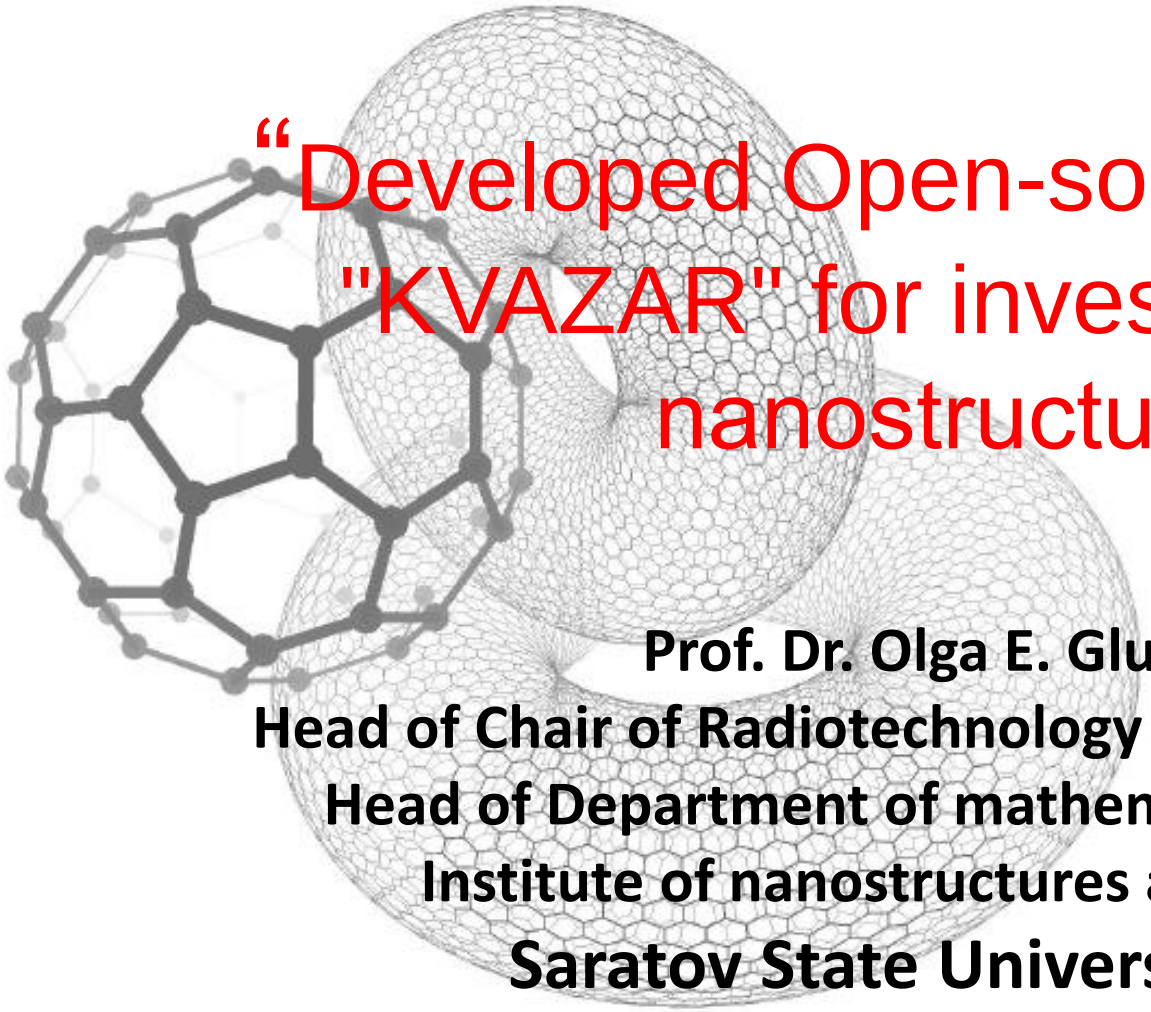


“Developed Open-source software "KVAZAR" for investigations of nanostructures“

Prof. Dr. Olga E. Glukhova,
Head of Chair of Radiotechnology and Electrodynamics,
Head of Department of mathematical modeling of
Institute of nanostructures and biosystems
Saratov State University, Russia

glukhovaoe@info.sgu.ru

Department of Computer Simulations

High-Performance Computing Division

Parallel Computing Algorhythms

Supercomputers maintenance

Databases construction and maintenance

Mathematical Modeling Division

FEM Modeling :

Biomechanics;

Construction mechanics;

Solid structures mechanics;

Structural mechanics;

Composite mechanics

Mechanics of Nanostructures :

Mechanical properties of nanostructures;

Mechanical properties of bionanoobjects;

Multiscale modeling

Nanoelectronics:

Electronic structure;

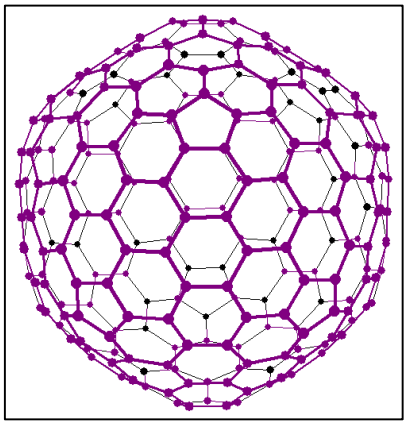
Emission properties;

Electronic cunductivity

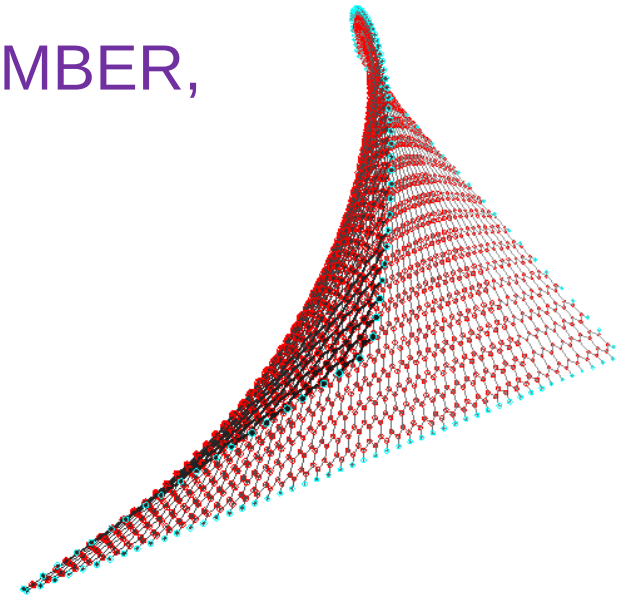
Radiotechnology and Electrodynamics Chair

- Modeling of nanodevices, based on carbon nanoclusters, nanoelectronics, nanobiosystems mechanics, molecular electronics, mathematical modeling of physical processes
- 3D displays, mathematical logic methods, mathematical modeling in biology and medicine
- Theoretical and applied electrodynamics of micro- and extremely high wave frequences
- Radiotechnical research methods of superconductors as the objects for recording, storage and processing of information and optimization of transtormator chains for powerful impulse generators

COMPUTATIONAL METHODS: QUANTUM MECHANICS, MOLECULAR DYNAMICS, MOLECULAR MECHANICS



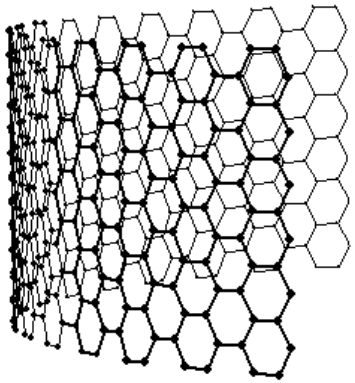
SCC DFTB MD, TBMD, REBO, AMBER, MARTINI and PM(3,6,7)



I. Graphene: electron and mechanical properties

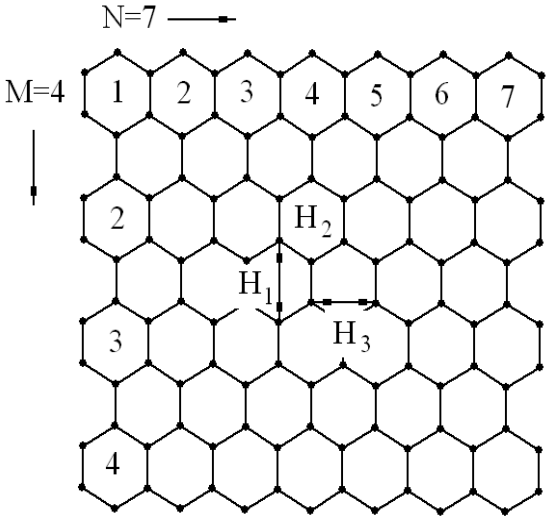
Graphene: electron properties

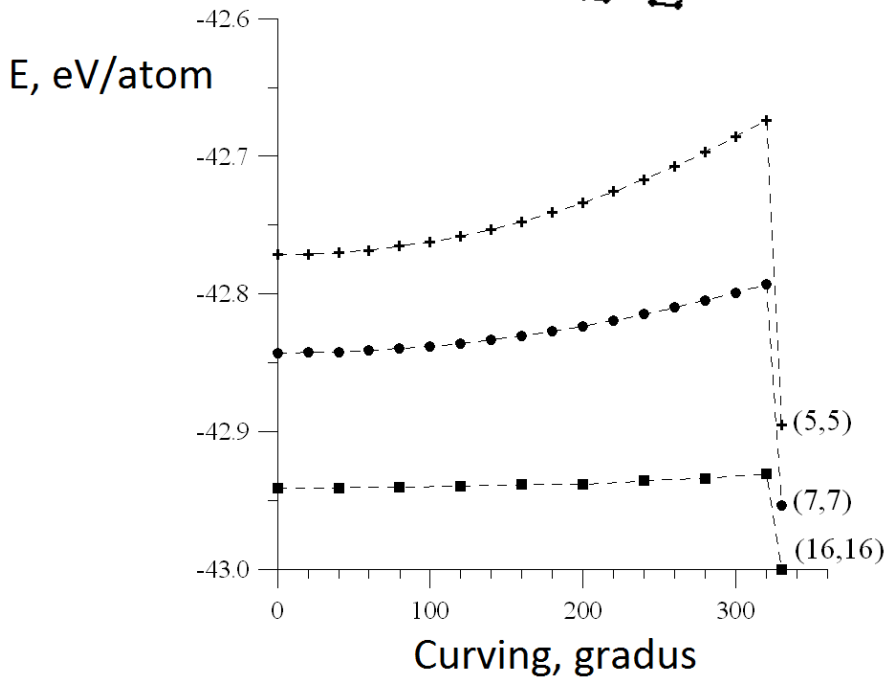
Scroll of nanoribbon (finite size effect)

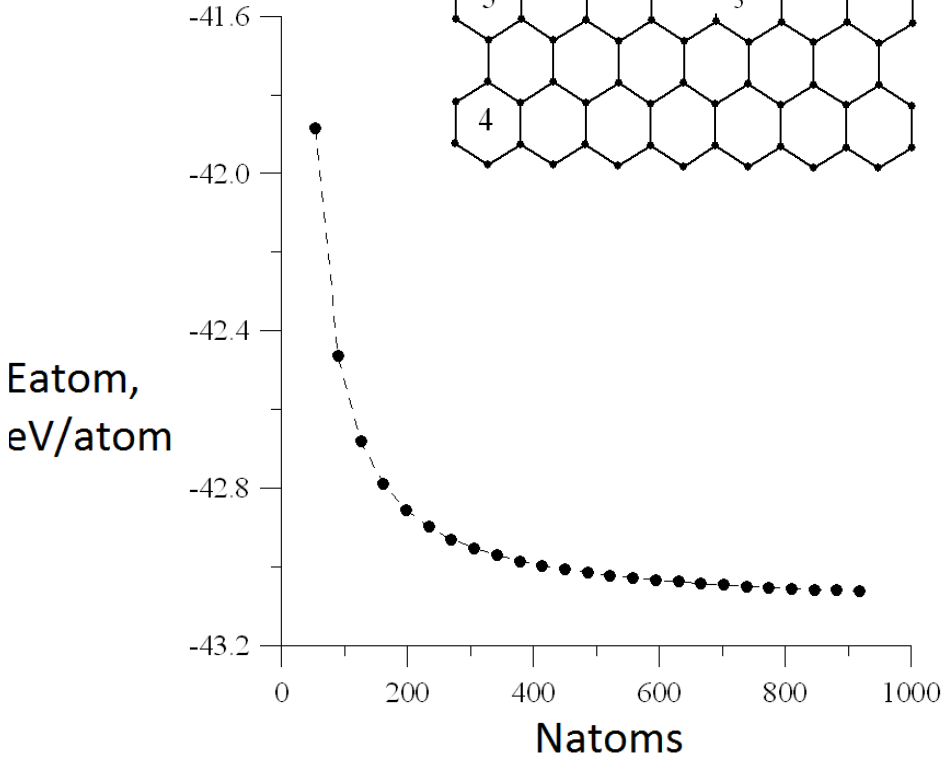


With increasing of the number of atoms the nanoribbon becomes stable

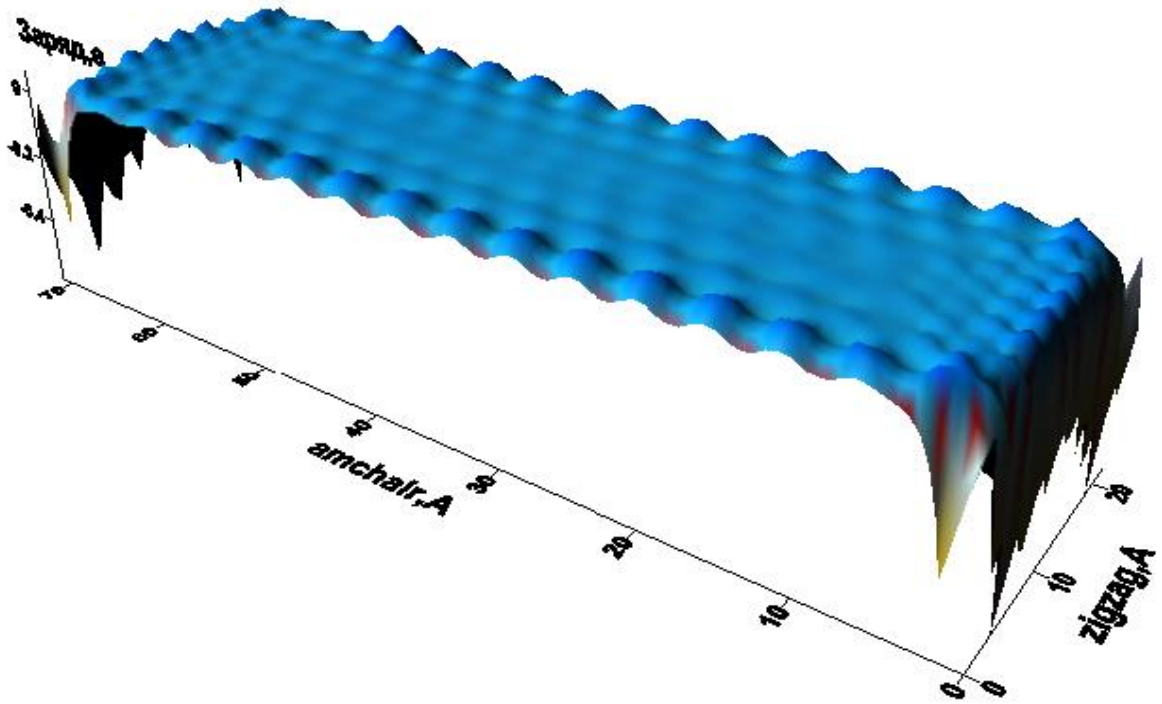
(finite size effect)

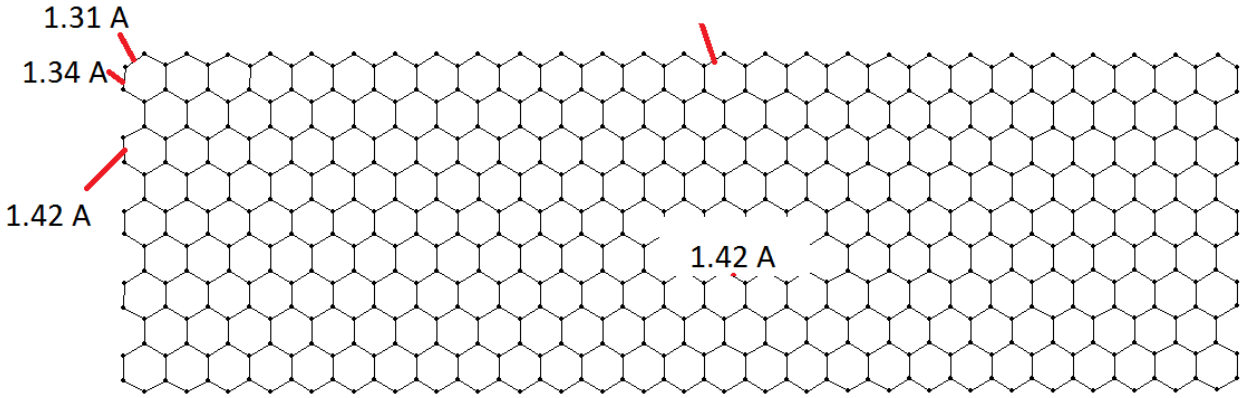




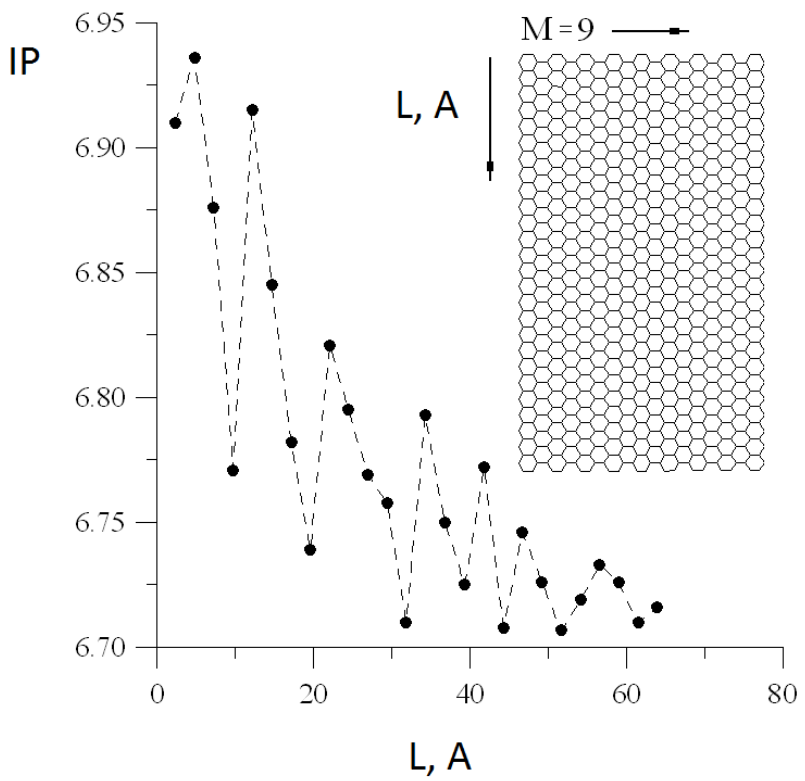


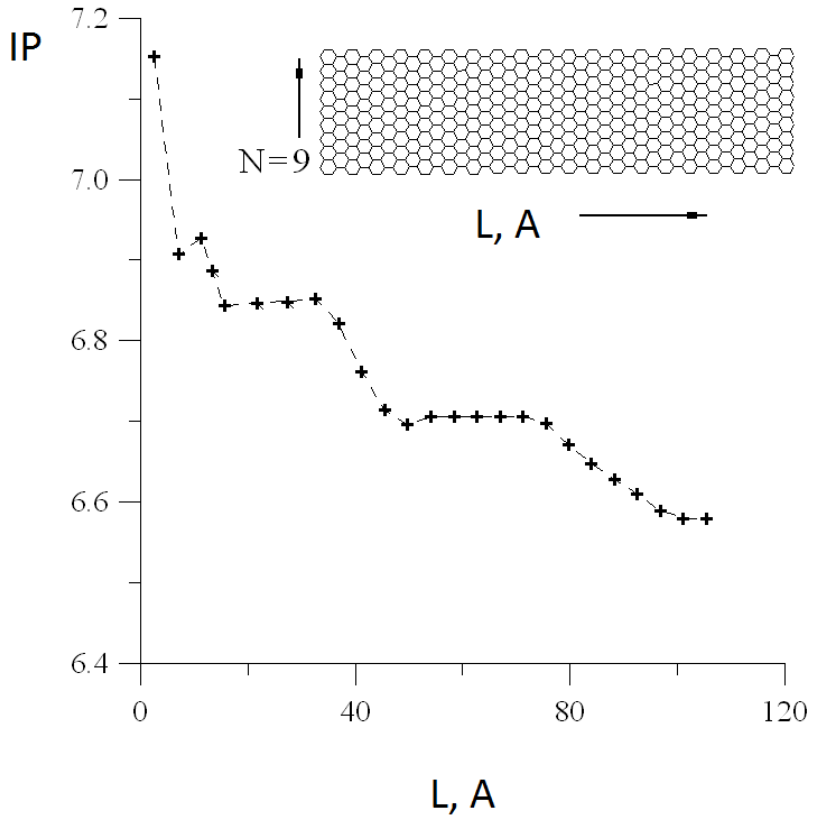
Density of Mulliken charge of carbon atoms of nanoribbon



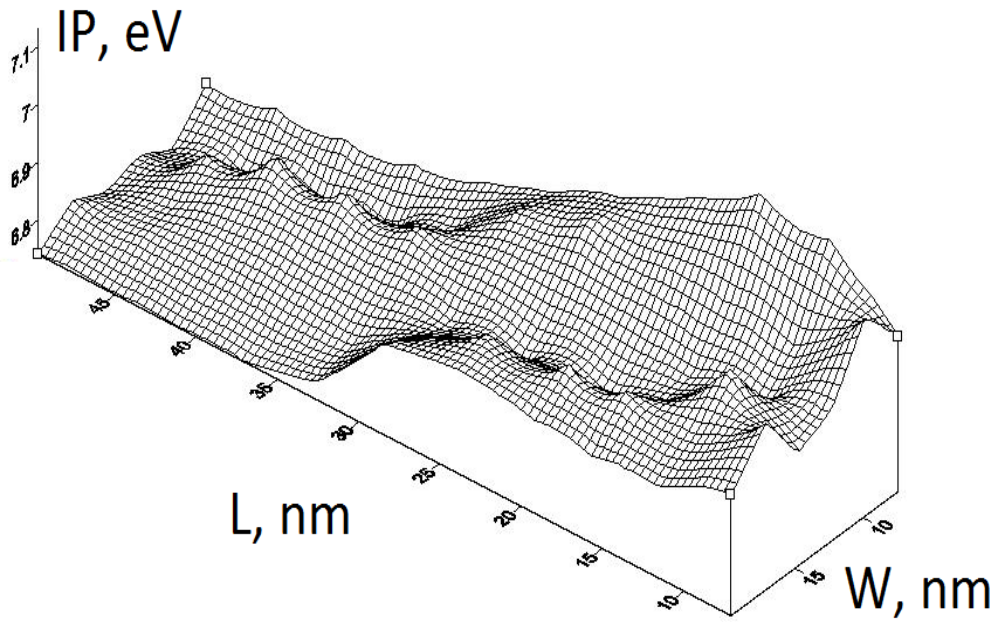


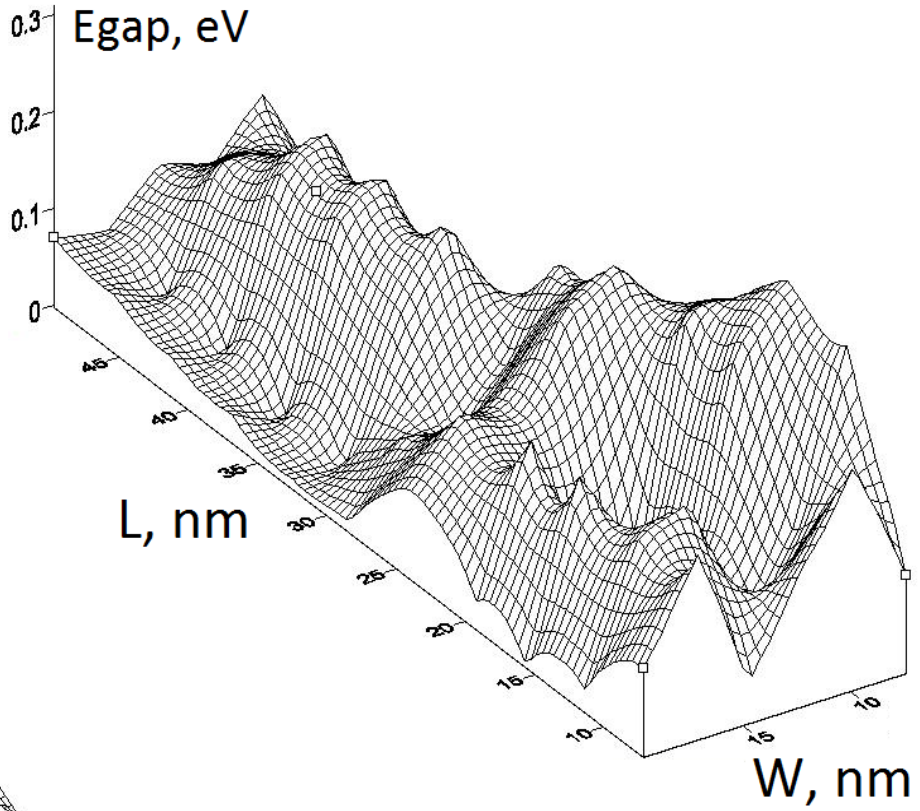
The dependency of IP on the nanoribbon length (finite size effect)





