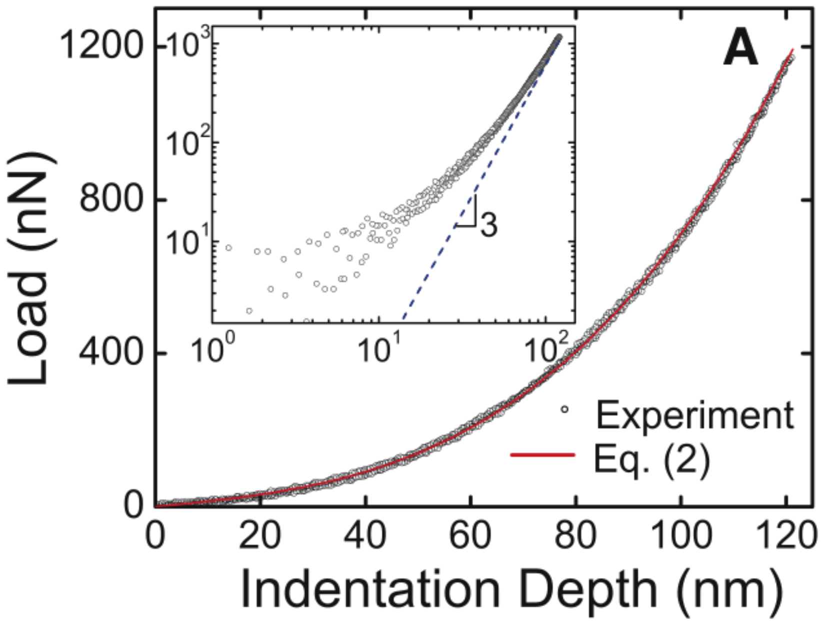


The corresponding force is obtained through the derivative of $E(a_2)$

Graphene as a membrane: bending experiments



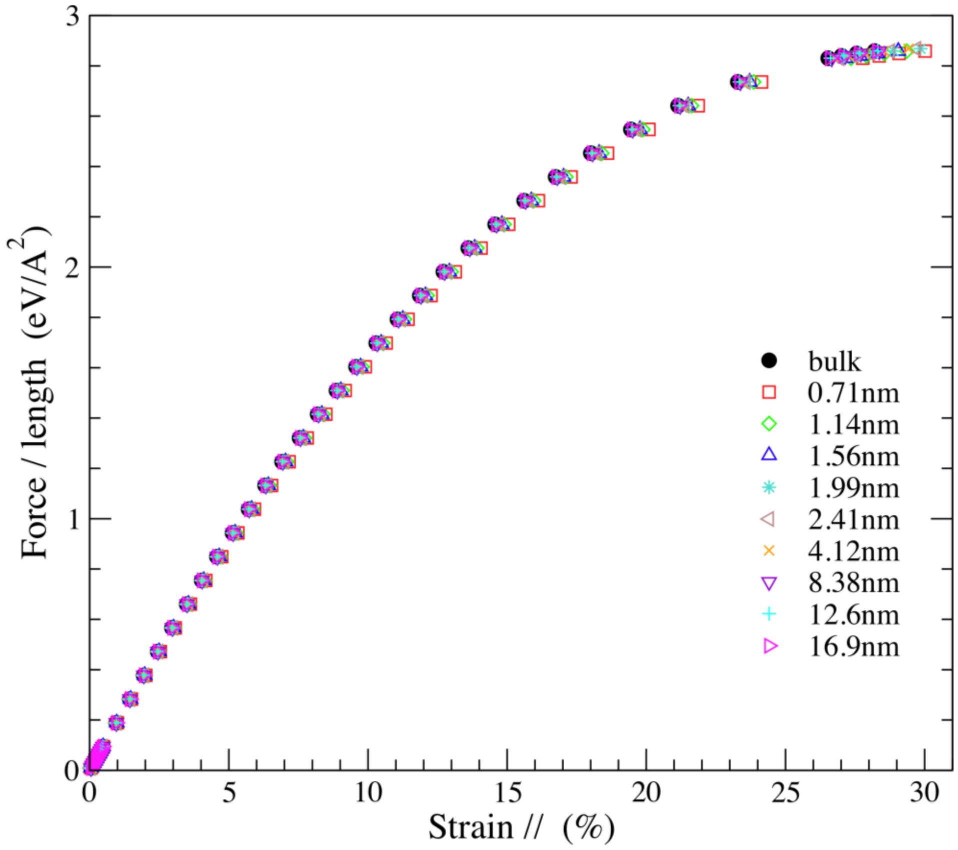
Measurement of the mechanical properties of monolayer graphene suspended over open holes onto SiO_2 substrate using AFM nanoidentation