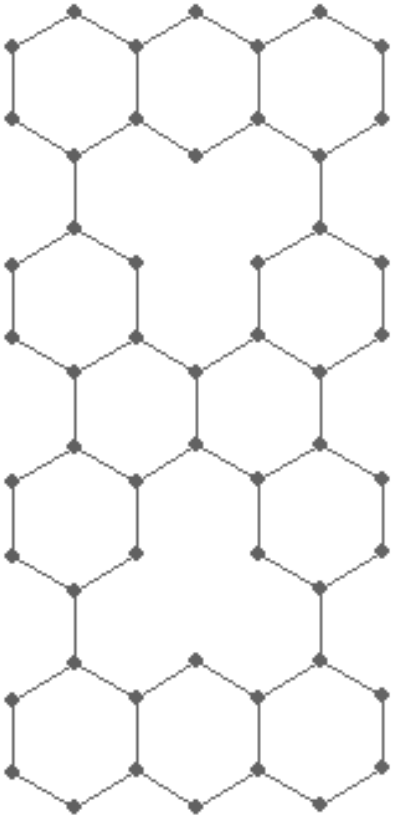
IP of nanoribbons





Energy gap of nanoribbons

Defected nanoribbons



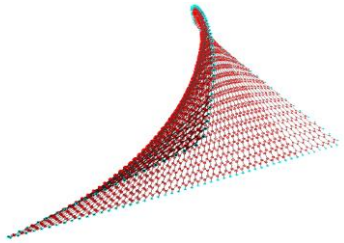
The dependency of IP on the concentration of defect

	0 %	1,8 %	3,6 %	5,4 %
IP, eV	7,15	7,11	7,14	7,15

The dependency of the energy gap on the concentration of defect

	0 %	1,8 %	3,6 %	5,4 %
Egap, eV	0,28	0,14	0,07	0,03

II. MECHANICAL PROPERTIES OF GRAPHENE



Study of deformations and elastic properties of nanoparticles and nanoribbons was implemented on the following algorithm

1) Optimization of atomic structure by entire system energy minimization on atomic coordinates (the atomic structure obtained from previous optimization);
2) Tension or compression of the atomic network of nanoribbon and reoptimization of atomic structure with fixed atoms on the nanoribbon ends;
3) Calculation the Young's pseudo-modulus for the elastic tension of nanoribbon on 1% on formula:

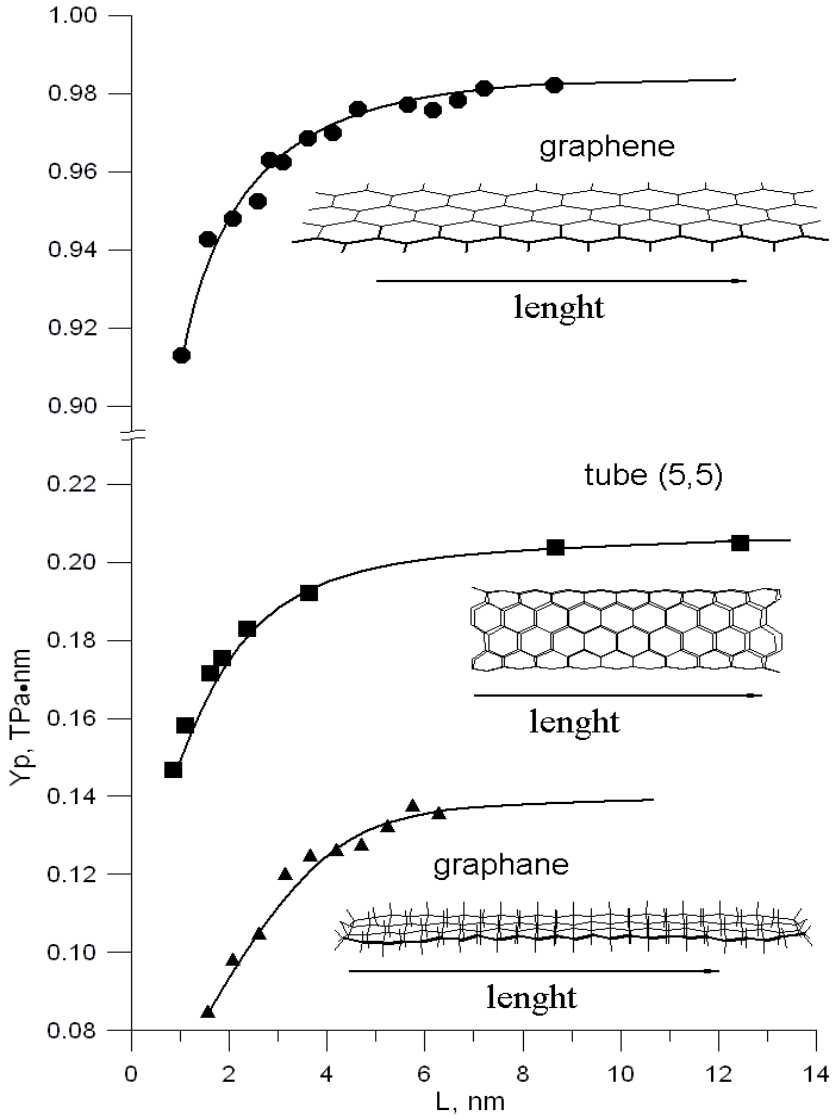
$$Y_p = \frac{F}{D}\frac{L}{\Delta L}$$

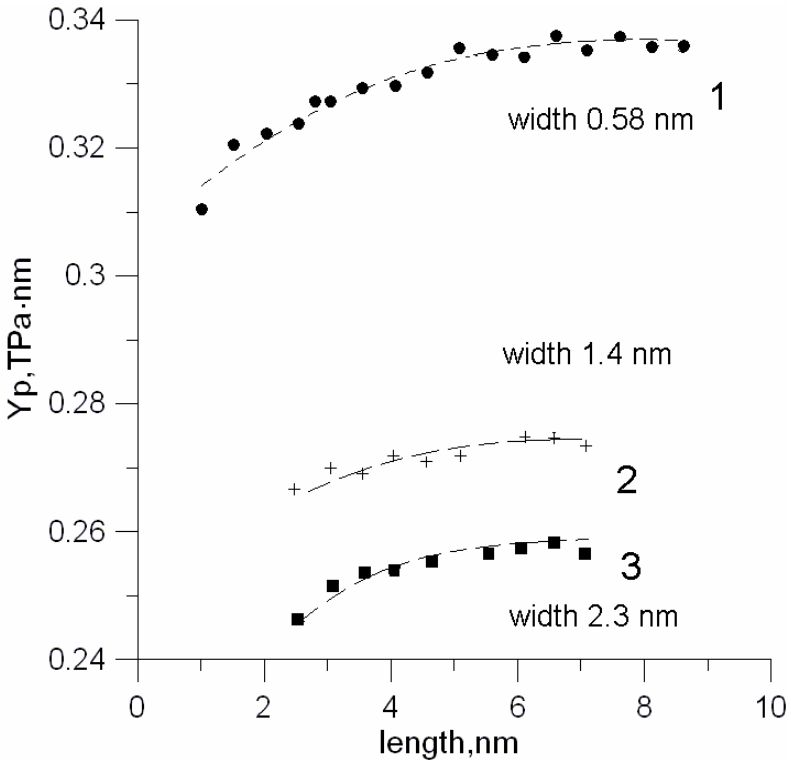
where a deformation force is given by $F = \frac{2\Delta E}{\Delta L}$. Here ΔE is the strain energy, namely, the total energy at a given axial strain minus the total.

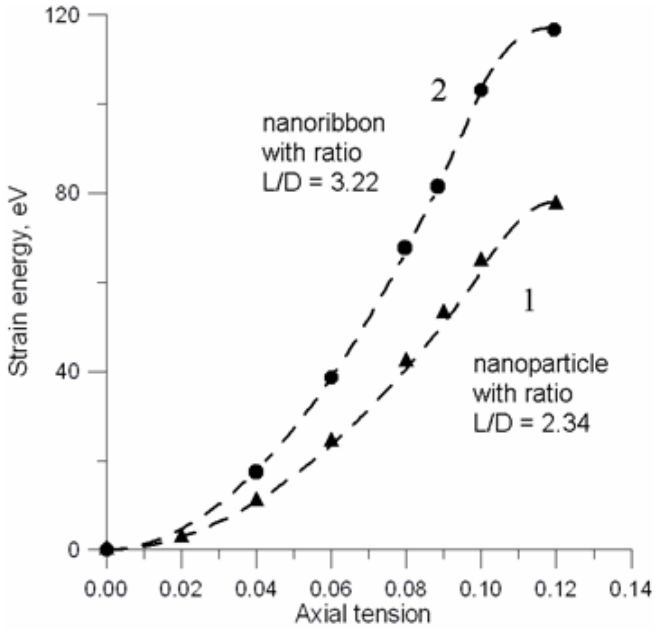
4) Calculation the Young's modulus for the elastic tension of nanoribbon on 1% on formula:

$$Y = \frac{F}{S}\frac{L}{\Delta L}$$

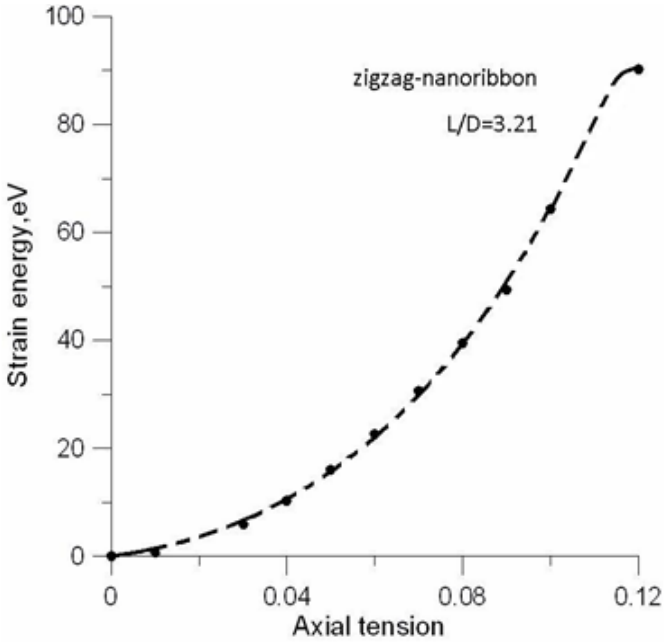
Young's pseudo-modulus (Y^{2D}) of nanoribbons. $Y^{3D} = Y^{2D} * 0.34$ nm



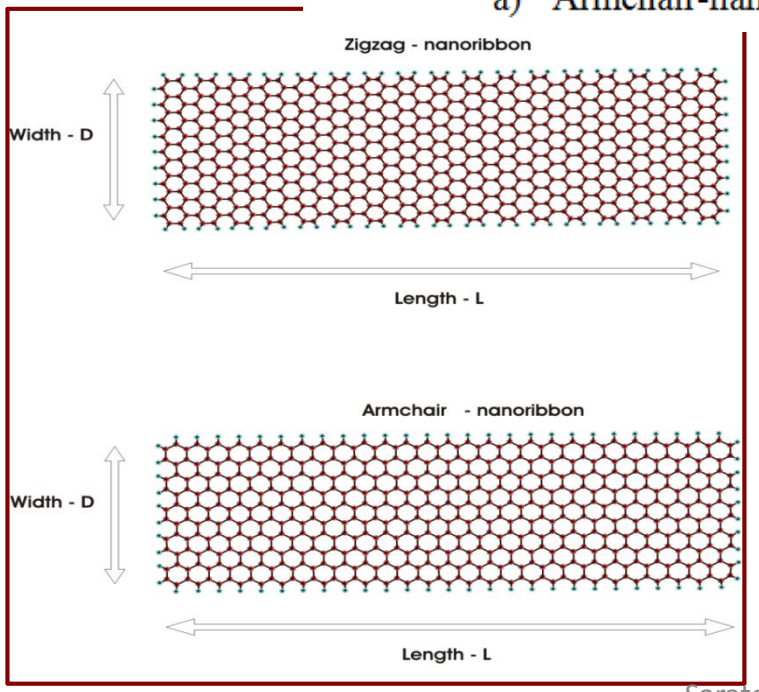




a) Armchair-nanoribbons



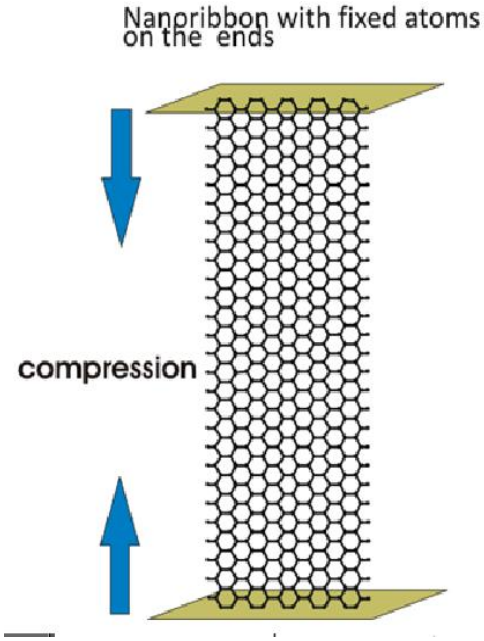
b) Zigzag-nanoribbons

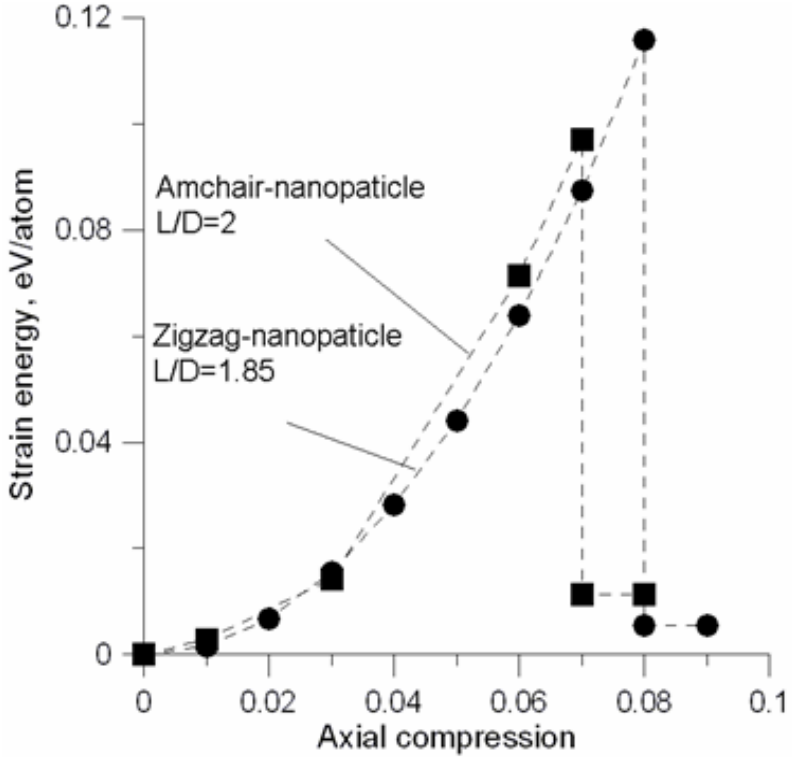


Strain energy of nanoribbons undergoing axial tension

O.E. Glukhova, A.S. Kolesnikova // Physics of the Solid State (Springer). 2011. Vol. 53. No.9 P. 1957-1962.

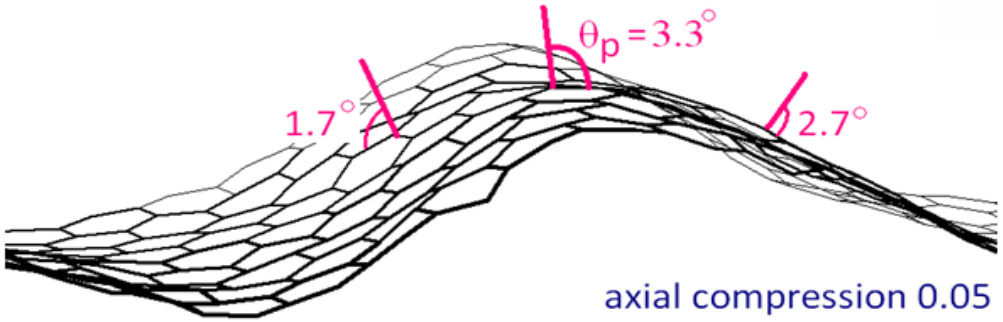
Nanoribbon undergoing axial compression





pyramidalization angles

$\theta_p = \theta_{\sigma\pi} - \pi/2$



O.E. Glukhova, I.N.Saliy, R.Y.Zhnichkov, I.A.Khvatov, A.S.Kolesnikova and M.M.Slepchenkov // Journal of Physics: Conference Series 248 (2010) 012004

The local stress field of the atomic grid of nanostructures: original method (Olga Glukhova and Michael Slepchenkov //Nanoscale, 2012, 4, 3335–3344)

It is proposed to carry out the calculation of the local stress field according to the following algorithm.

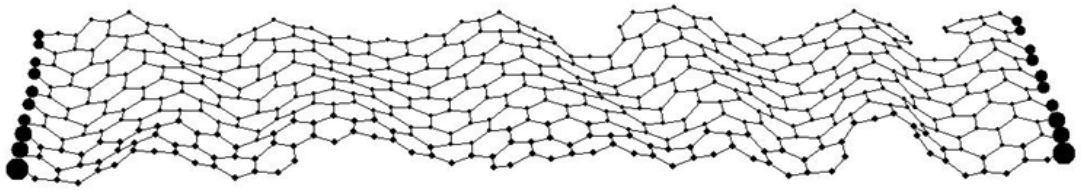
(1) Optimization of the initial structure by means of the quantum-chemical method.

(2) Calculation of distribution of the bulk energy density per atom using the empirical method.

(3) Search of the atomic configuration of the nanostructure subjected to the external influence as a result of the energy minimization for coordinates, using the quantum-chemical method.

(4) Calculation of the distribution of the bulk energy density per atom in the structure subjected to the external influence, using the empirical method.

(5) Calculation of the local stress in the atomic grid according to the difference between the values of the bulk density of energy for the atoms of the structure subjected to the external influence, and the initial structure.



The bulk energy density w_i of the atom i was calculated by the formula:

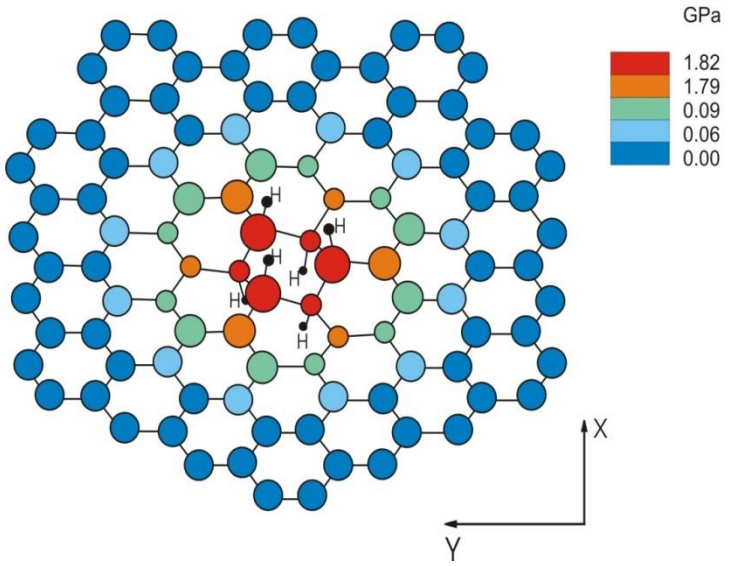
$$w_i = \left(\sum_{j(\neq i)} \left(V_{\mathrm{R}}(r_{ij}) - B_{ij} V_{\mathrm{A}}(r_{ij}) \right) + \sum_{j \neq i} \left(\sum_{k \neq i,j} \left(\sum_{l \neq i,j,k} V_{\mathrm{tros}}(\omega_{ijkl}) \right) \right) + \sum_{j(\neq i)} V_{\mathrm{vdW}}(r_{ij}) \right) \Big/ V_i$$

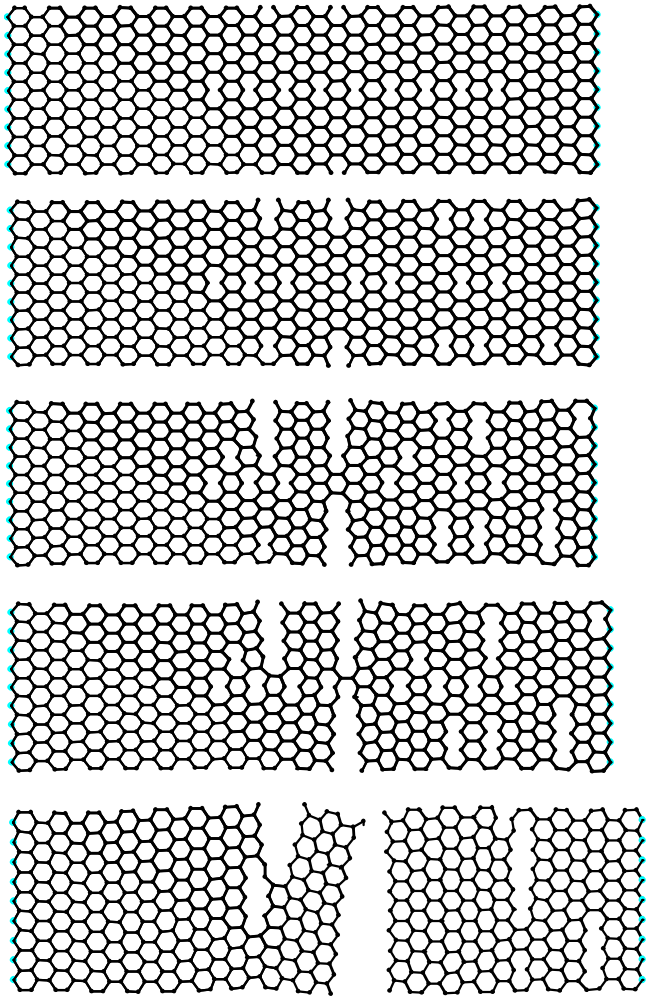
$$V_i = \frac{4}{3} \pi r_0^3$$

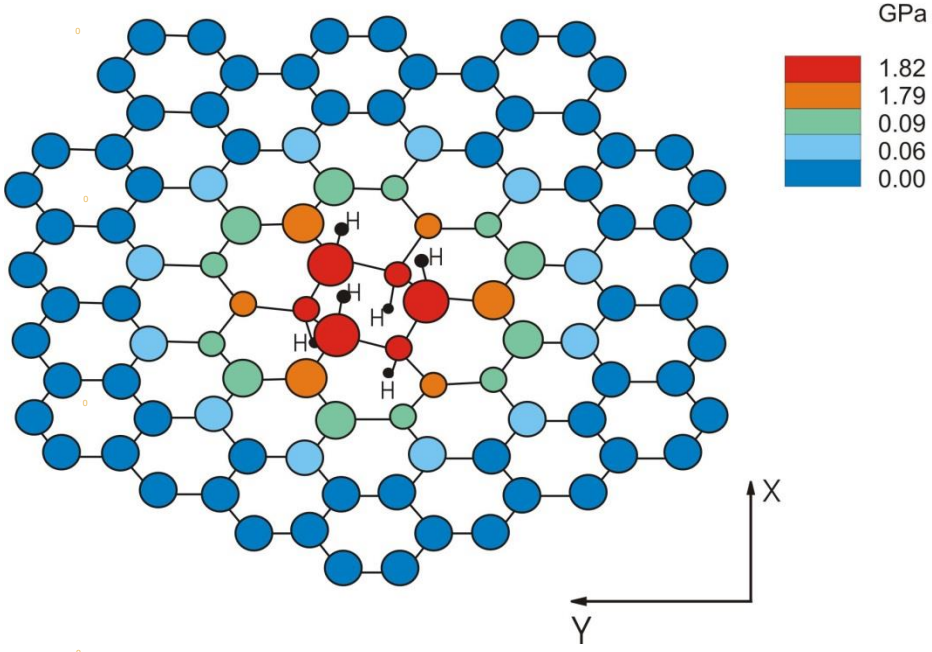
The stress of the atomic grid near the atom with number i is calculated as:

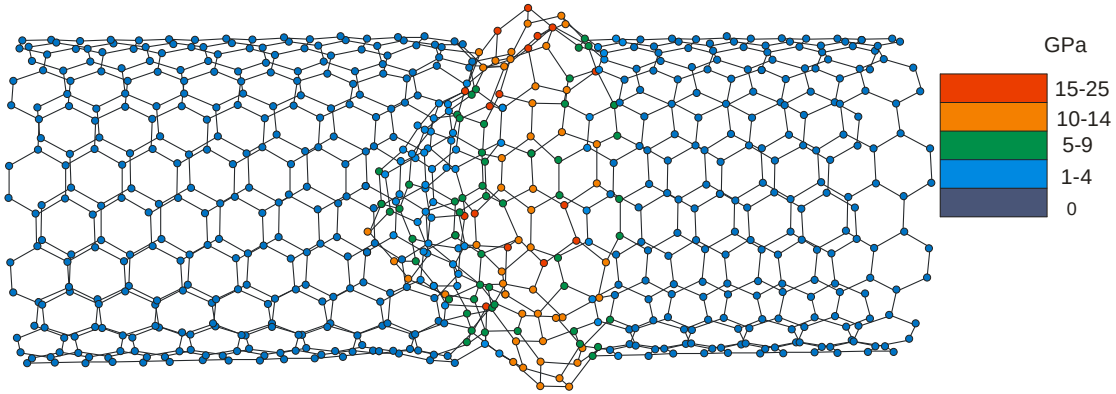
$$\sigma_i = |w_i - w_i^0|$$

where w_i^0 is the bulk energy density of the i^{th} atom of the graphene sheet which is in equilibrium; w_i is the bulk energy density of an atom of the graphene sheet subjected to the external influence (deformation, defect formation, *etc.*). The value of w_i^0 in the centre of the graphene sheet is equal to −58.60 GPa. At the edges of the graphene sheet the bulk energy density is higher since the atoms of the edges have only two links with other carbon atoms. It is equal to −41.54 GPa on an armchair edge and on the zigzag edge is equal to −40.64 GPa. It is suggested that without an external influence the stress equals to zero for the atoms in the centre and at the edges of the graphene sheet.

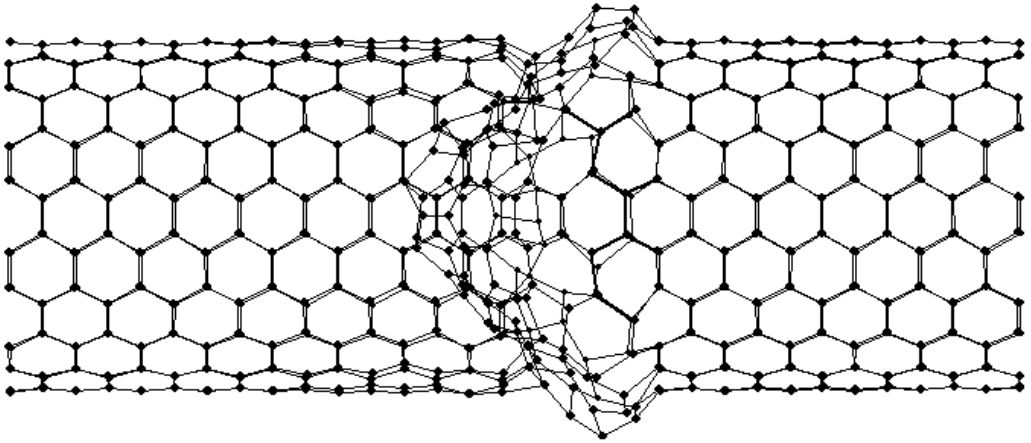


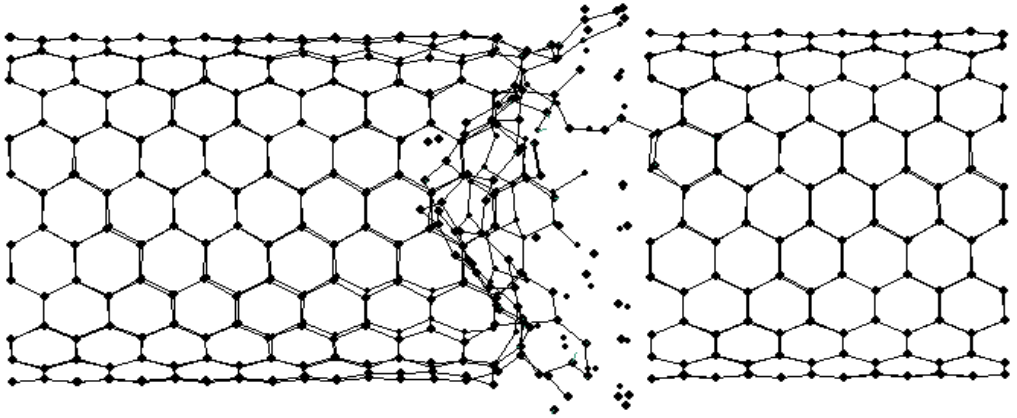



GPa
1.82
1.79
0.09
0.06
0.00
X
Y

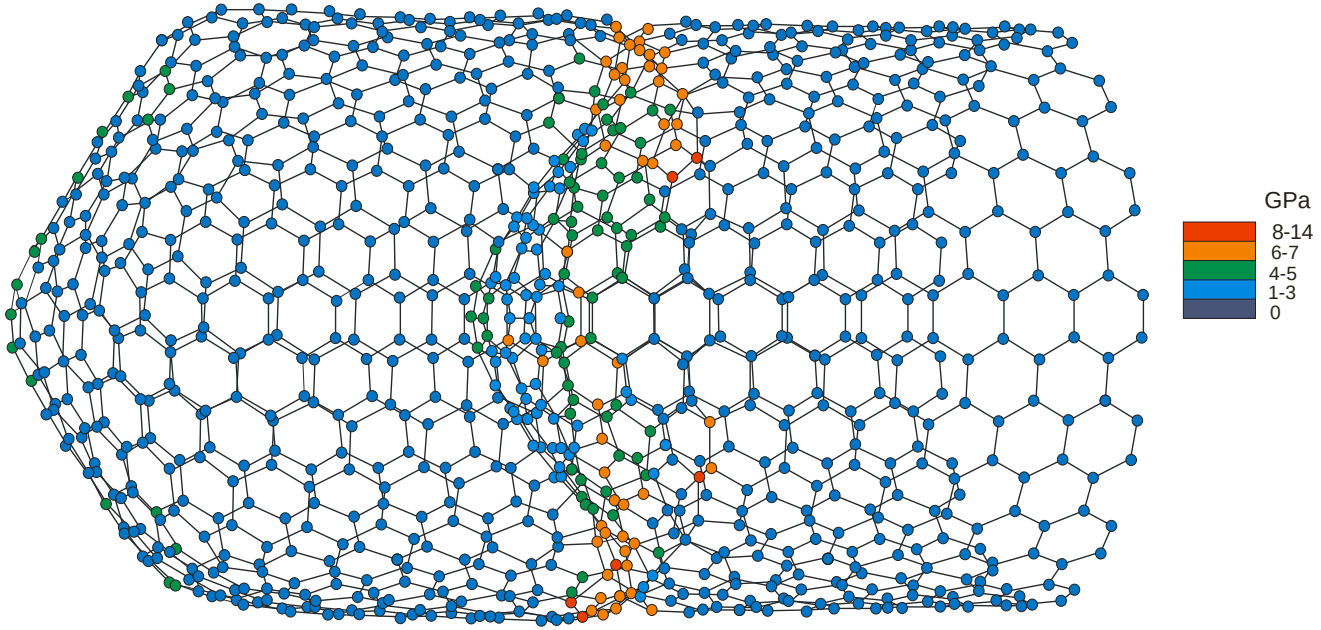


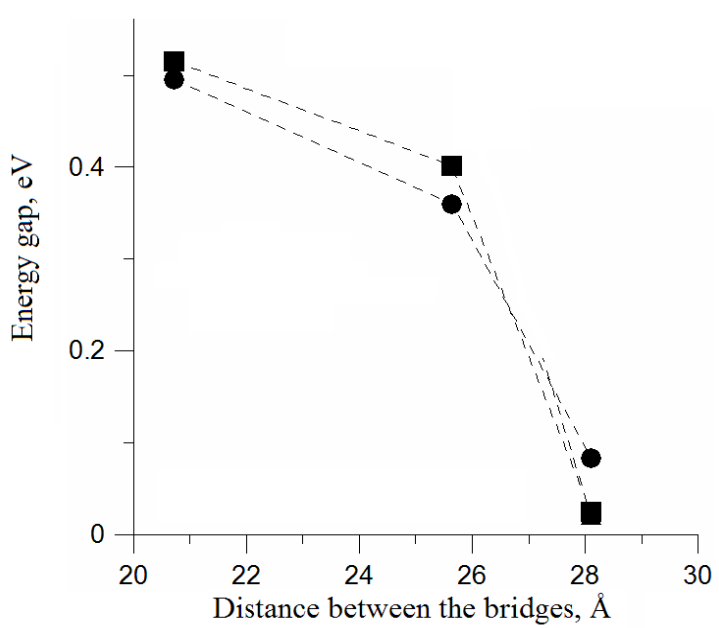
Destruction of the structure of bamboo-like CNT during the increase of the temperature

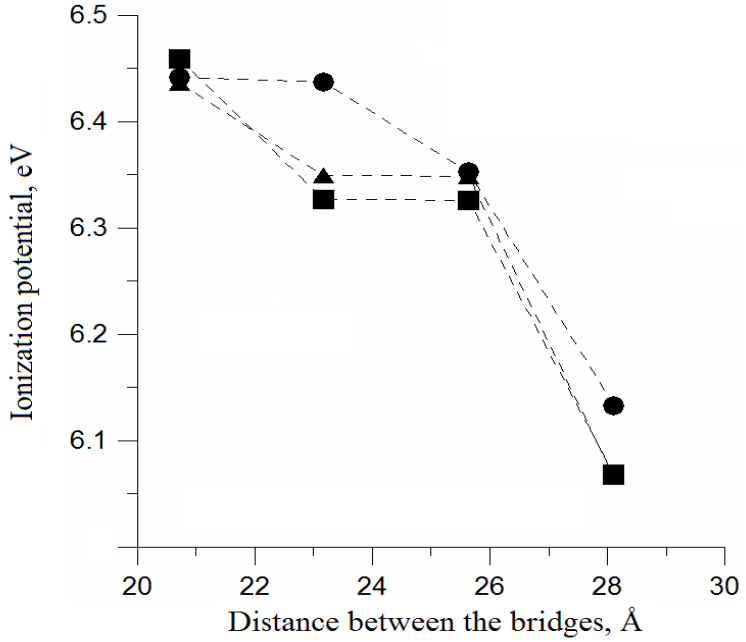




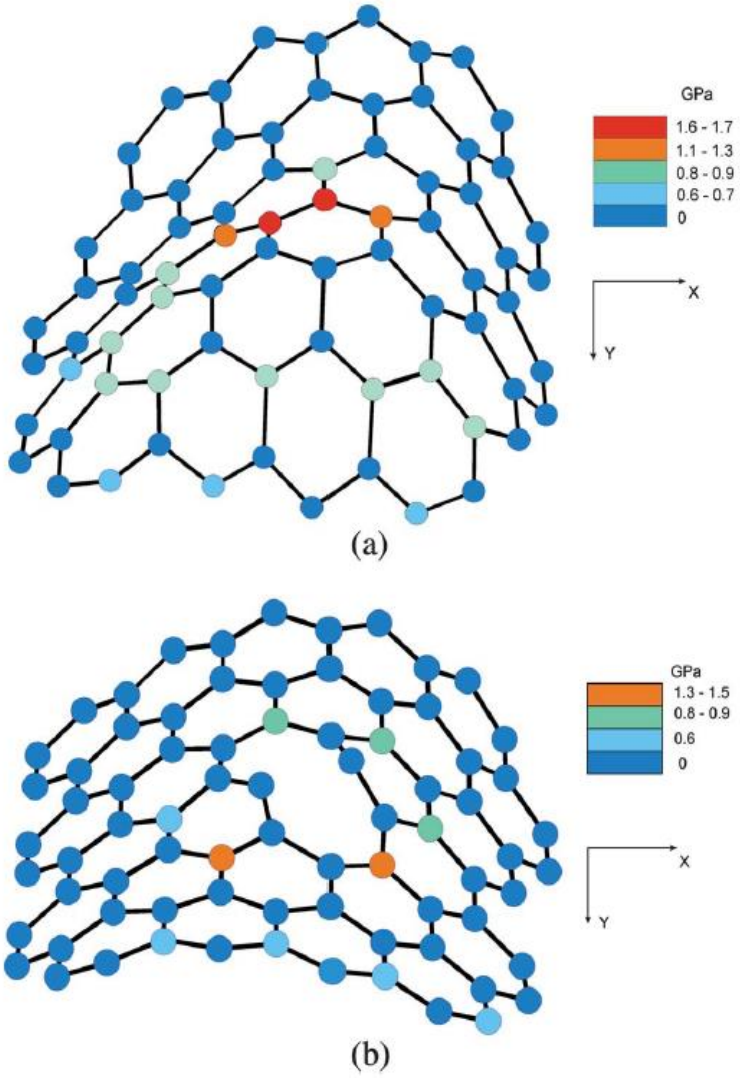
O.E. Glukhova, I.V. Kirillova, A.S. Kolesnikova, E.L. Kossovich, G.N. Ten // Proc. of SPIE. 2012. Vol. 8233. P. 82331E-1-82331E-7.

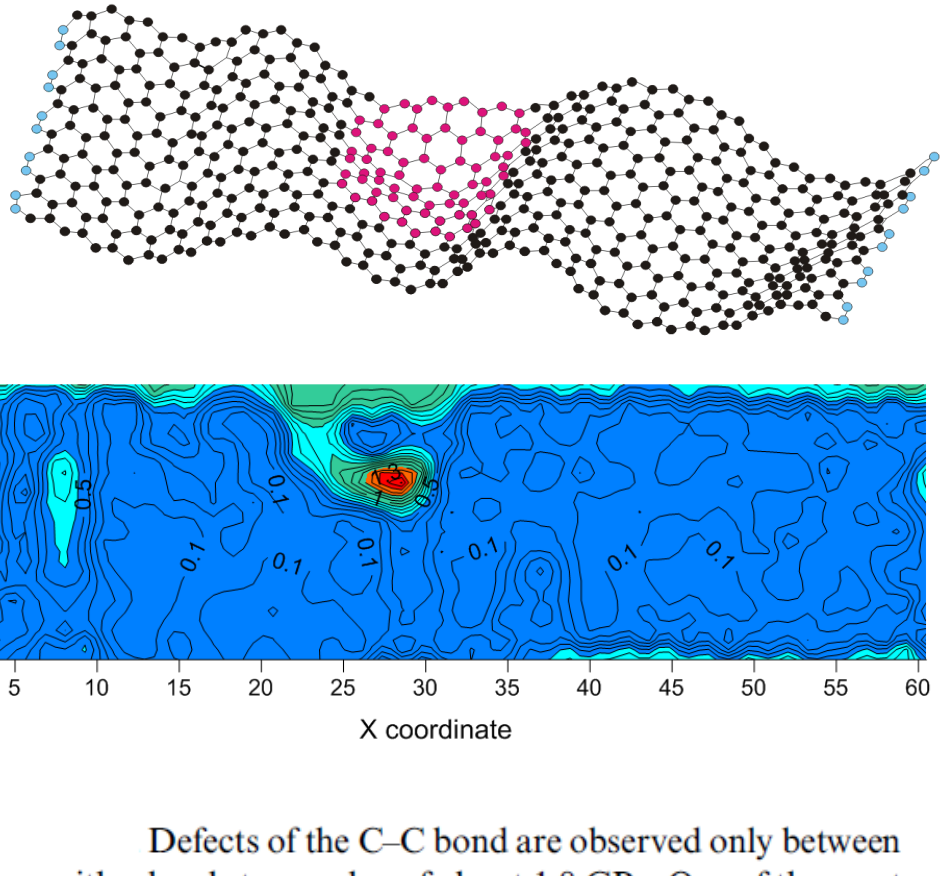

GPa
8-14
6-7
4-5
1-3
0


Energy gap, eV
0
0.2
0.4
20
22
24
26
28
30
Distance between the bridges, Å


Ionization potential, eV
6.1
6.2
6.3
6.4
6.5
20
22
24
26
28
30
Distance between the bridges, Å

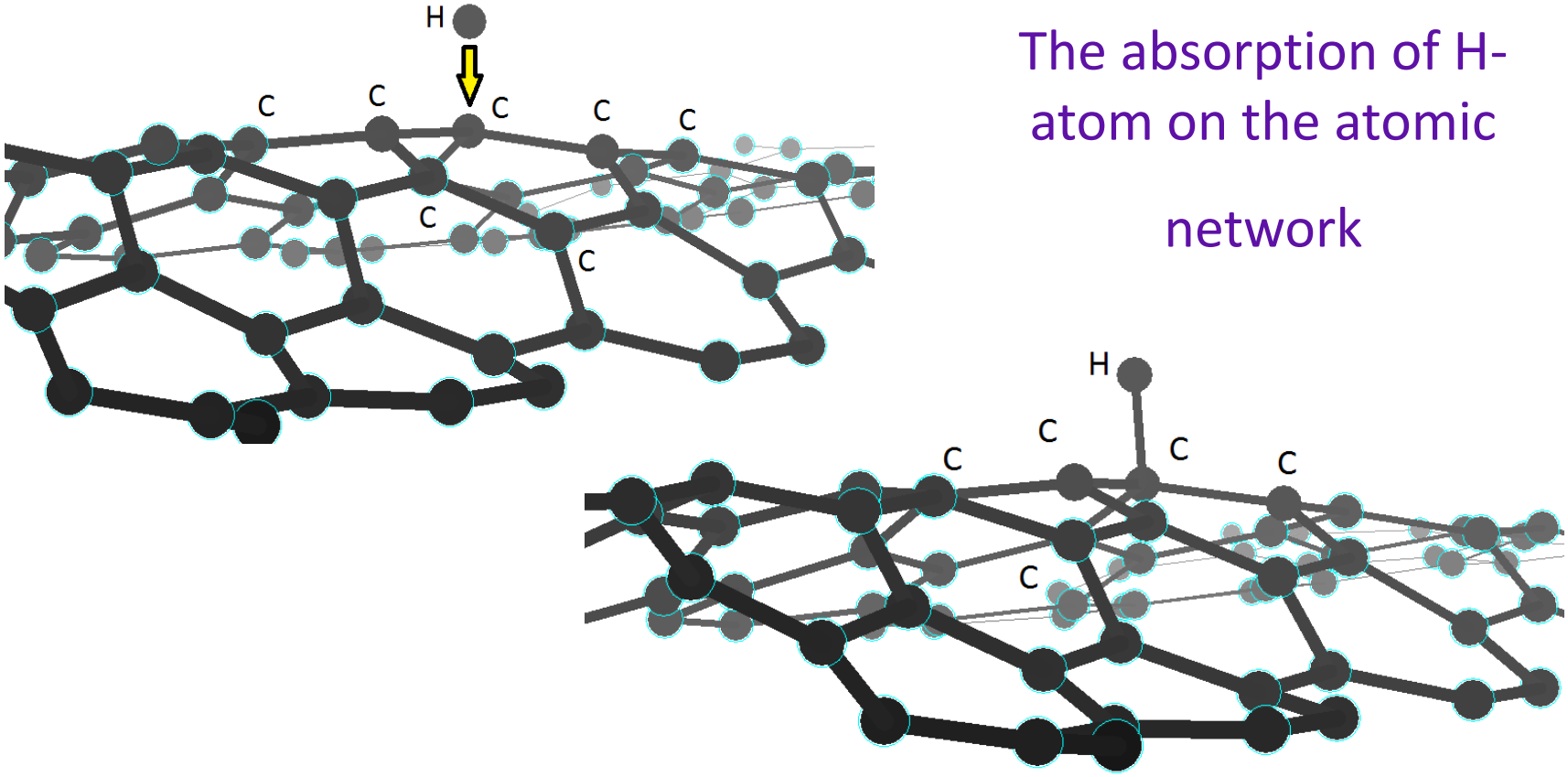
Prediction of the defects appearance





Defects of the C–C bond are observed only between atoms with a local stress value of about 1.8 GPa. One of the most stressed sections of the atomic grid containing a defect is presented in Fig. 4. From the Figure it is clearly seen that after C–C-bond breaking the atomic grid reconstructs and the stress decreases. The enthalpy of the defect formation equals 163.5 kcal mol^{-1}.

The influence of a curvature on the properties of nanostuctures

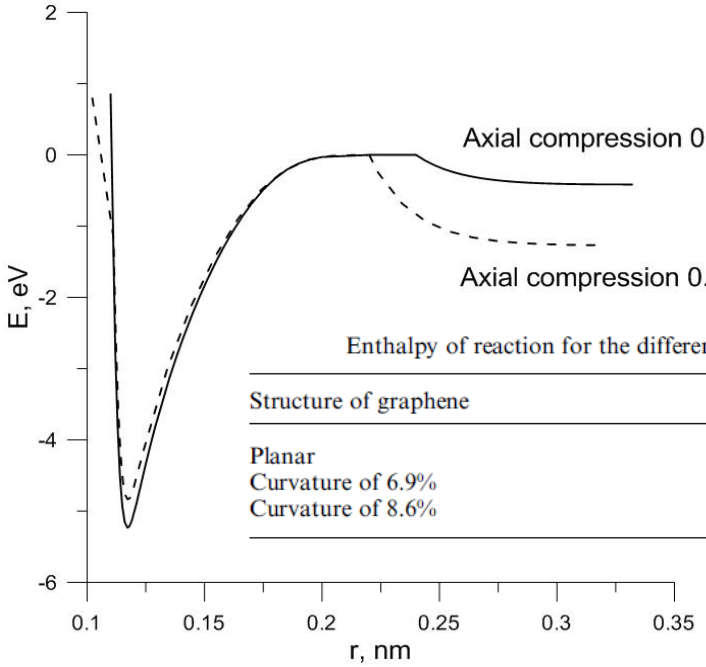


The absorption of H-atom on the atomic network

O.E. Glukhova, I.V. Kirillova, M.M. Slepchenkov The curvature influence of the graphene nanoribbon on its sensory properties // Proc. of SPIE. 2012. Vol. 8233. P. 82331B-1-82331B-6.
Olga E. Glukhova, Michael M. Slepchenkov Influence of the curvature of deformed graphene nanoribbons on their electronic and adsorptive properties: theoretical investigation based on the analysis of the local stress field for an atomic grid // Nanoscale 2012. Issue 11. Pages 3335-3344. DOI:10.1039/C2NR30477E.

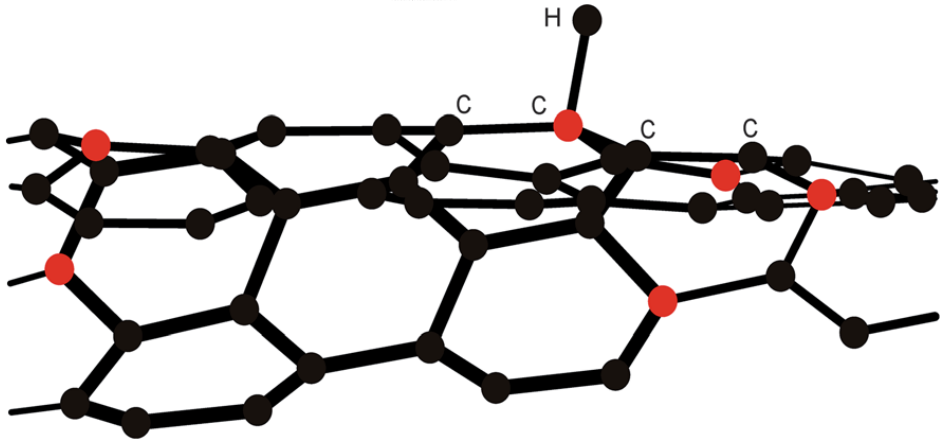
The total energy of the structure depends on the distance between the hydrogen atom and the carbon atom.