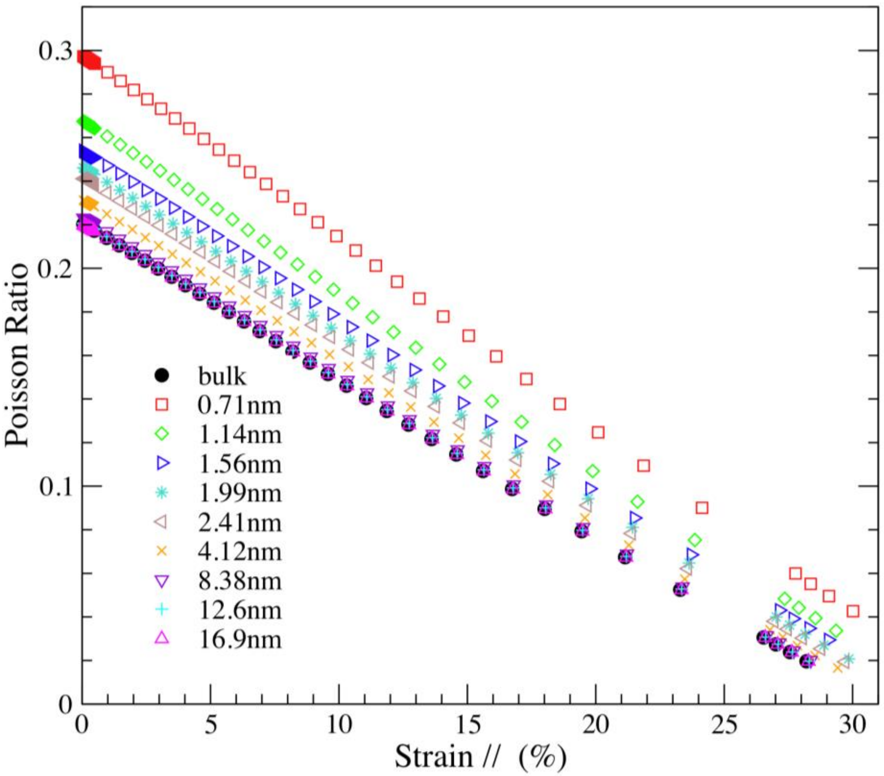


A value of E=340±50 N/m has been derived from fitting an approximate function F=f(δ) to the experimental data

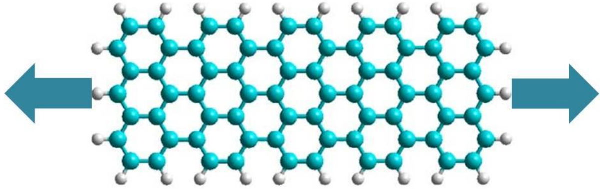
Lee, Wei, Kysar, Hone, *Science* **321**, 385 (2008)