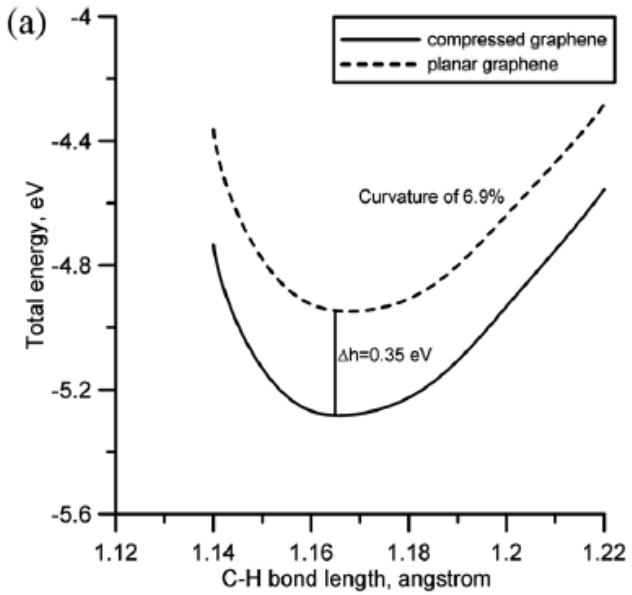
(The dashed line is the interaction of the hydrogen atom with planer graphene nanoribbon; the solid line is the interaction of the hydrogen atom from wave-like graphene nanoribbon)

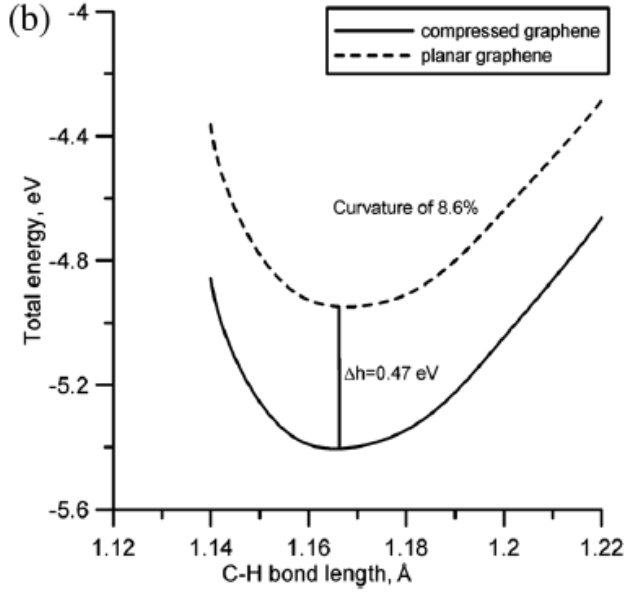


Enthalpy of reaction for the different graphene structures

Structure of graphene	Enthalpy of reaction
Planar	−23.31 kcal mol^{-1}
Curvature of 6.9%	−28.13 kcal mol^{-1}
Curvature of 8.6%	−31.59 kcal mol^{-1}



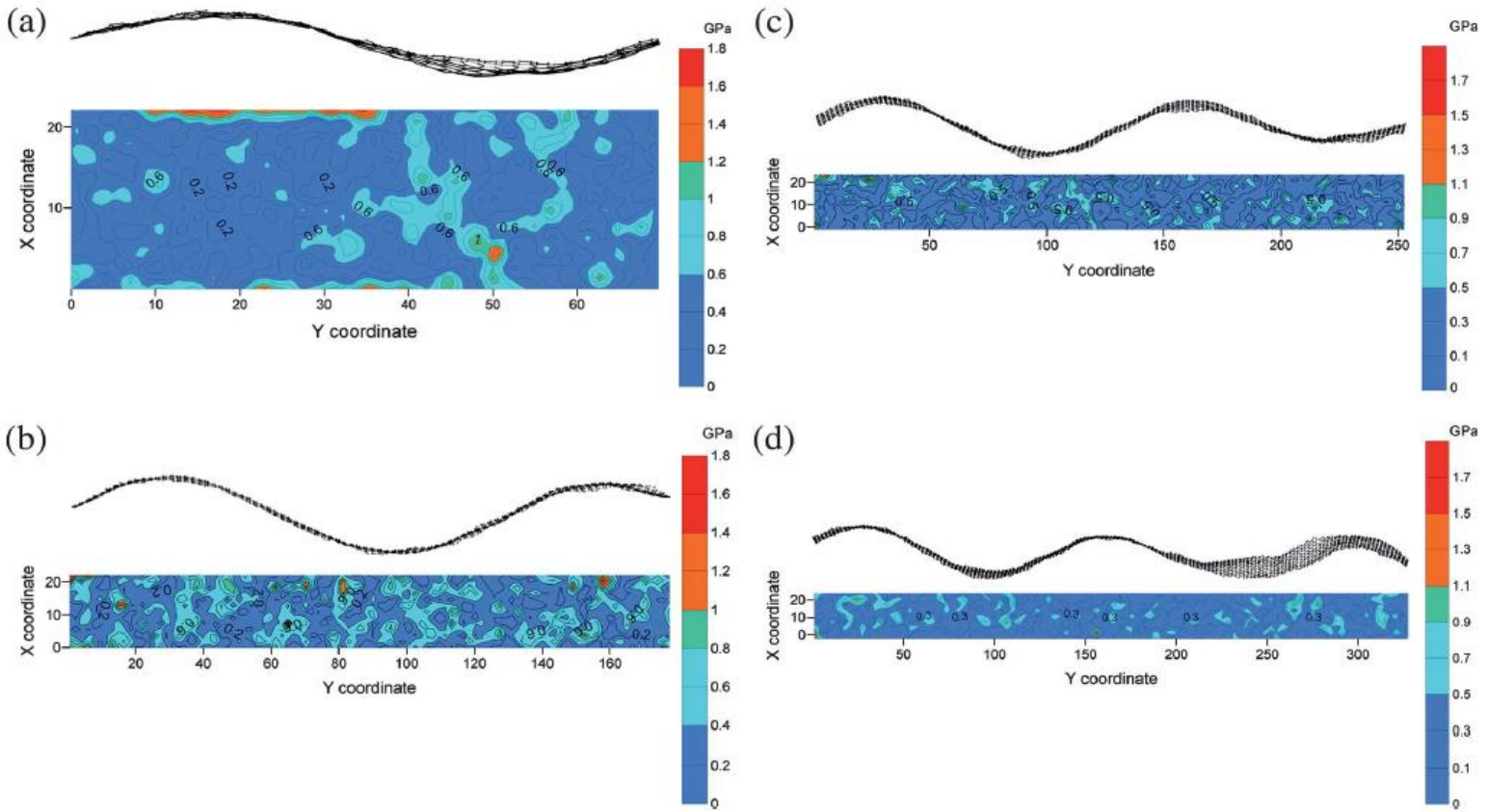




The dependence of the chemical C–H interaction energy on the length of the C–H bond for the planar and compressed graphene nanoribbon: (a) with curvature of 6.9%; (b) with curvature of 8.6%.

Geometrical characteristics of the curved armchair graphene nanoribbons compressed up to 98% of initial length

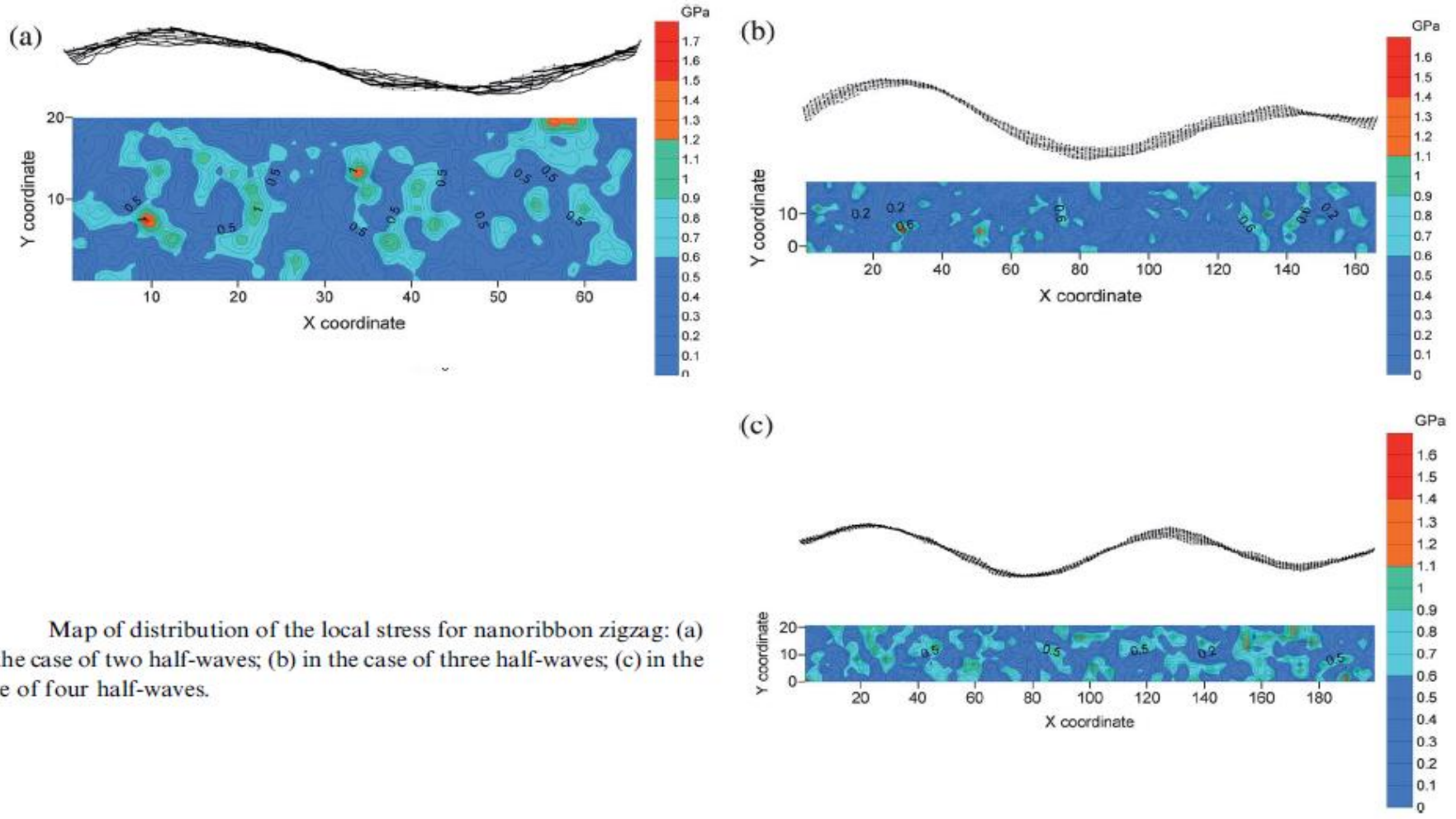
Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	646	71.0	35.5	2.2	9	22.4
3	1634	181.7	60.5	5.3	14	
4	2318	258.4	64.6	5.65	15	
5	3002	335.12	66.2	5.4	15	



Map of distribution of the local stress for the nanoribbon armchair: (a) in the case of two half-waves; (b) in the case of three half-waves; (c) in the case of four half-waves; (d) in the case of five half-waves.

Geometrical characteristics of the curved zigzag graphene nanoribbons compressed up to 98% of the initial length

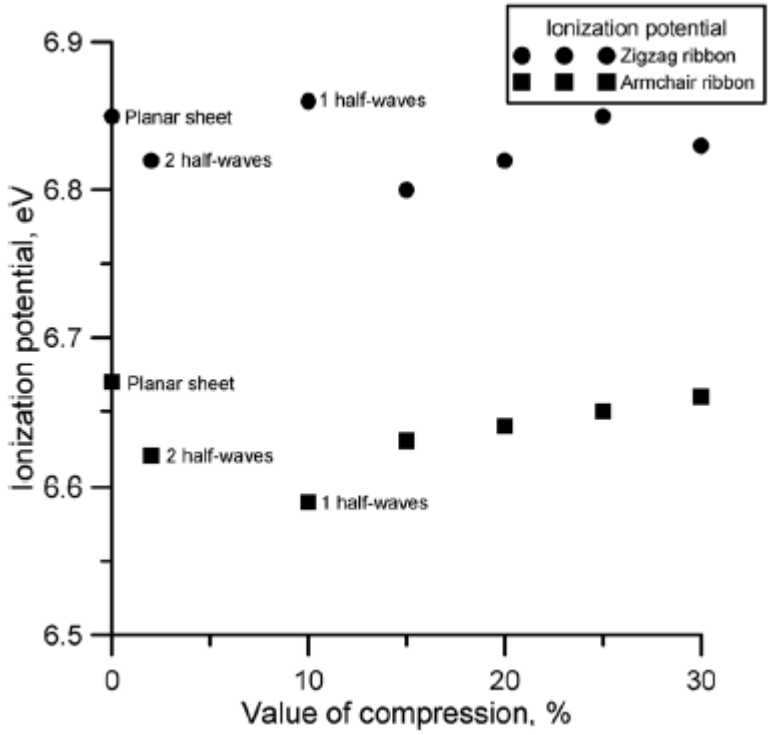
Number of half-waves	Number of atoms in structure	Length of nanoribbon/Å	Length of half-wave/Å	Amplitude of half-wave/Å	Number of hexagons in half-wave	Width of nanoribbon/Å
2	550	65	32.5	2.8	12	19.88
3	1390	165.18	55.06	5.4	20	
4	1670	198.7	49.6	5.6	20	

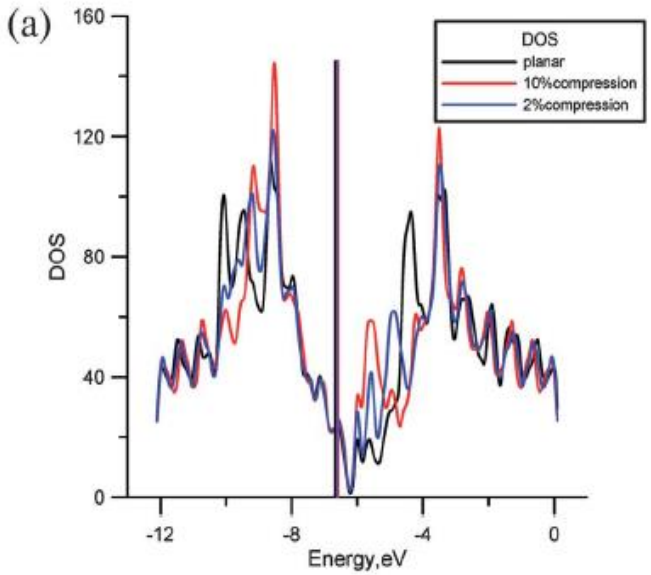


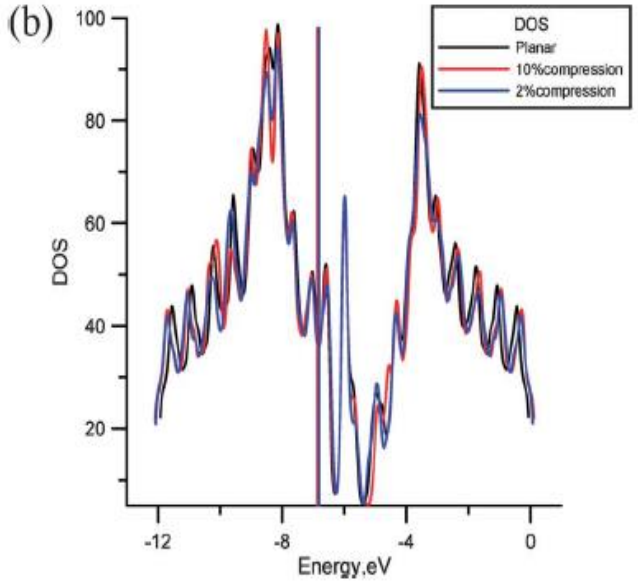
Map of distribution of the local stress for nanoribbon zigzag: (a) in the case of two half-waves; (b) in the case of three half-waves; (c) in the case of four half-waves.

Some parameters of the electronic structure of nanoribbons

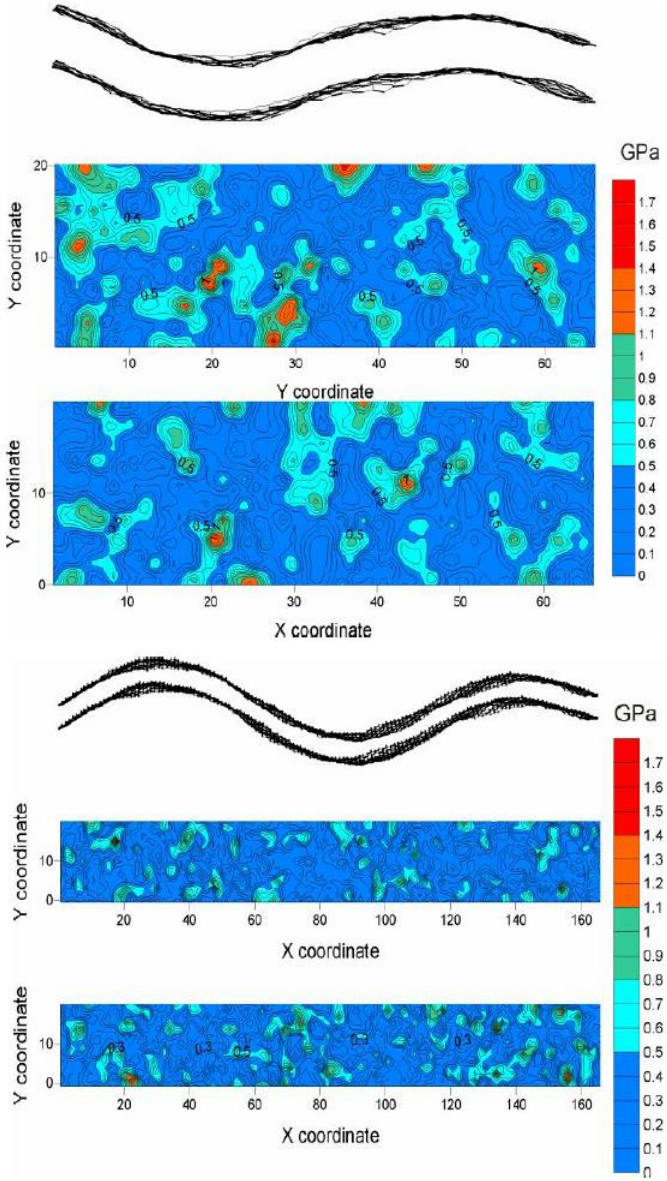
Number of half-waves	Length of half-wave/Å	IP/eV	E_{gap}/eV
Armchair ribbon of width 22.4 Å			
2	71.0	6.63 (6.65)	0.04 (0.03)
3	181.7	6.50 (6.53)	0.04 (0.03)
4	258.4	6.44 (6.47)	0.02 (0.01)
5	335.12	6.41 (6.44)	0.04 (0.02)
Zigzag ribbon of width 19.88 Å			
2	65	6.82 (6.84)	0.04 (0.02)
3	165.18	6.79 (6.81)	0.01 (0.01)
4	198.7	6.80 (6.81)	0.01 (0.01)

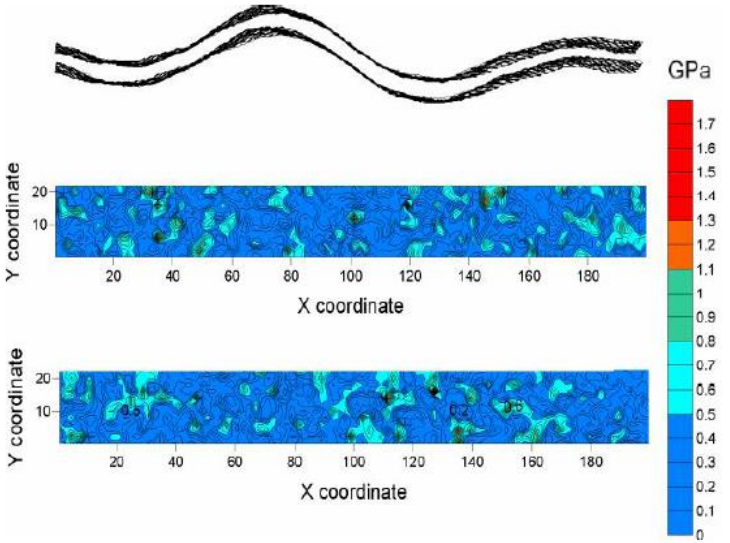






The compression process of bi-layer graphene



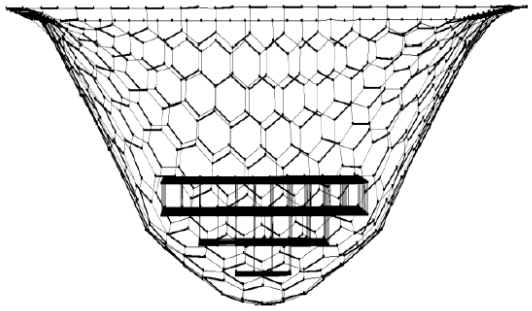


Geometrical characteristics of the curved zigzag bi-layer graphene nanoribbons compressed up to 98% of the initial length

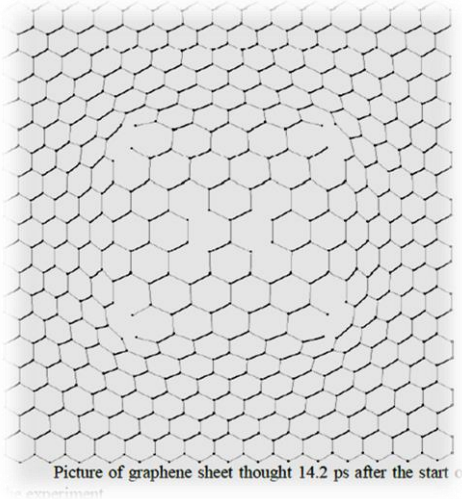
Number of half-waves	Number of atoms in structure	Length of nanoribbon, Å	Length of half-wave, Å	Amplitude of half-wave, Å	Number of hexagons in half-wave	Width of nanoribbon, Å
2	1100	65	32.3	3.1	13	
3	2780	165.18	55.4	5.48	20	19.88
4	3340	198.7	49.8	5.55	20	

Investigation of the one-layer graphene plate

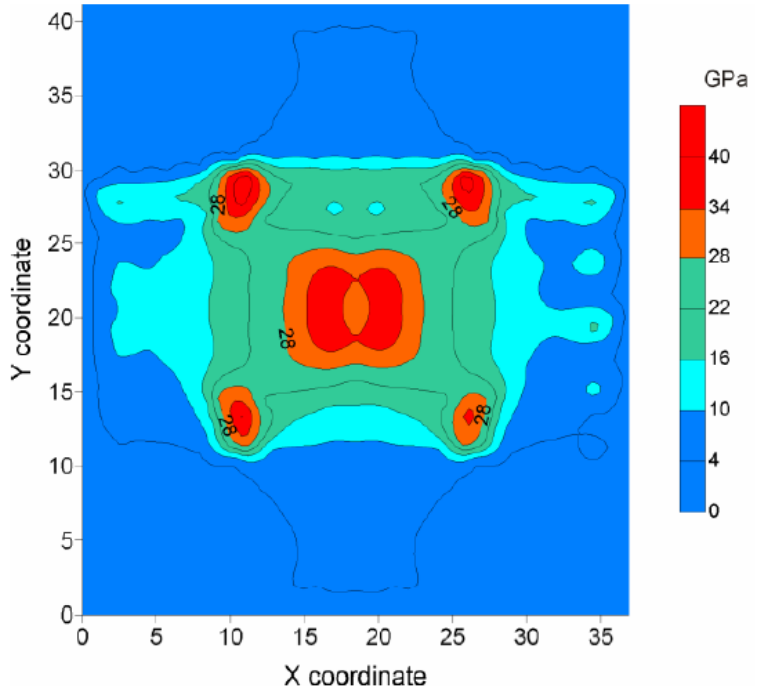
The deflection of the graphene sheet (620 atoms) by means of the platinum pyramid (376 atoms).