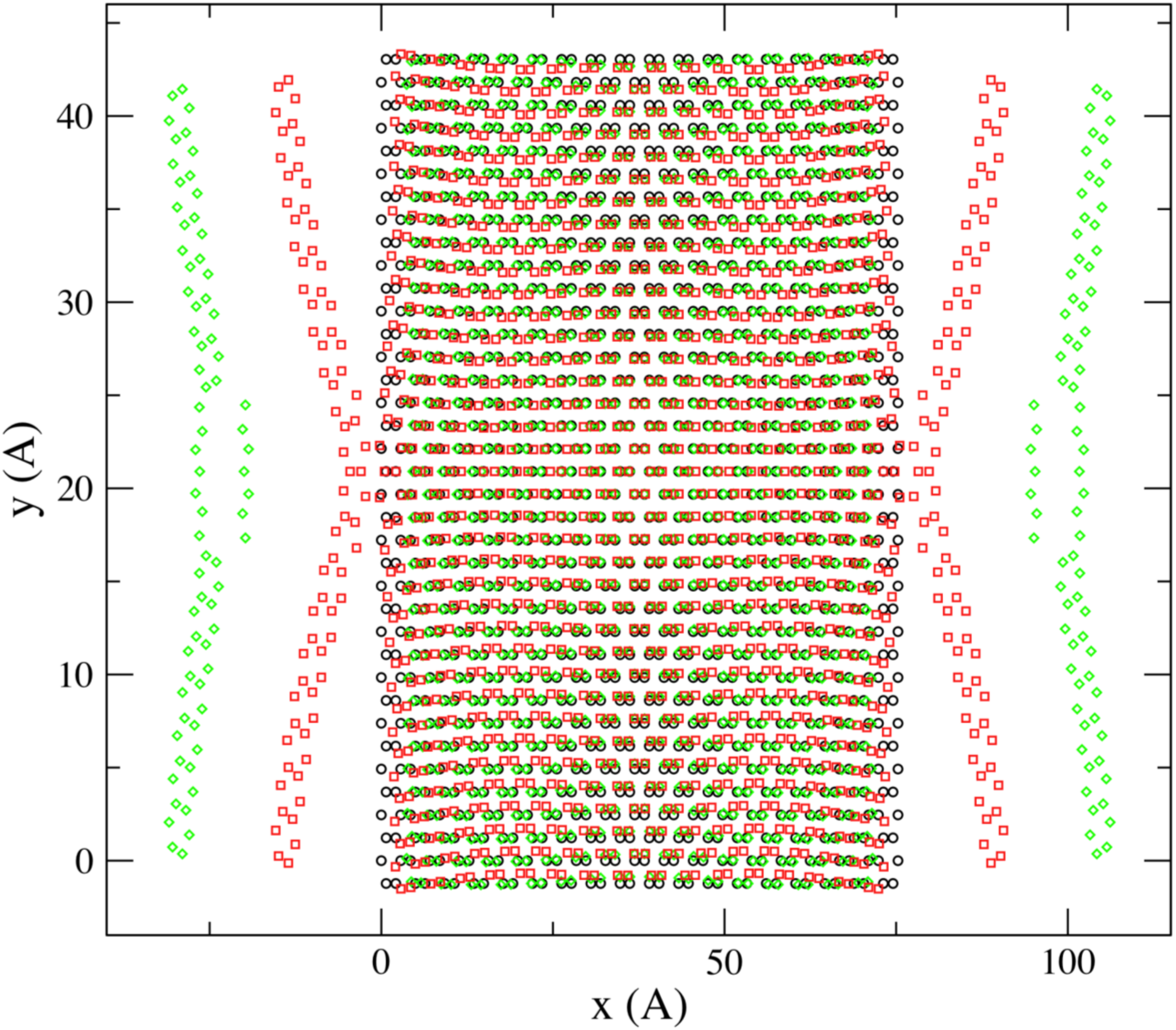
Graphene nanoribbons II



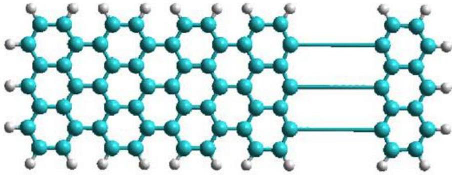


Fracture under uniaxial stress I



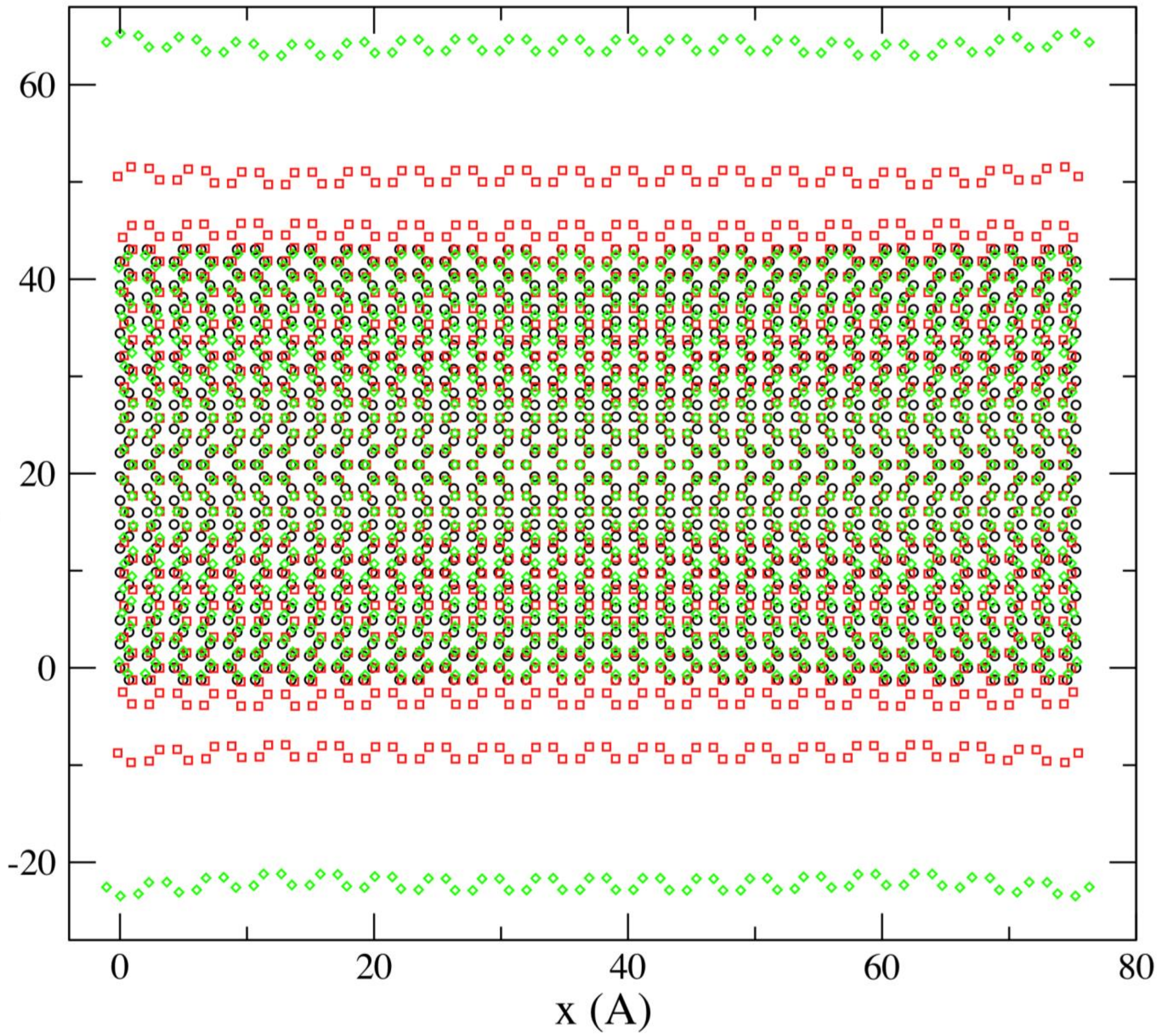


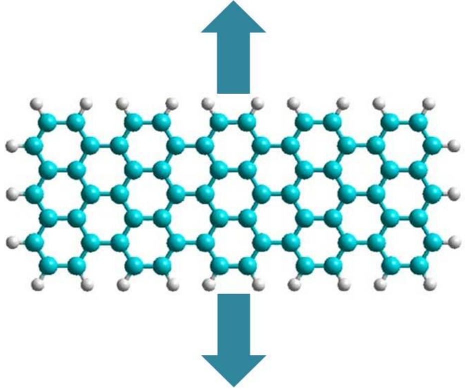
F = 2.5 eV/A



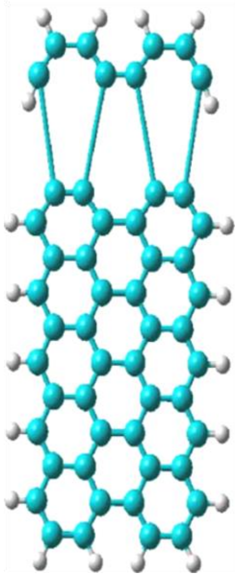
Gao, Hao, *Physica E* **41**, 1561 (2009)