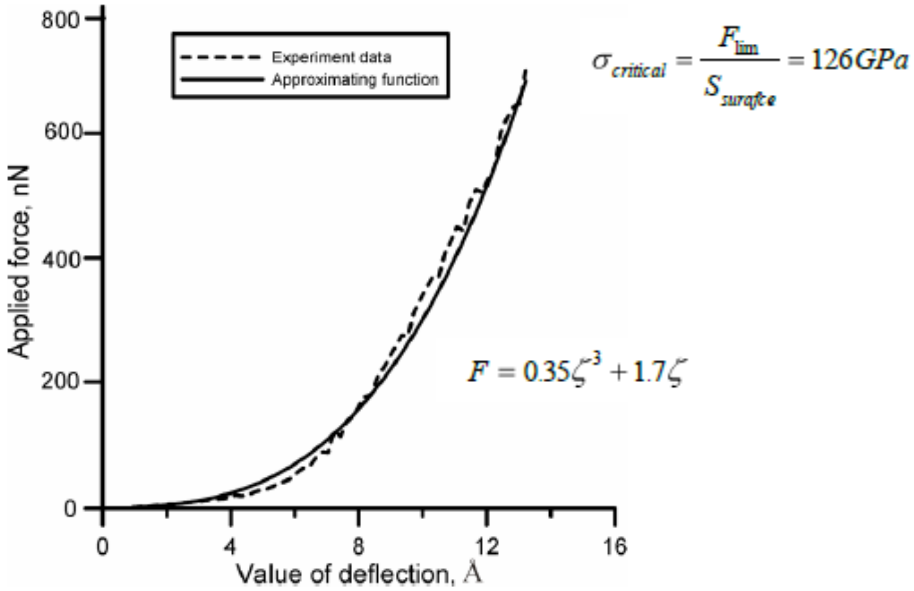
The image of the platinum pyramid and graphene sheet through 13.2 ps after the start of the experiment.



Picture of graphene sheet thought 14.2 ps after the start

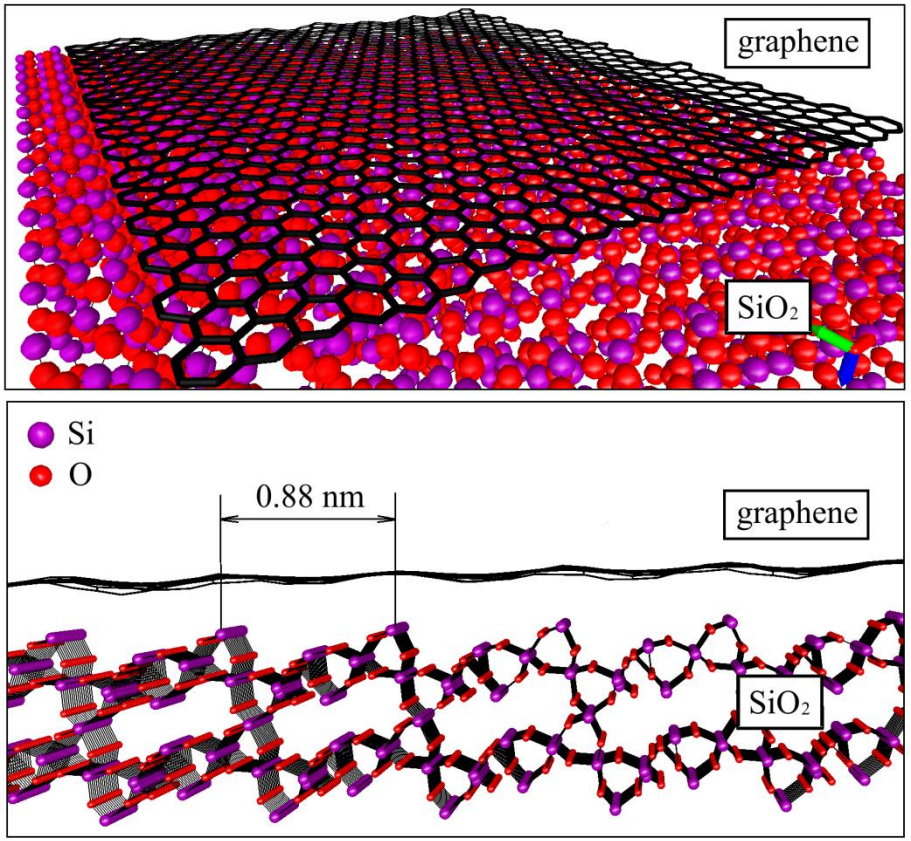


Map of the local stress, calculated thought 13ps after the start of the experiment.



The dependence of the applied force on the bending deflection in the center of the upper plate bi-layer graphene plate. The dashed line corresponds to data obtained in the experiment, the solid - approximated function.

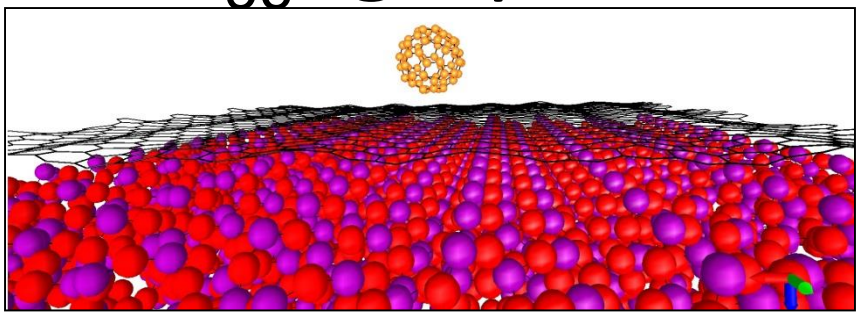
The control of movement of C60 on rippled graphene located on substrate SiO_2

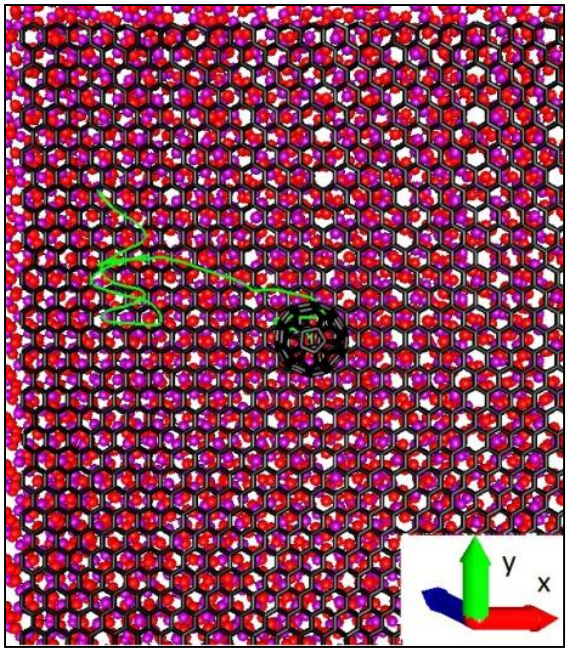


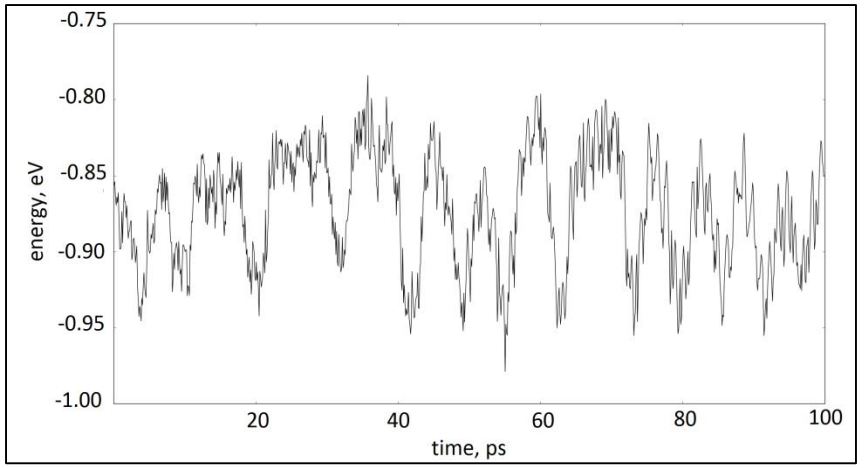
The average distance of the graphene-substrate is ~0.3 nm, the adhesion is 1.8 eV/nm2 that well agrees with the experimental studies [NATURE NANOTECHNOLOGY | VOL 6 | SEPTEMBER 2011].

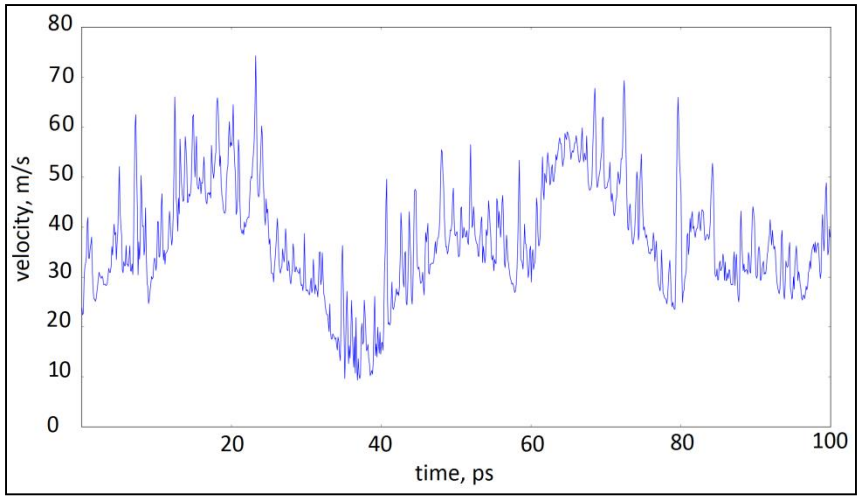
Monolayer graphene on a substrate

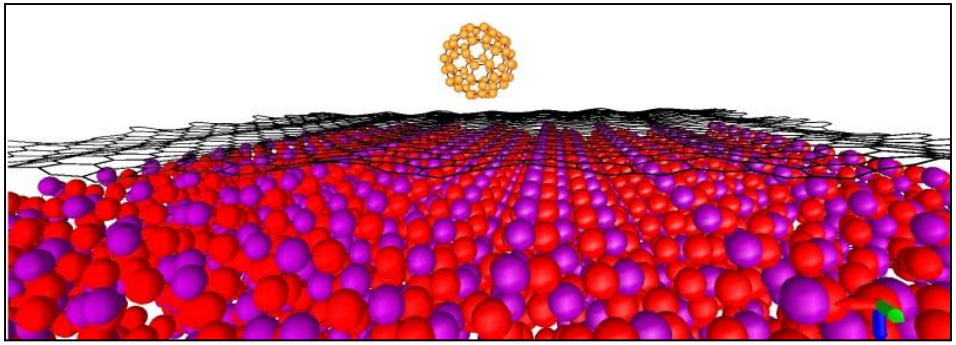
C_{60}+graphene on the ideal surface

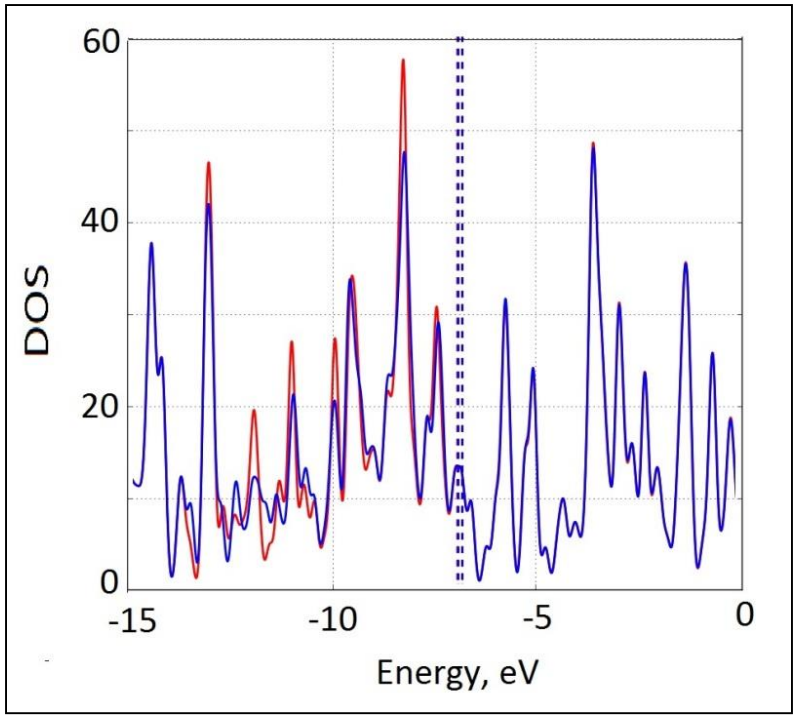






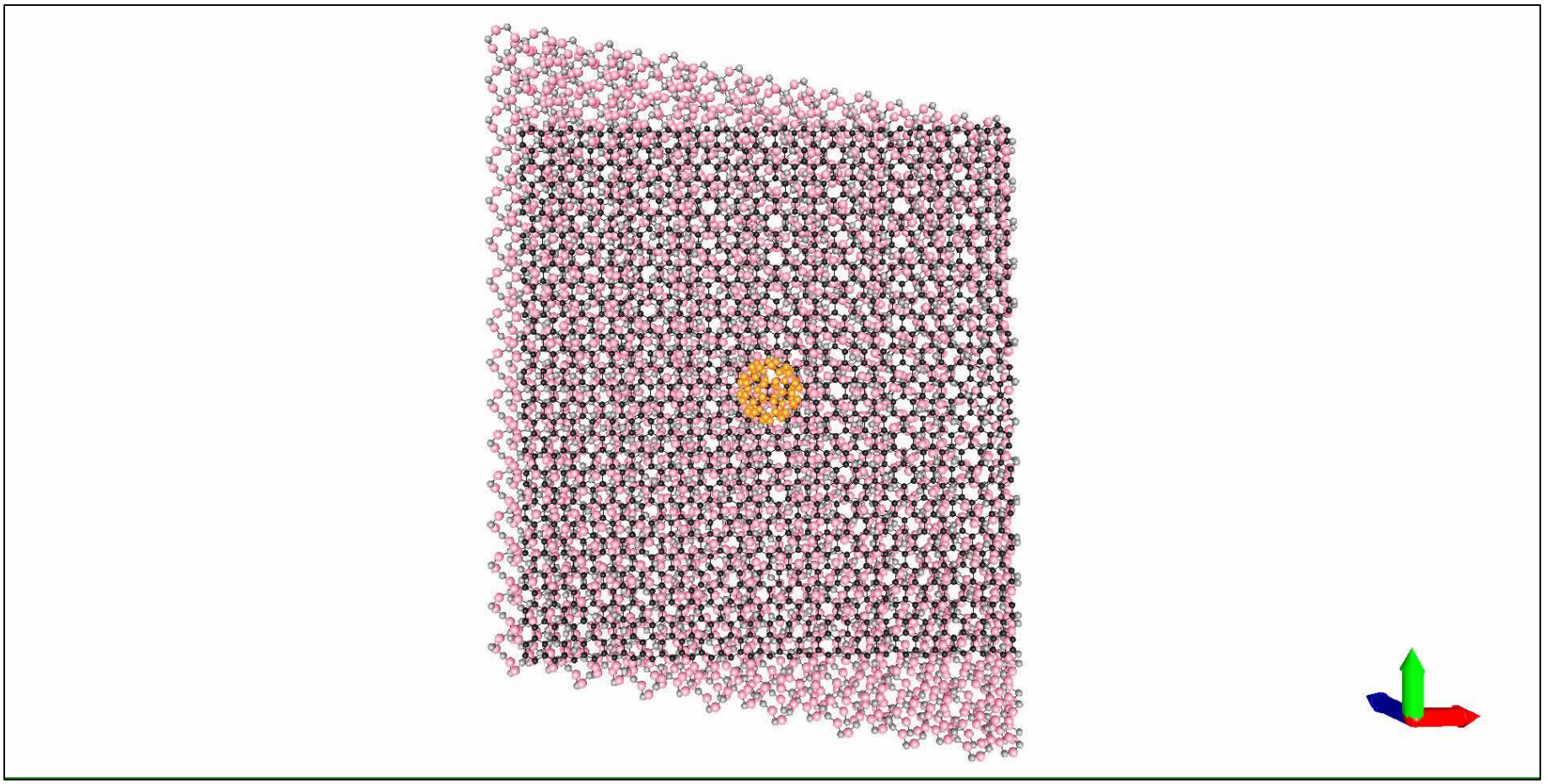




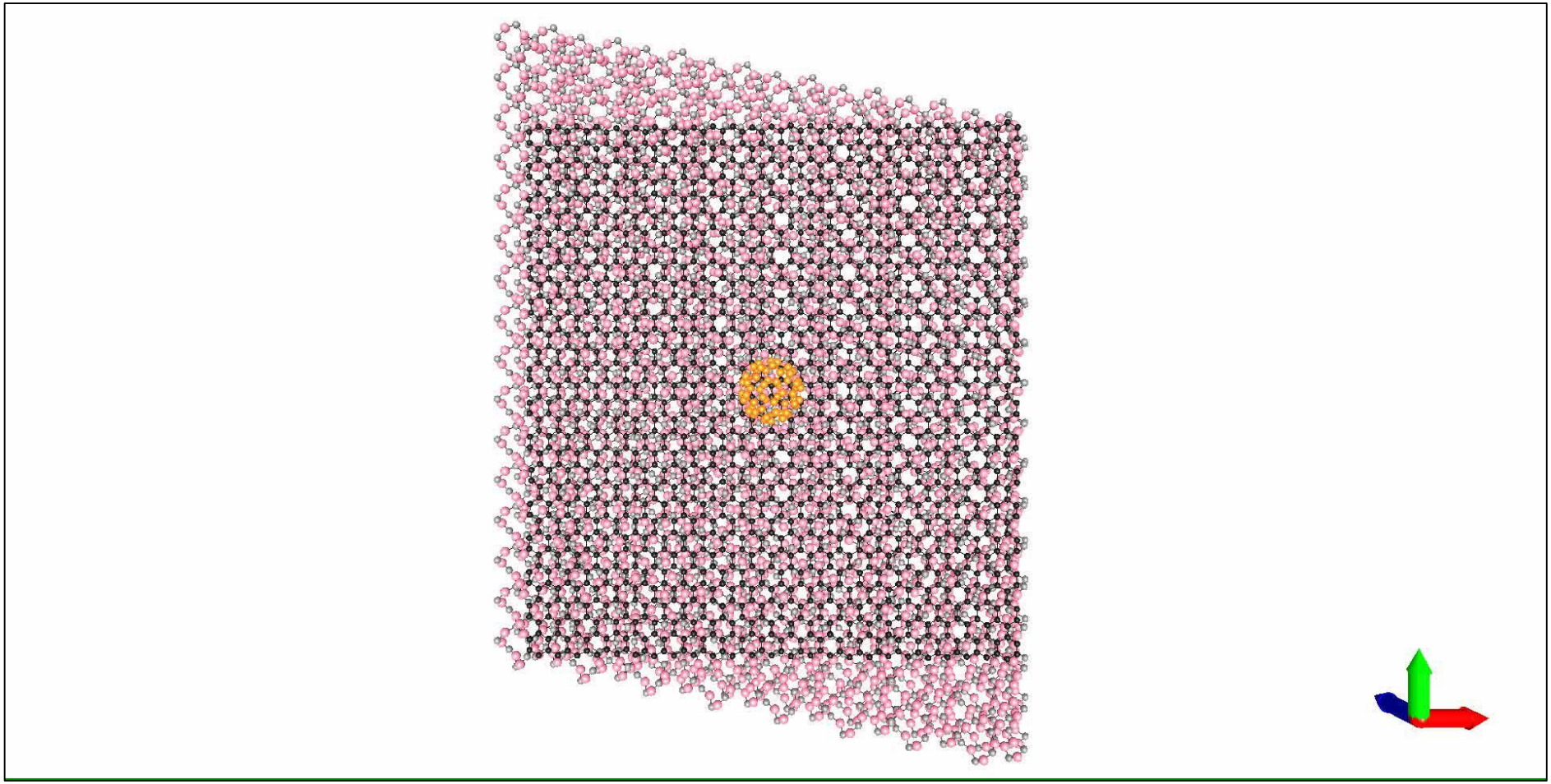


The density of electron states of complex C60+graphene near the last filled HOMO-level (vertical dotted lines indicate the position of the HOMO level).

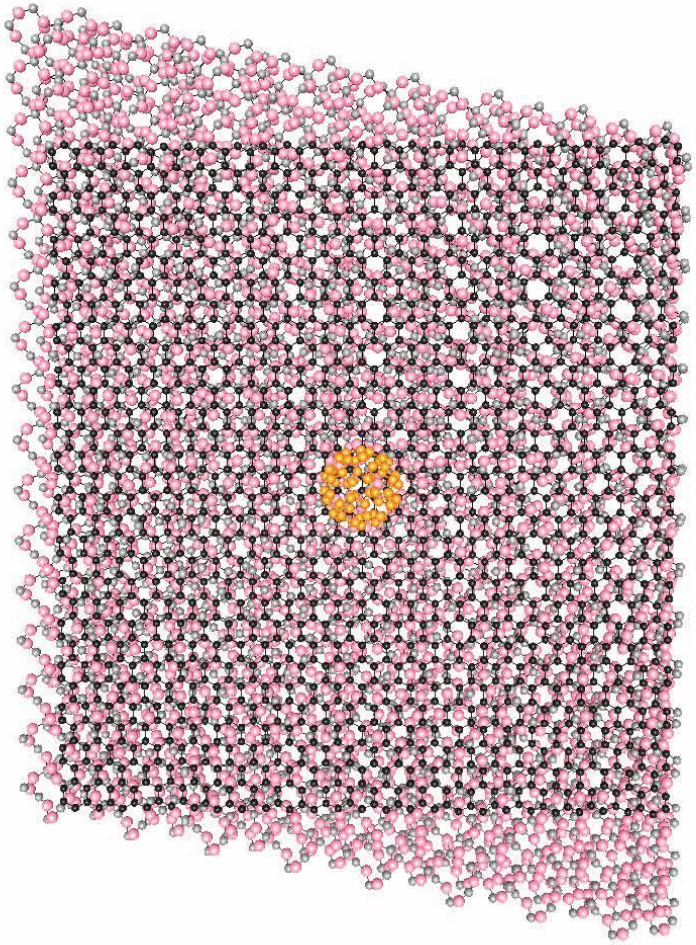
The red curve corresponds to the case without account of additional overlap of the electron clouds of the fullerene and graphene, blue – to the case with account.