Fracture under uniaxial stress II



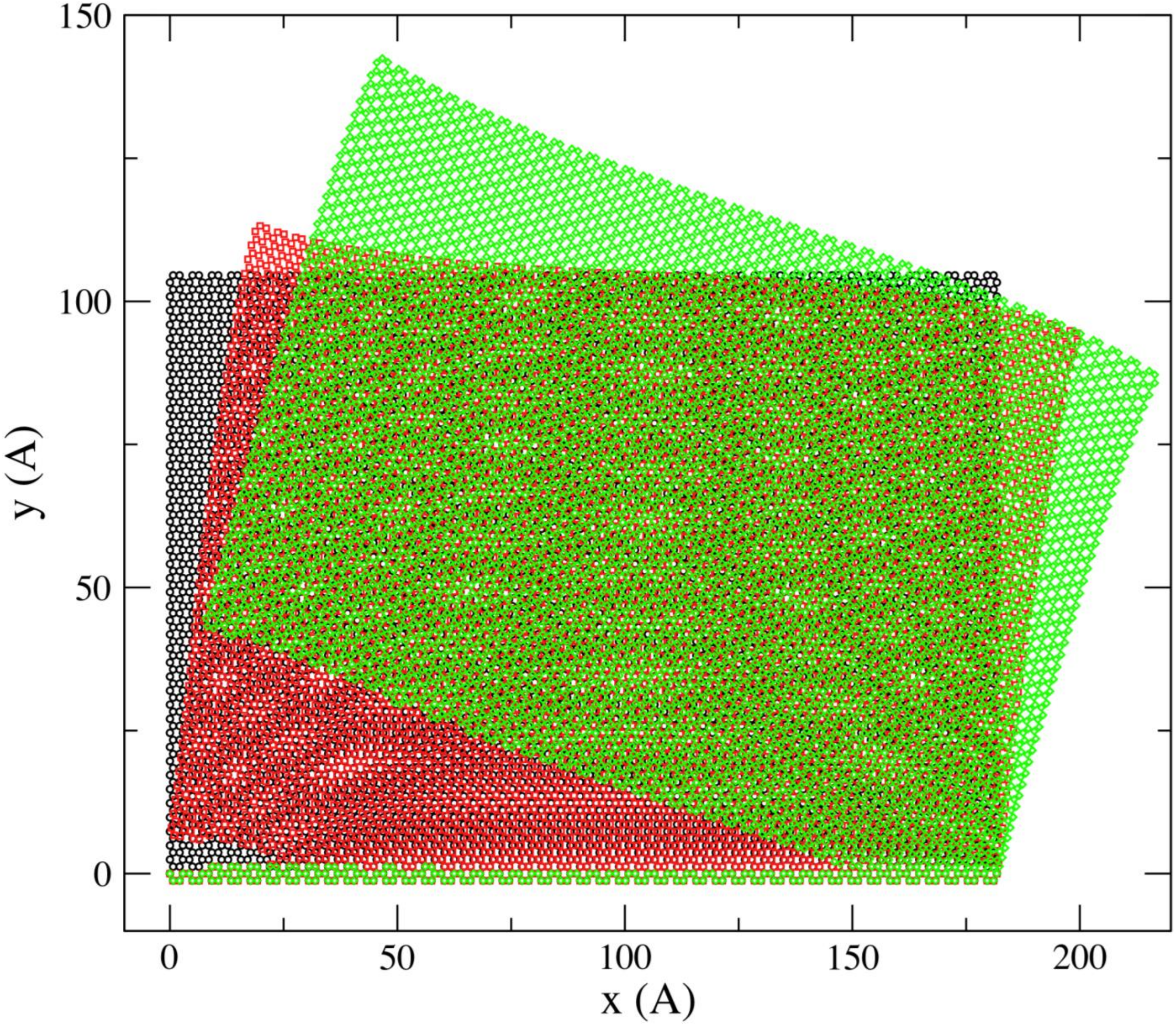


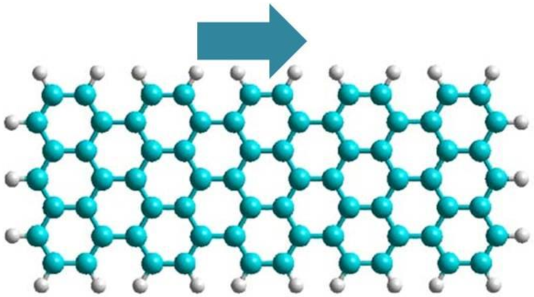
F = 3.1 eV/A



Gao, Hao, *Physica E* **41**, 1561 (2009)

Fracture under shear stress





F = 0.8 eV/A

Graphene distortion under shear stress