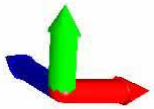


On the ideal surface SiO2

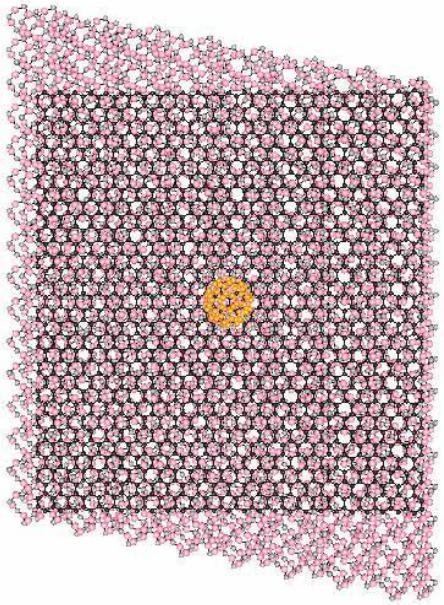


F_y = 10 V/mkm

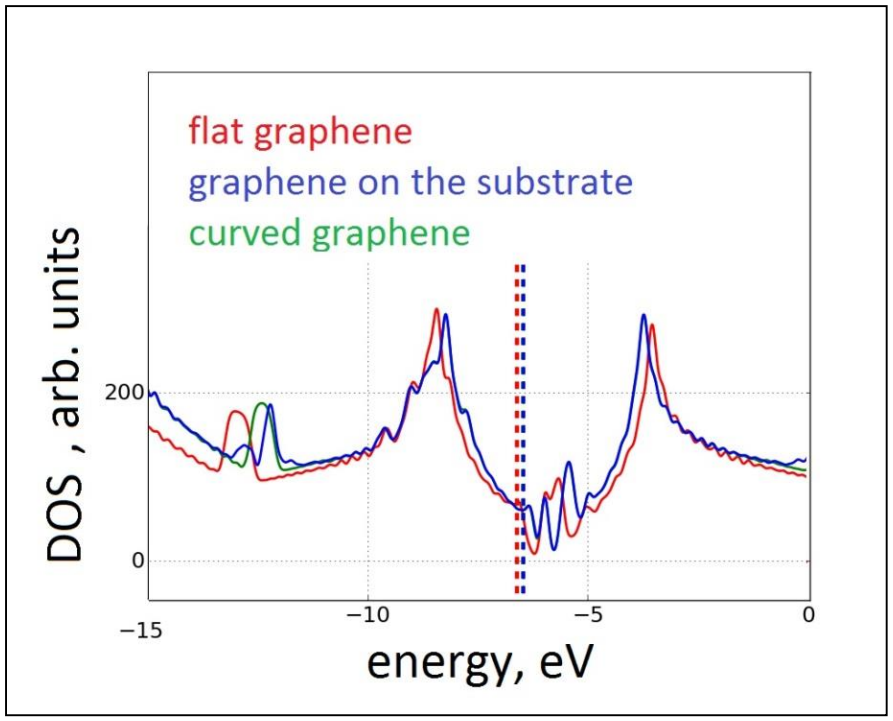


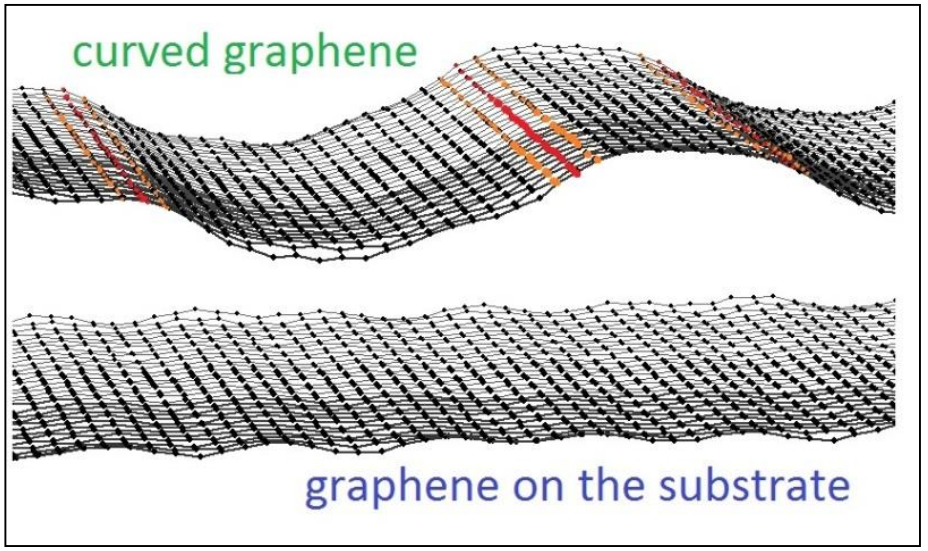


F_y=50 V/mkm



F_y=100 V/mkm





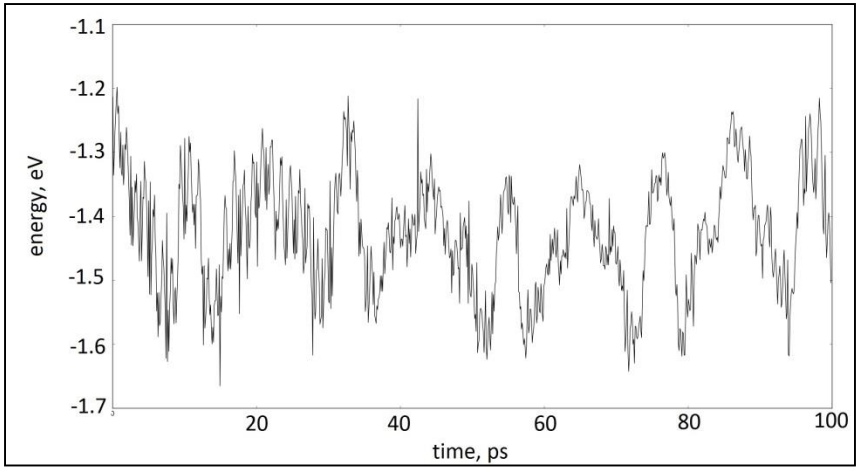
Graphene on a substrate:

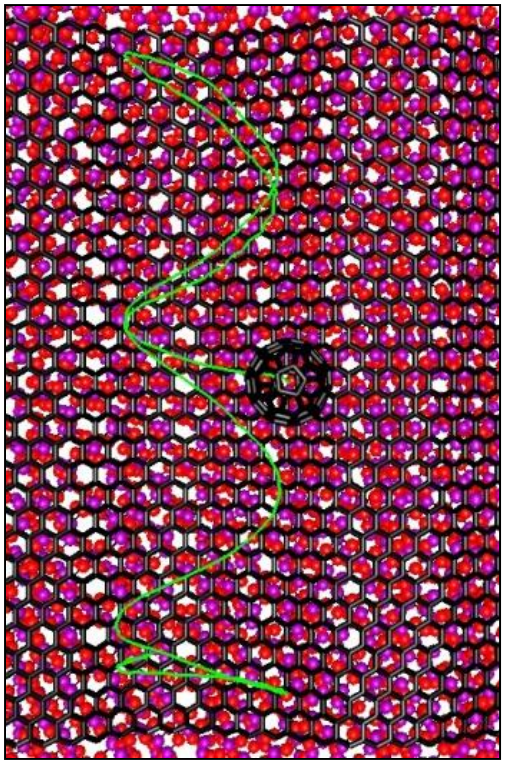
a) the density of electronic states of graphene on an ideal and corrugated substrate (dashed lines indicate the position of HOMO-levels);

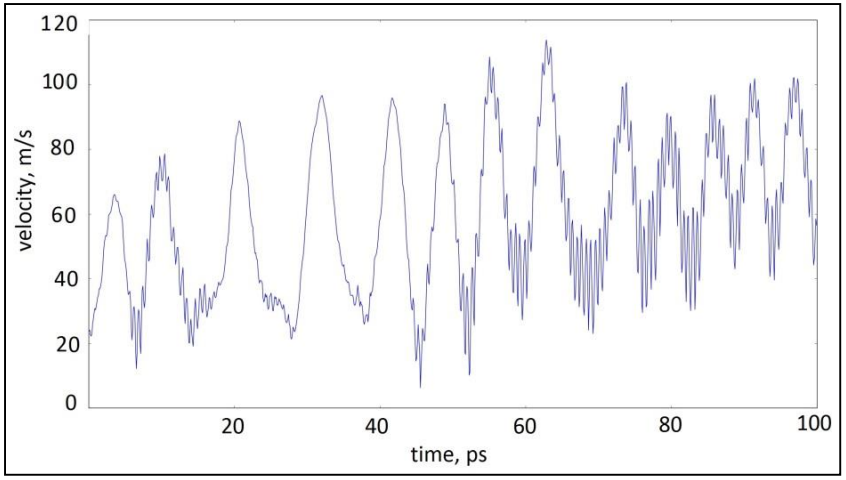
b) fields of atomic mesh with rehybridizated electron clouds (the maximum degree of rehybridization belongs to the atoms marked with red dots and orange).

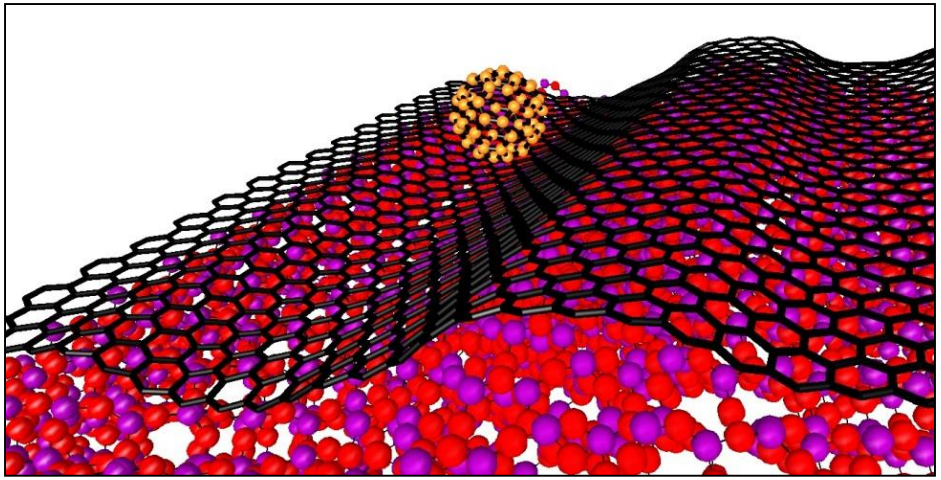
Some of the electrons (red highlighted) will be eventually located in $sp^{2.02}$.

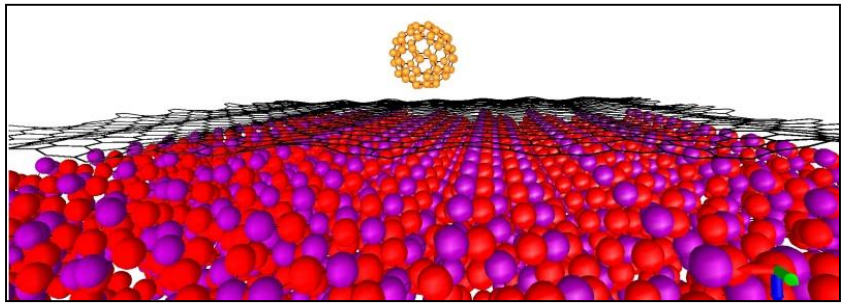
Fullerene on the corrugated substrate at T = 300 K:
- general view,
- the trajectory of the mass center,
- changes of velocity,
- the oscillations of the interaction energy.

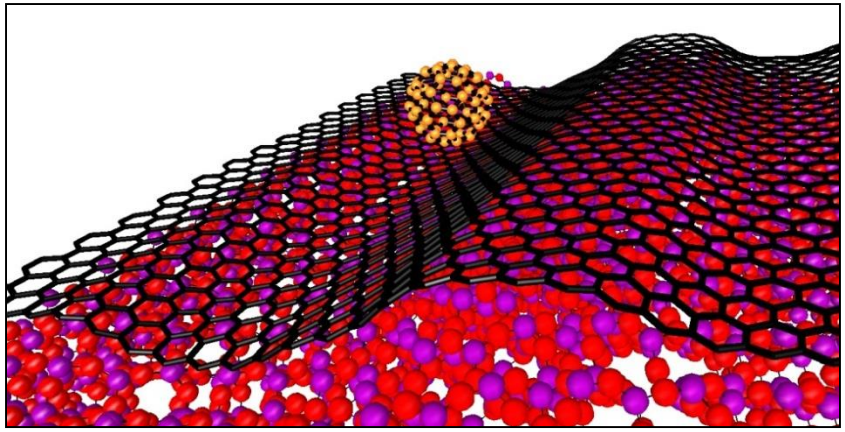


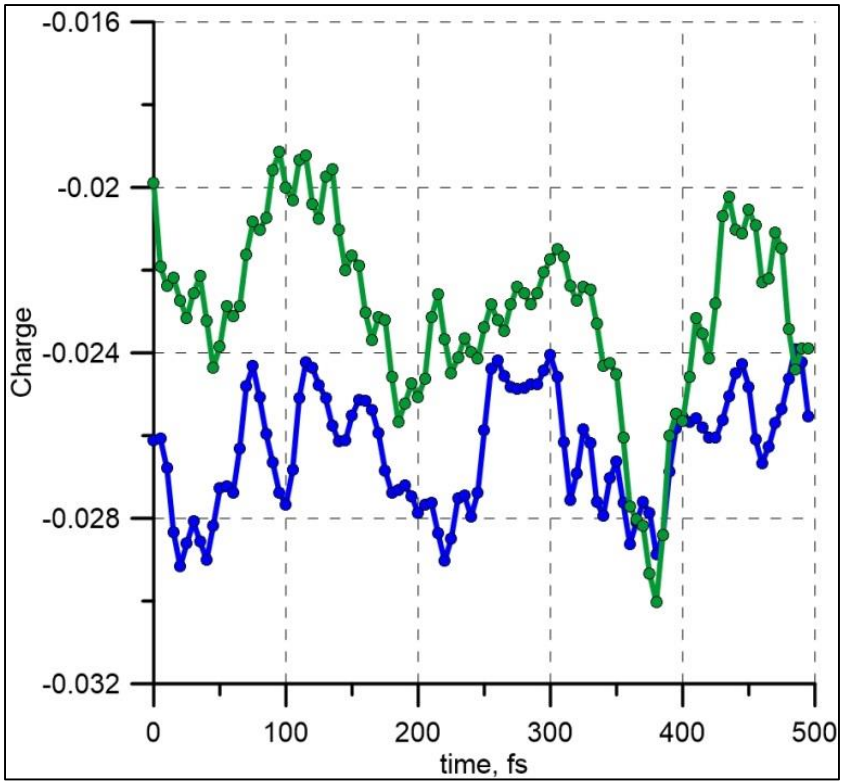




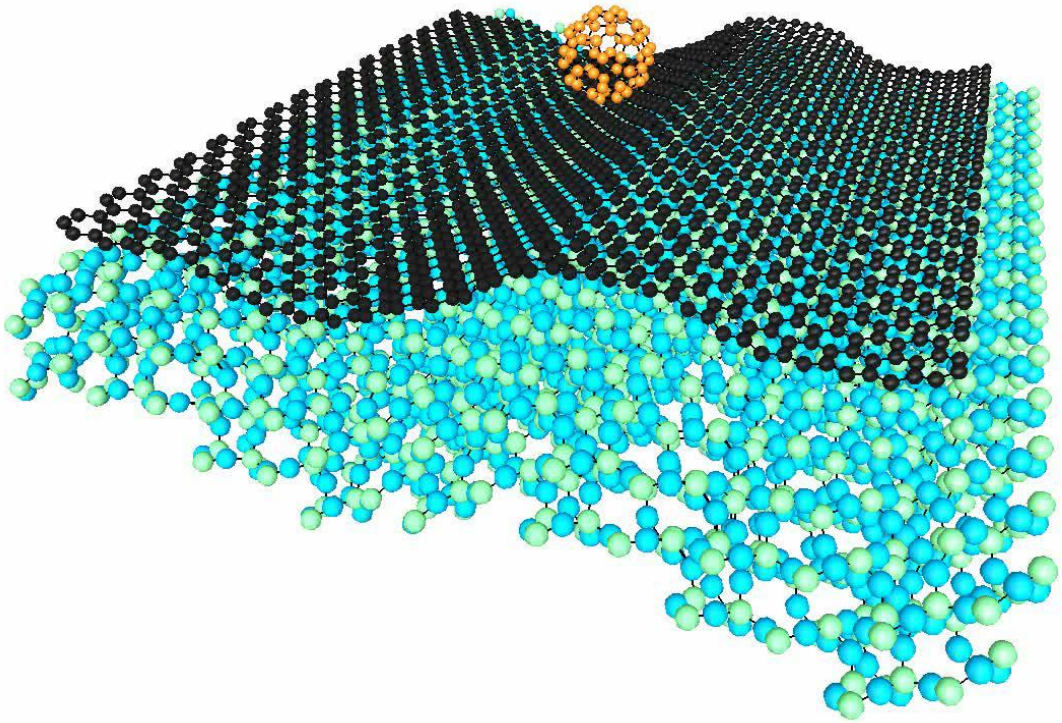




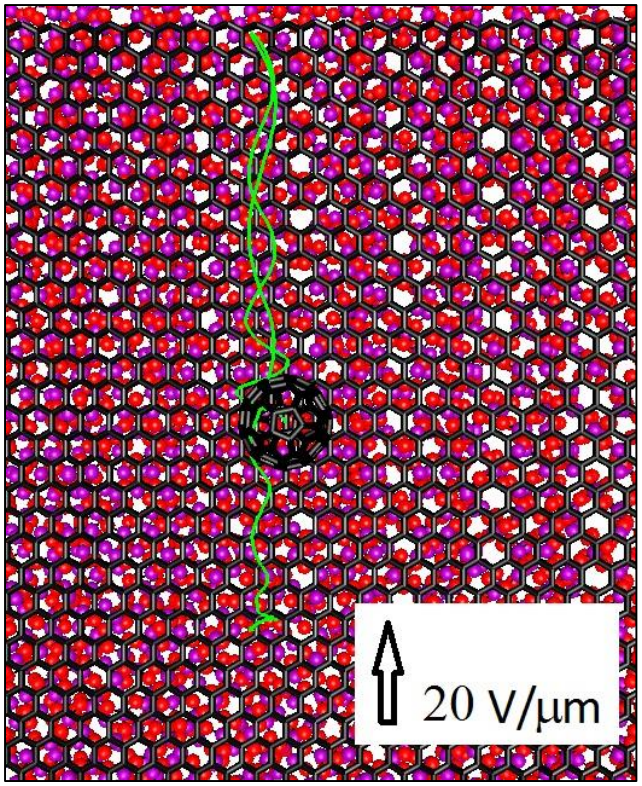


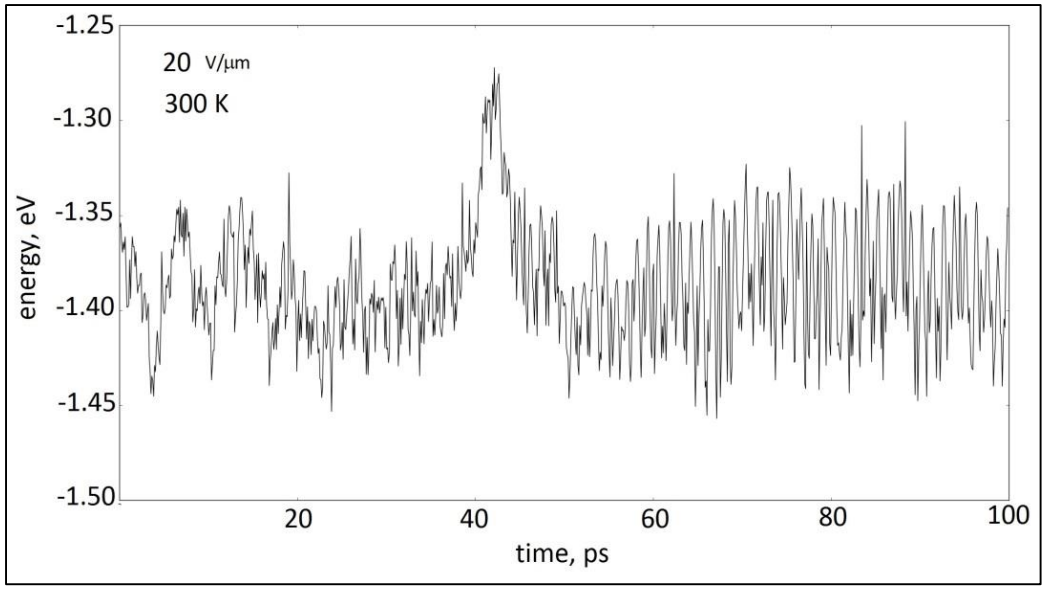


Change of charge on fullerene during its motion on graphene:
blue curve – movement on ideal defectless substrate SiO2.
The current flowing within 10-20 fs can reach 14-17 nA;
green curve – motion on graphene in corrugated substrate.
Thus the current in the molecular complex reaches 16 nA.
T = 300 K, time step – 5 fsek.

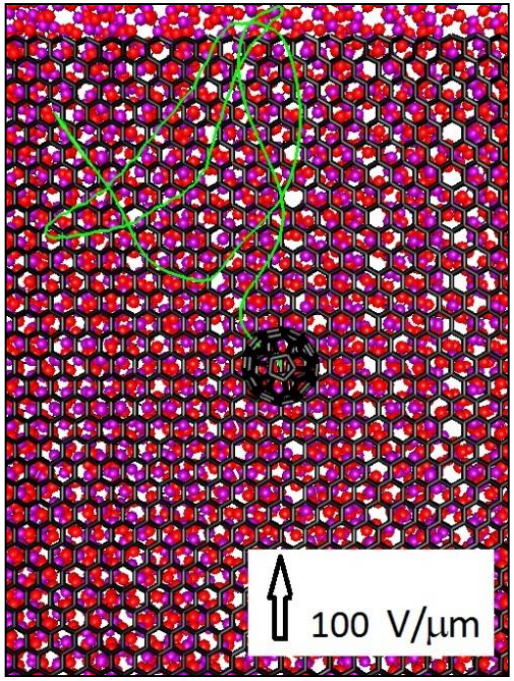


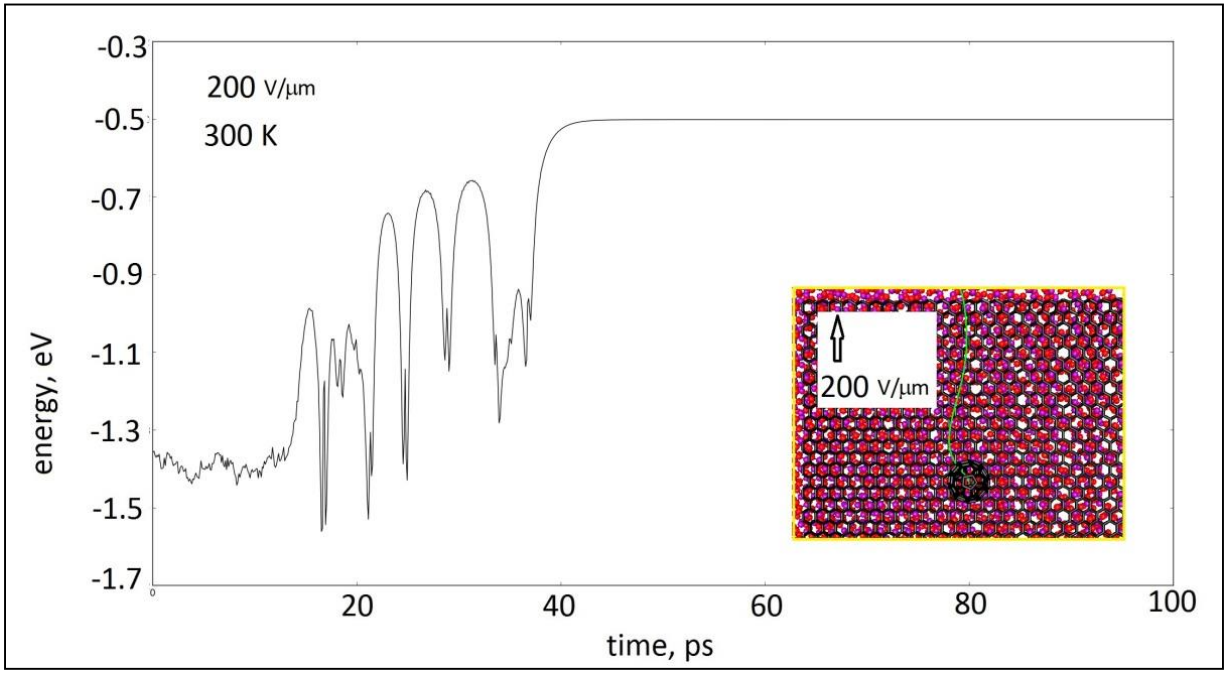
On the corrugated SiO2





Fullerene on the corrugated substrate in external electric field at T = 300 K:
- the trajectory of the mass center and the change in the interaction energy for 100 psec at a field strength of 20 V/ mkm





Fullerene on the corrugated substrate in external electric field at T = 300 K:
- at a field strength of 100 V/mkm;
- at a field strength of 200 V/mkm

Giga- and terahertz range nanoemitter based on a peapod structure

M.M. Slepchenkov[1], A.S. Kolesnikova[1], G.V. Savostiyanov[1], Igor S. Nefedov[2], Ilya V. Anoshkin[3], Alexandr V. Talyzin[4], Albert G. Nasibulin[3,5], Olga E.Glukhova[1]

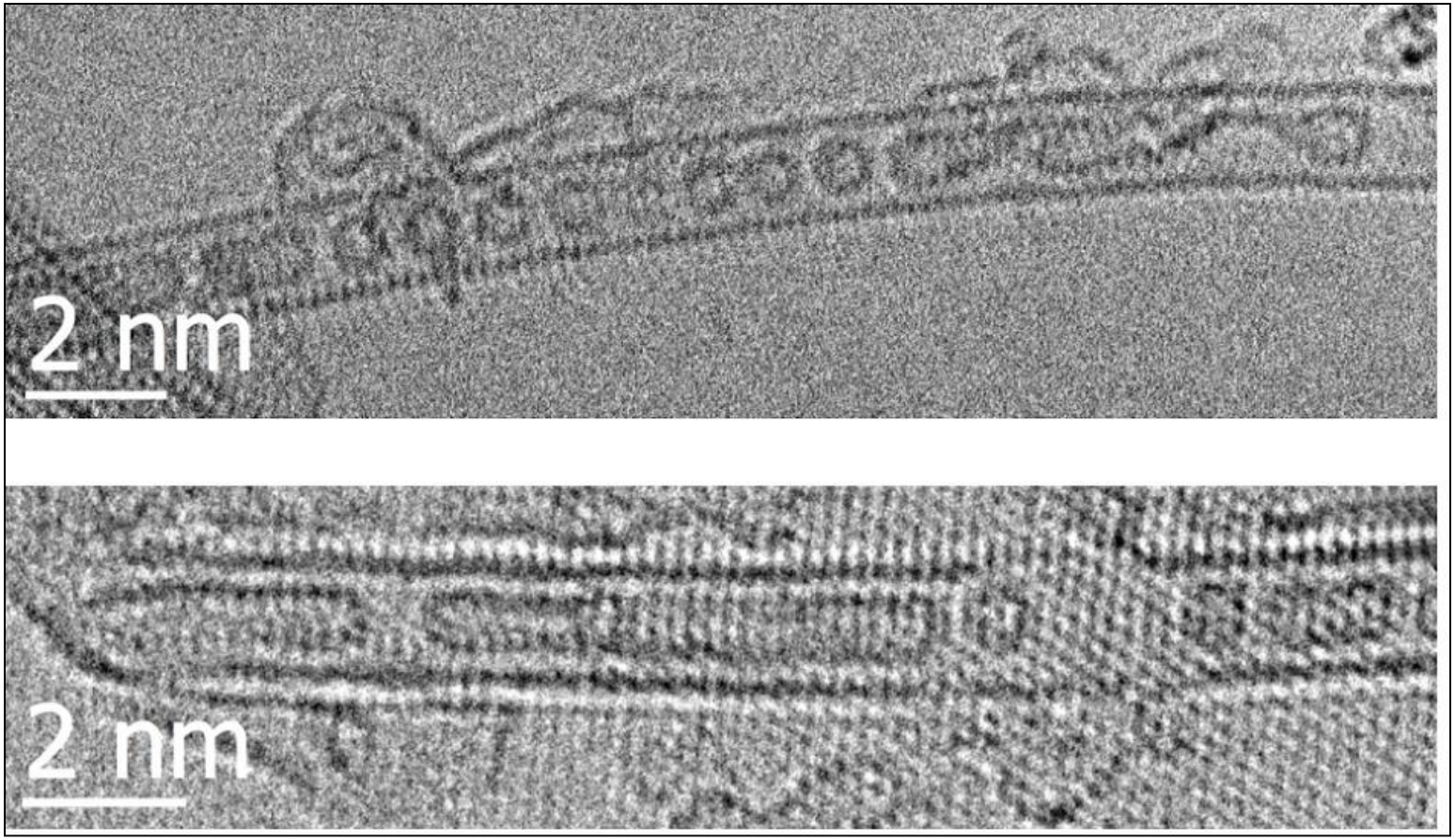
[1] Saratov State University, Department of Physics, Russian Federation

[2] Aalto University School of Electrical Engineering, Department of Radio Science and Engineering, Finland

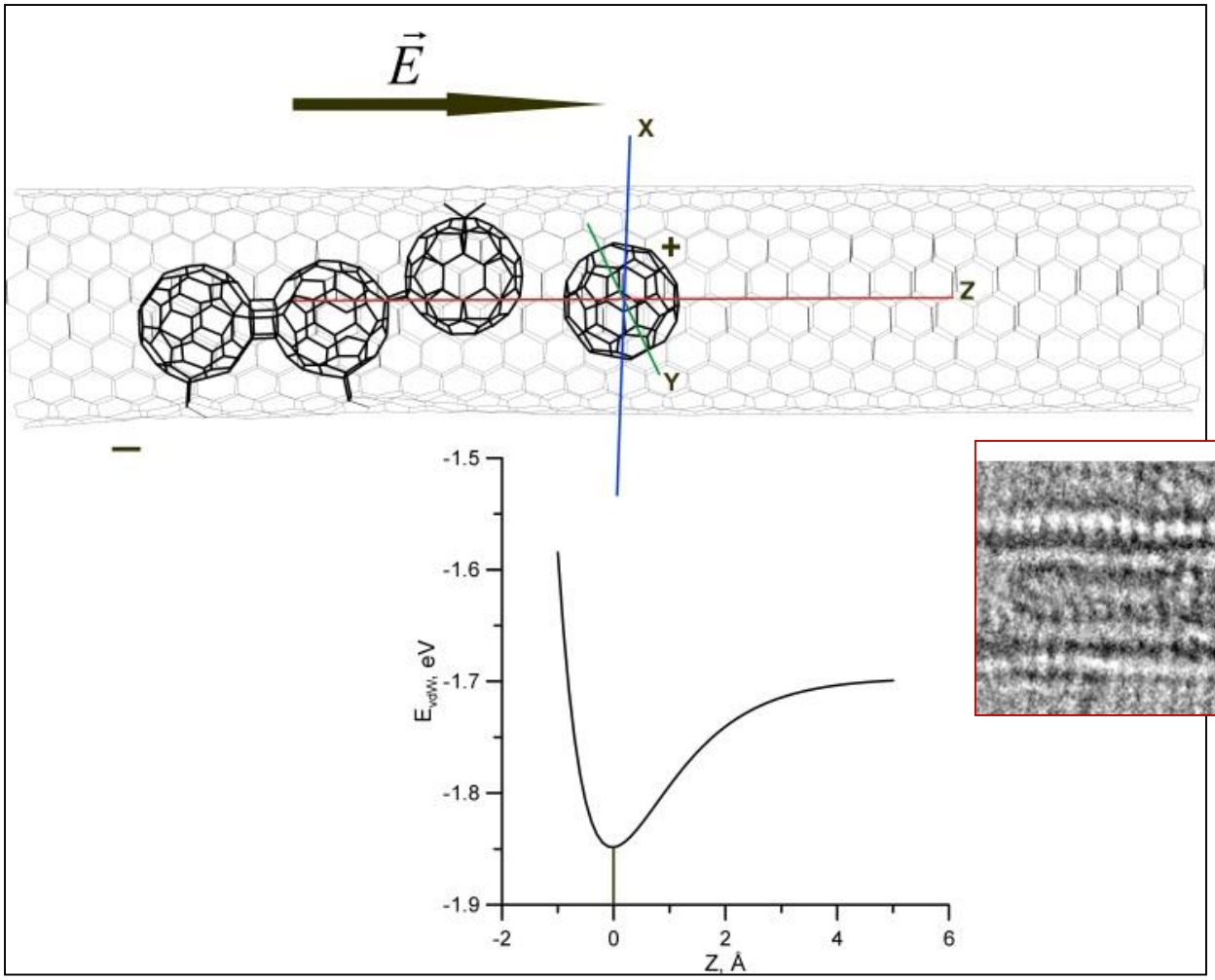
[3] Aalto University School of Science, Department of Applied Physics, Espoo, Finland

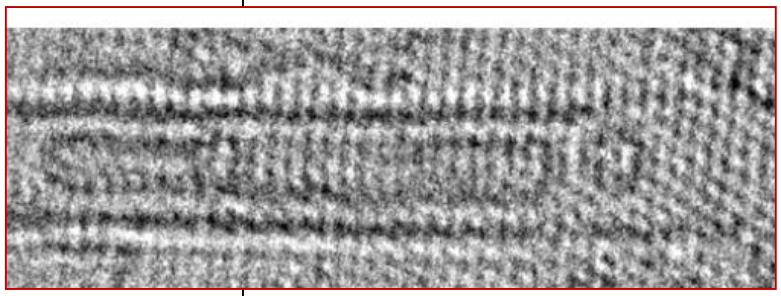
[4]Umeå University, Department of Physics, S-90187 Umeå, Sweden

[5]Skolkovo Institute of Science and Technology, 100 Novaya st., Skolkovo, 143025, Russia

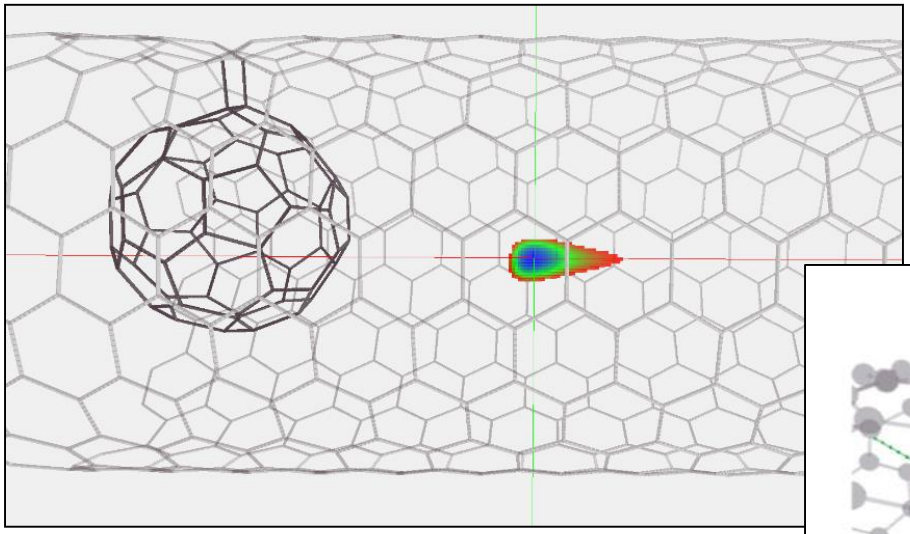


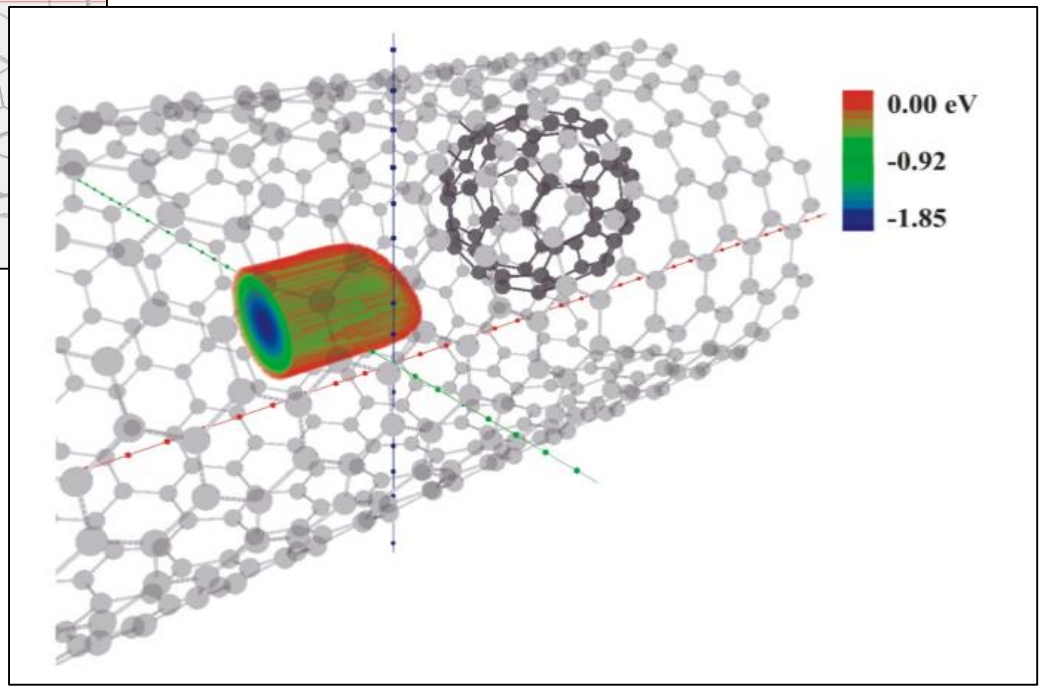
HR-TEM images illustrating the partial polymerization of fullerene molecules inside CNTs





Model of a nanoemitter: configuration of fullerenes inside (10,10) carbon nanotube





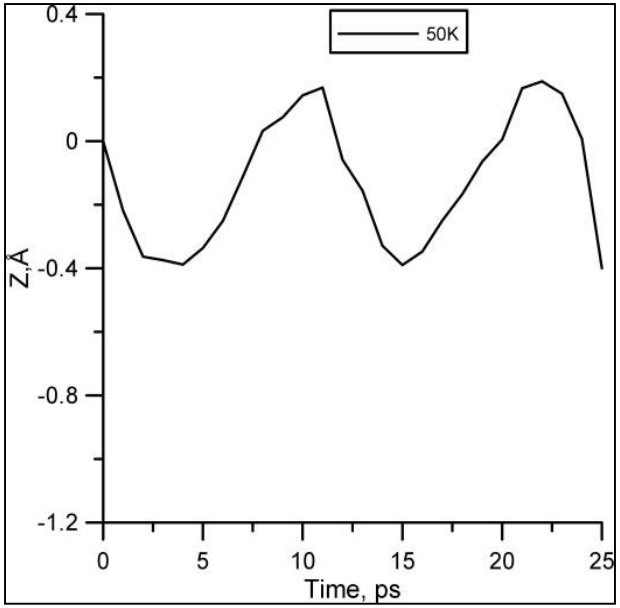
Color image of the potential well for free charged C60;
field image of the center of gravity for charged C60.
Only one attached to the CNT wall fullerene closest
to the free fullerene is shown here.

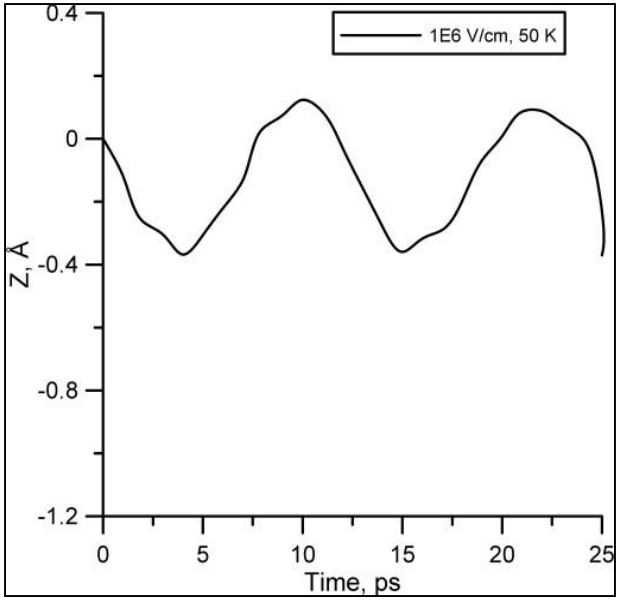
C_{60}^{+} oscillations in the potential well at T = 50 K:

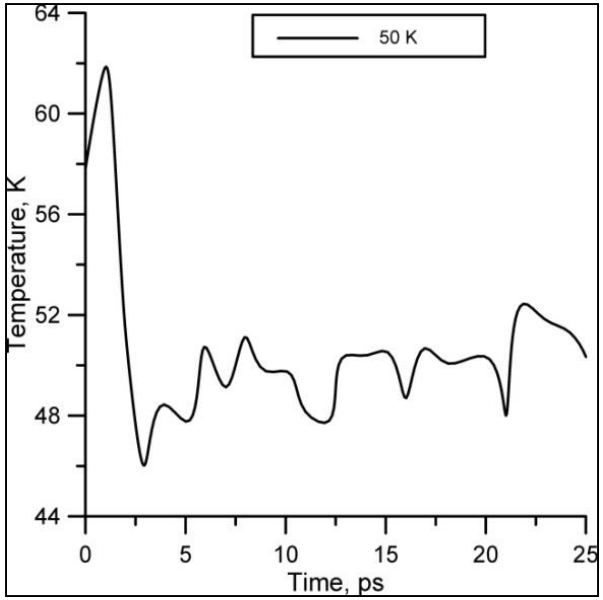
a) the position of the gravity center without electric field;

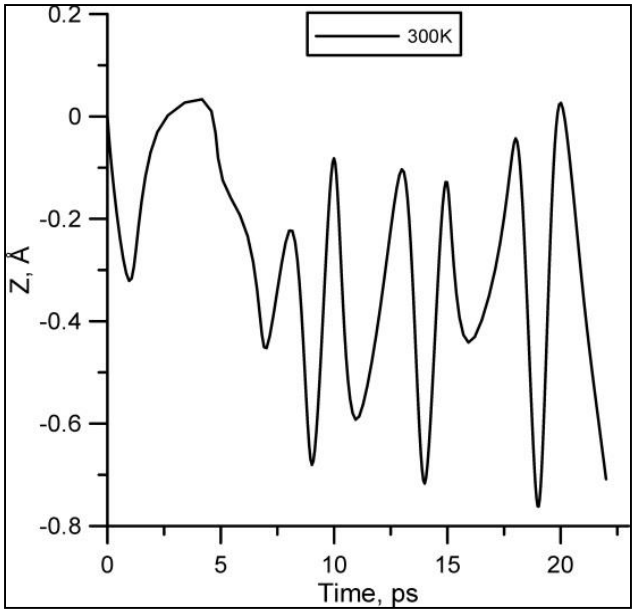
b) the position of the gravity center in the external electric field with the strength of 1 V/μm;

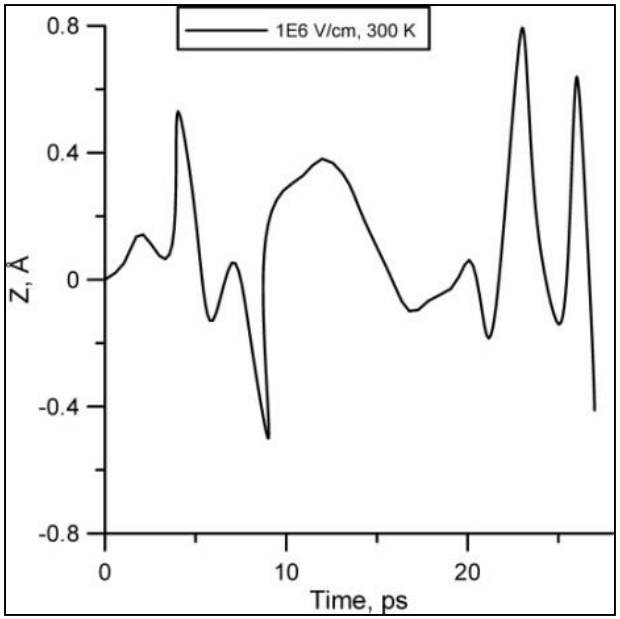
c) the change of the system temperature

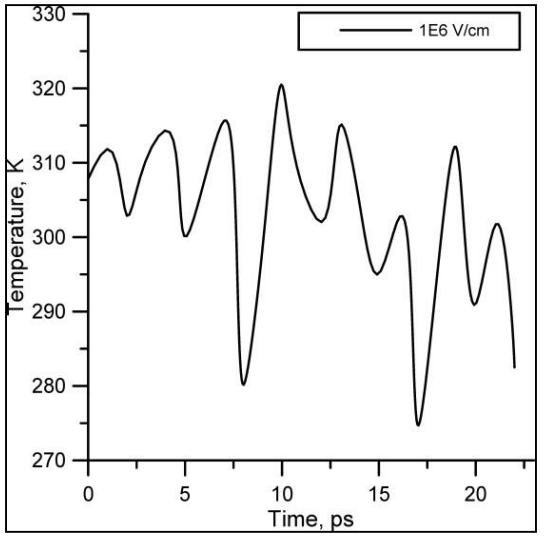












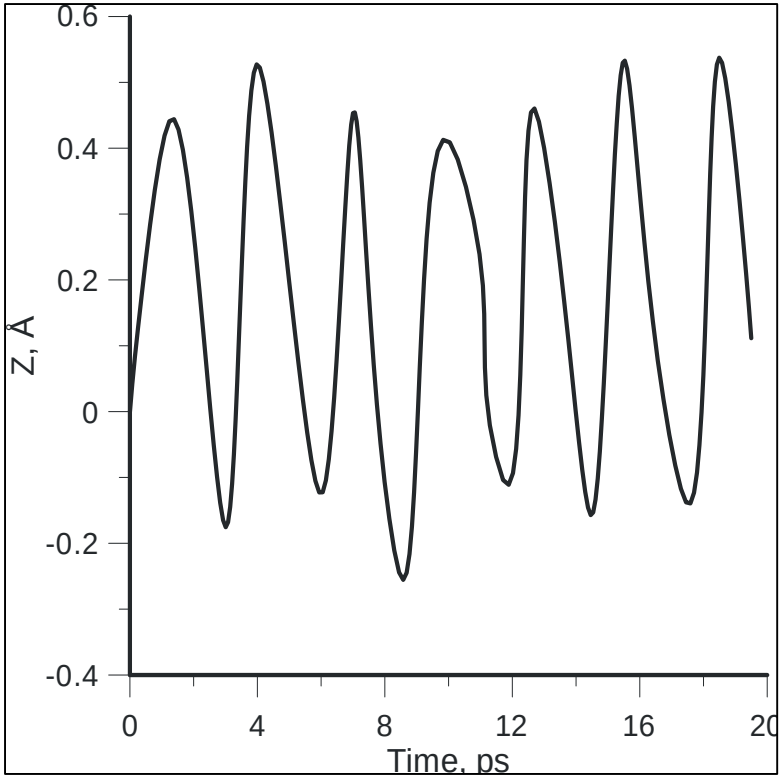
C_{60}^{+} oscillations in the potential well at T = 300 K:

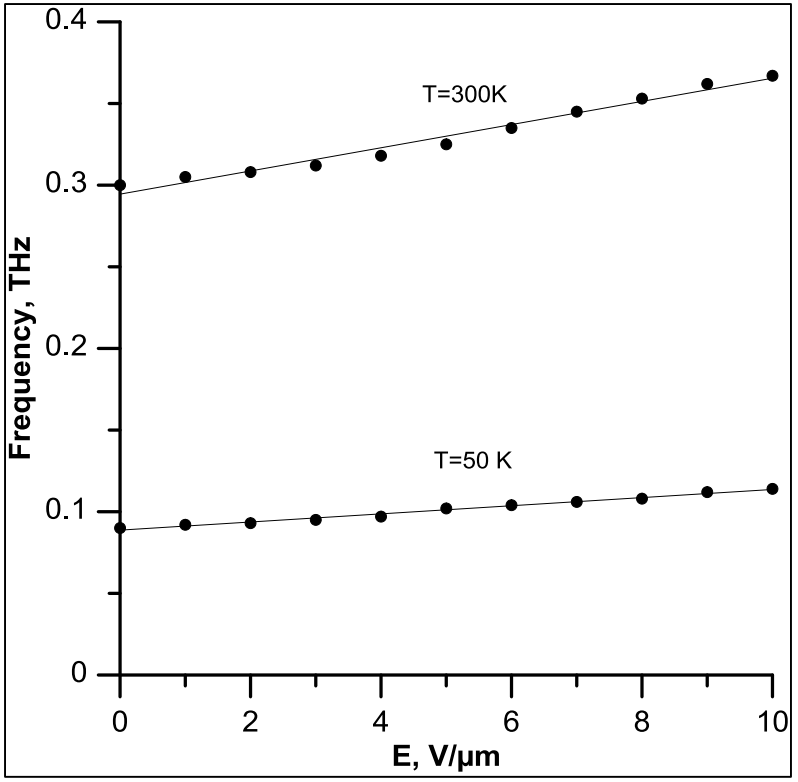
a) the trajectory of the center of gravity without field;

b) the trajectory of the center of gravity in external electric field with the strength of 1 V/μm;

c) the change of the system temperature

The C60+ oscillations in the GHz range are found to be stable at 50 K, while after the temperature increase to 300 K the C60+ oscillation frequency falls in the THz range.

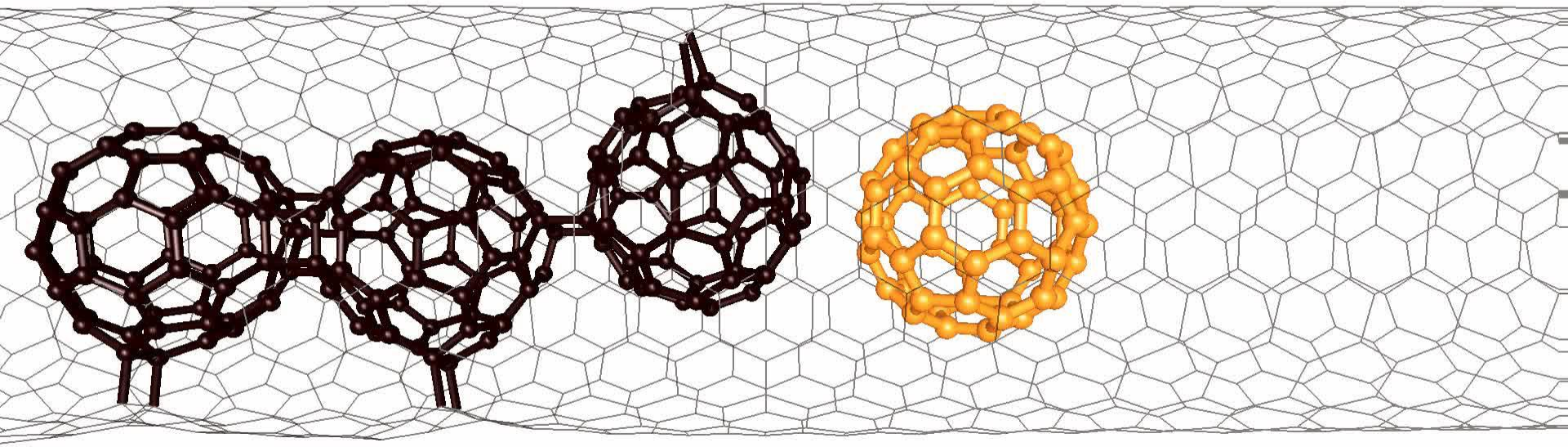




1) Position of the gravity center of C60 + oscillating in the potential well under the external field with the strength of 10 V/μm

2) Oscillation frequency versus intensity of the electric field strength.

The oscillations are generated only at the external electric field of 10 V/μm. We also demonstrated the experimental possibility to synthesize such kind of structures by hydrogen annealing of the carbon nanopeapods.

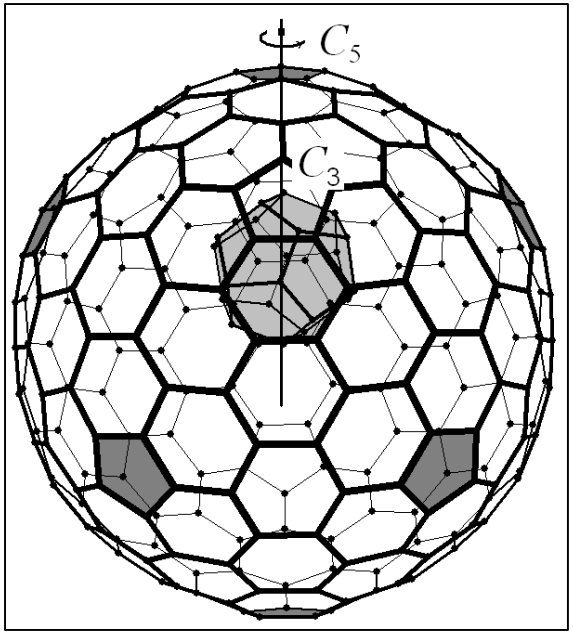


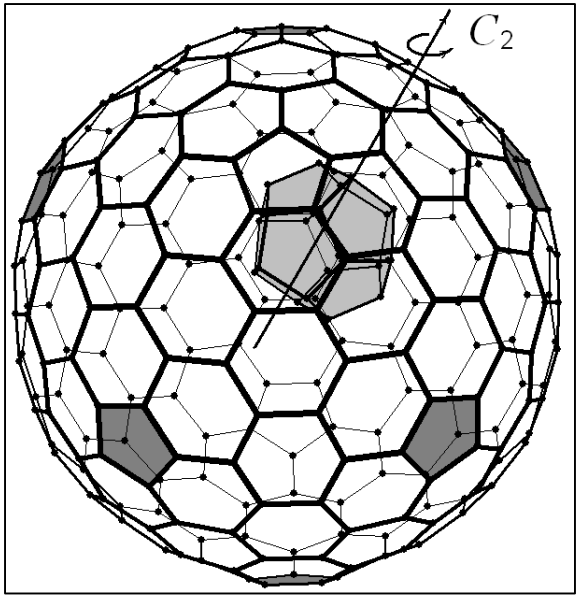
The radiation

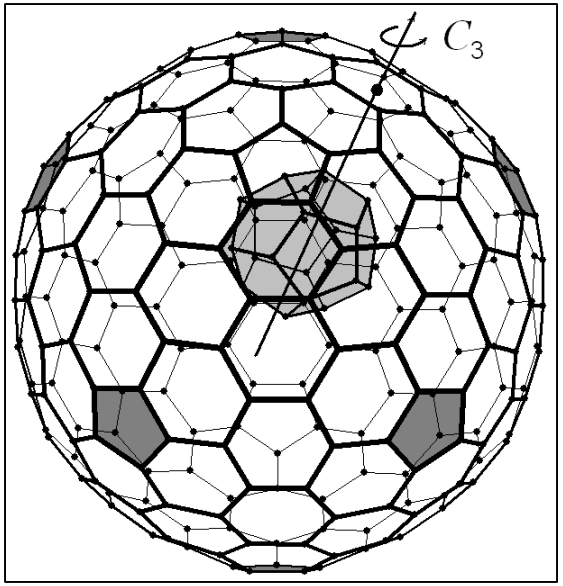
The theoretical investigation of bilayer fullerenes C60@C540 and C20@C240

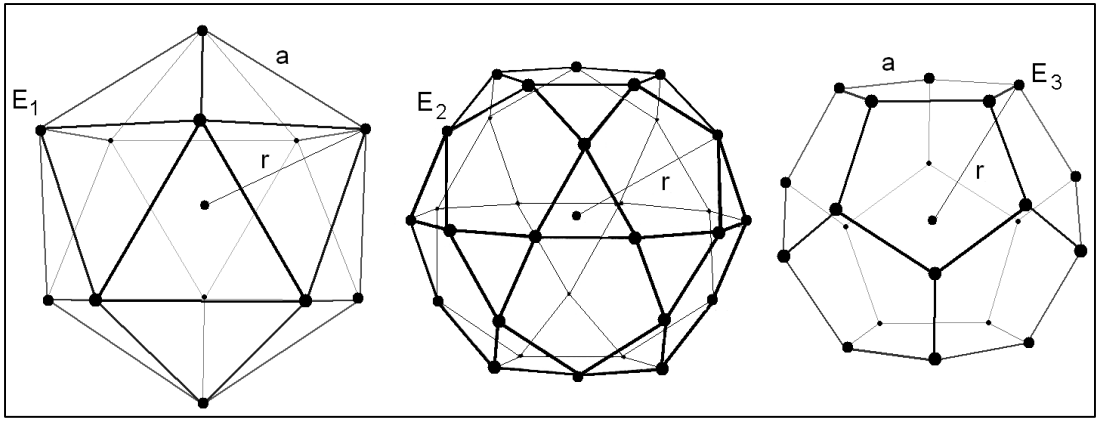
O.E. Glukhova, A.S. Kolesnikova, M.M. Slepchenkov, V.V. Shunaev Moving of Fullerene Between Potential Wells in the External Icosahedral Shell // J. Comput. Chem. 2014. 35(17):1270-7.

Positioning of the C20 in the field of fullerene C240 retaining potential a) for interaction energy *E1* b) for energy *E2*, c) for energy *E3*.

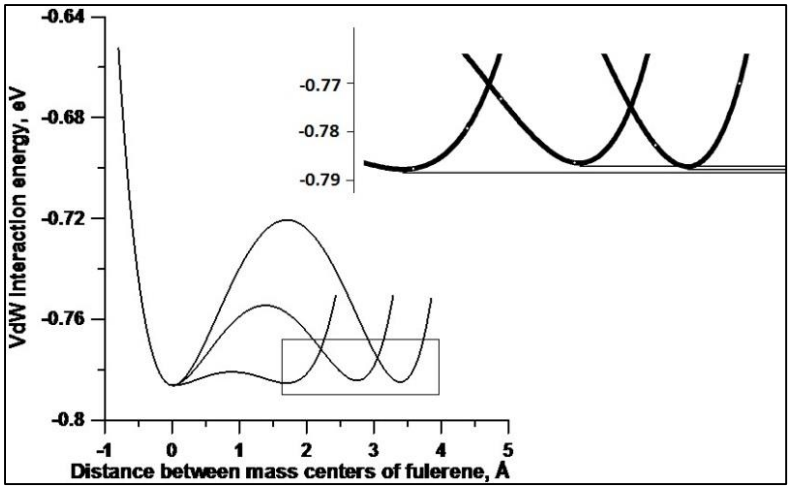


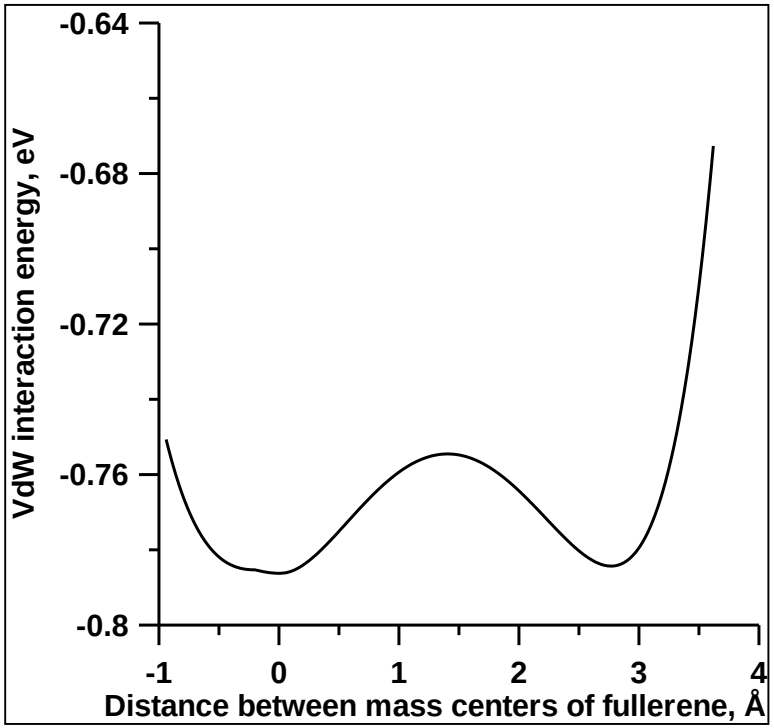






Surface relief of the van der Waals interaction energy between C20@C240 nanoparticle layers at different variants of C20 moving. a) from the well with energy E1 to the same well, from the well with energy E1 to the well with the energy E2from the well with energy E1 to the well with the energy E3;
b) from the well with the energy E2 to the well with the energy E3.

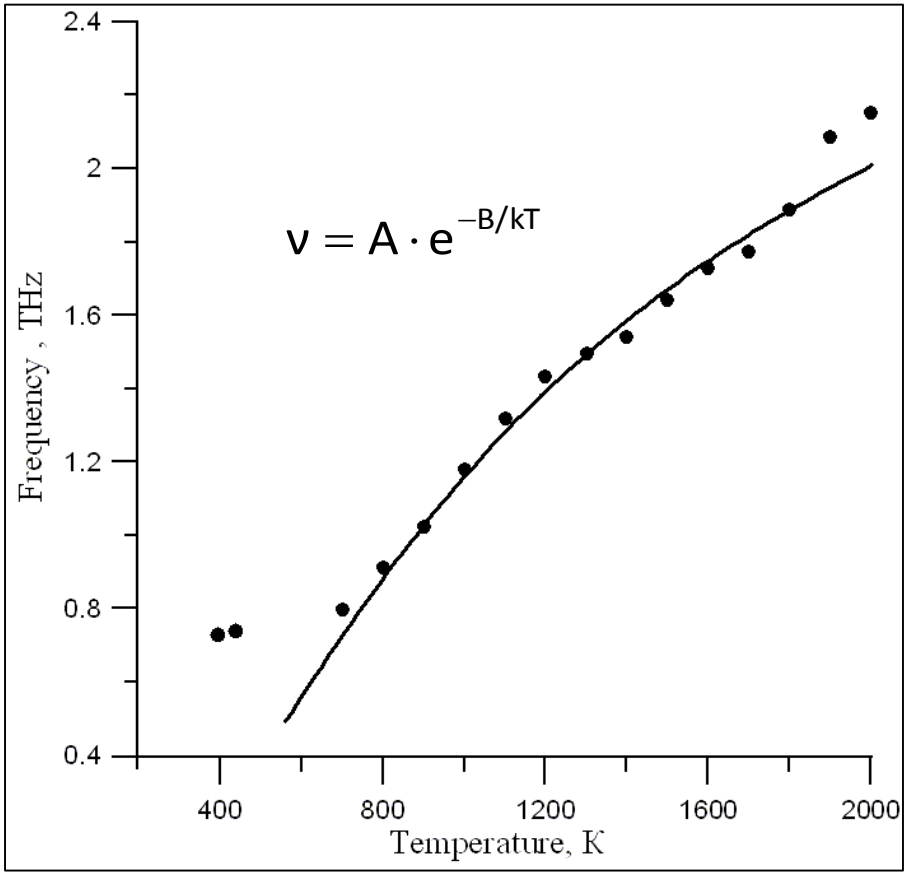




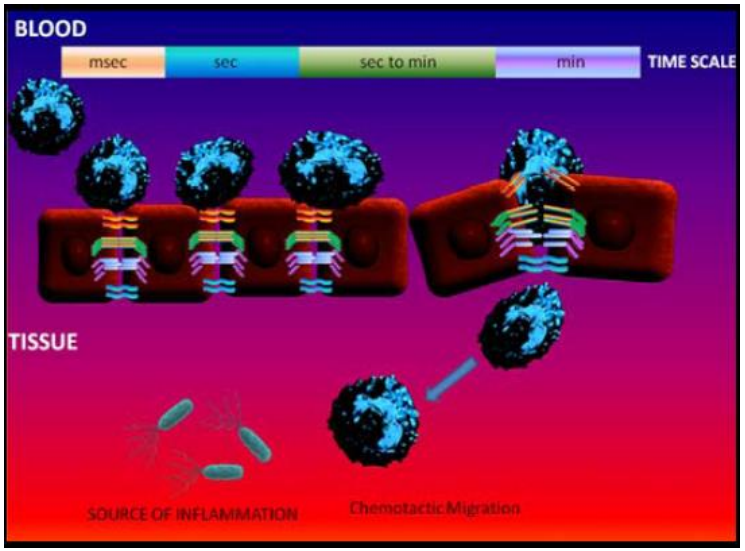
Geometry and Energy Parameters for Fullerenes of Nanoparticle $C_{20}@C_{240}$

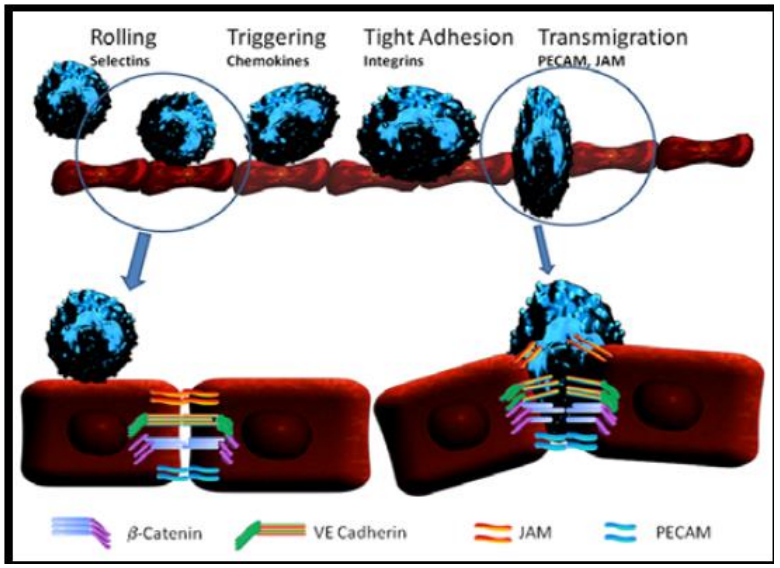
C_n	E_g, eV	P_{ioniz}, eV	E_b, eV	ΔH, $\frac{kcal}{mol \cdot atom}$	R, Å	Min/max Bond length, Å
C_{20} (D_{3d})	2.88	6.71	6.34	25.10	2.06	1.43/1.51
C_{240} (I_h)	1.29	7.06	7.17	5.99	7.20	1.39/1.44

Dependence of jumping frequency on temperature in the case when fullerene C20 jumps from one potential well to another in the field of C240 keeping potential.

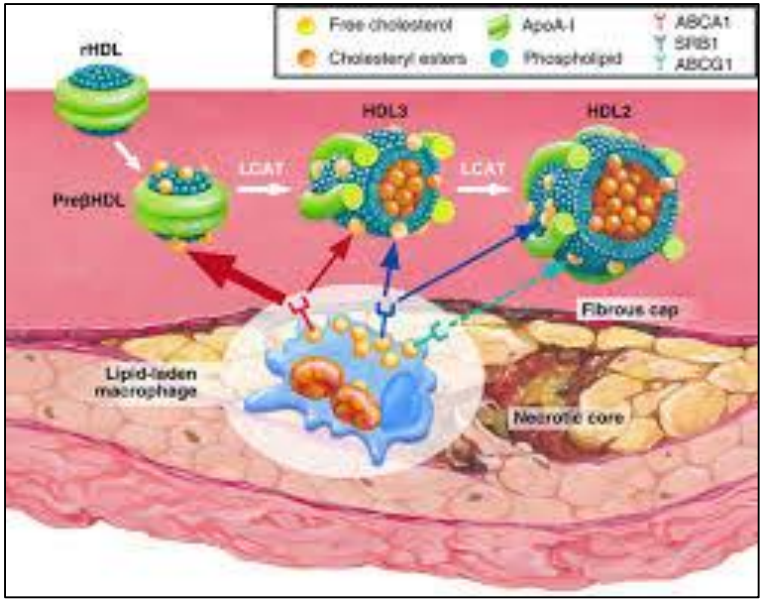


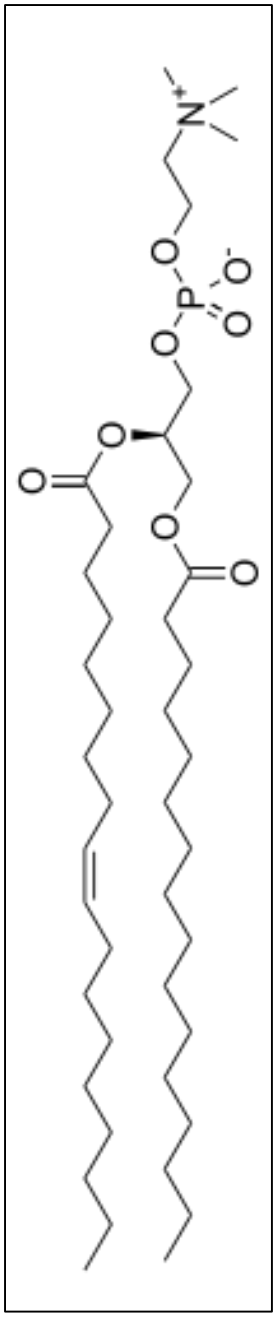
Nanoclusters with non-central effect	$C_{20}@C_{180}$	$C_{20}@C_{240}$	$C_{20}@C_{540}$	$C_{60}@C_{540}$	$C_{80}@C_{540}$
$\Delta H_{formation}\left(C_n@C_m\right)$, kcal/mol	-40.29	-25.72	-12.33	-2.00	-71.78
E_1, eV	-1.734	-1.126	-0.869	-1.972	-2.569
E_2, eV	-1.700	-1.114	-0.665	-1.691	-2.288
$E_2 - E_1$, K	394.6	139.2	2367.6	3261.3	3261.3
E_3, eV	-1.699	-1.113	-0.658	-1.643	-2.270
$E_3 - E_2$, K	11.6	64	81.2	557.1	208.9

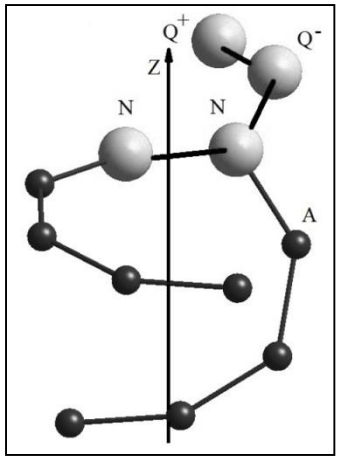


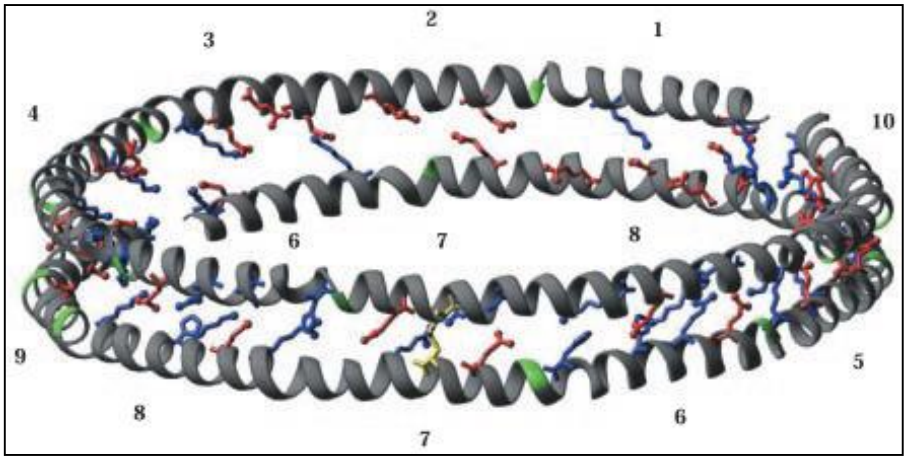


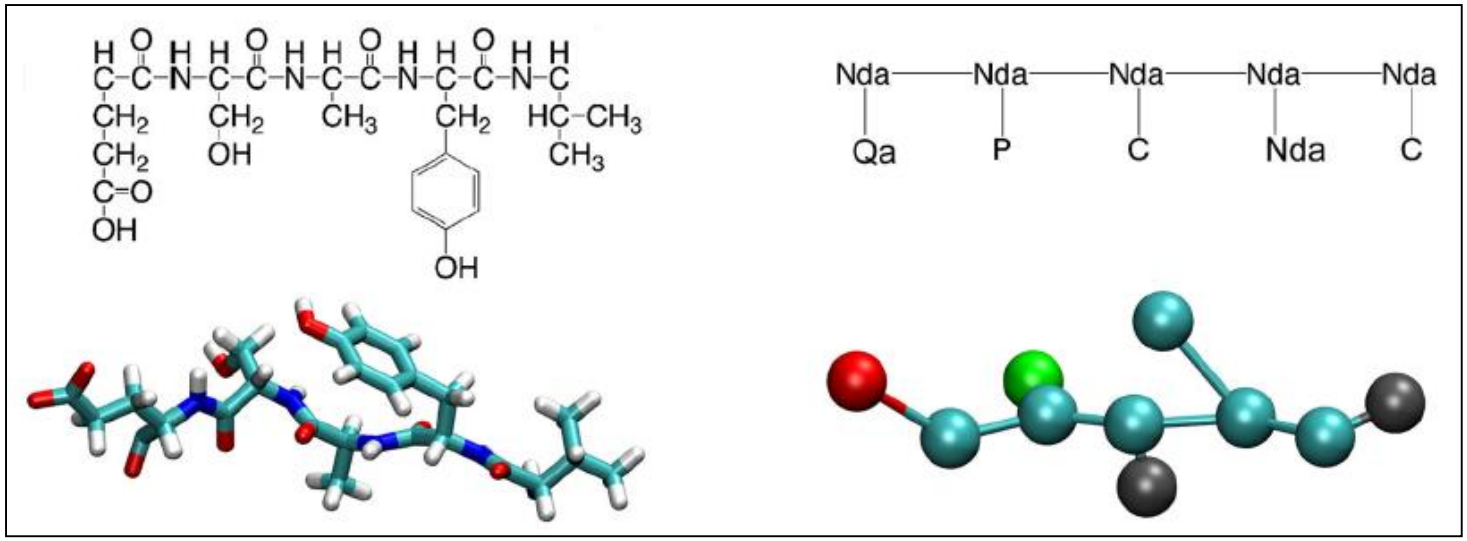
Behavior of High-density lipoprotein (HDL) on graphene





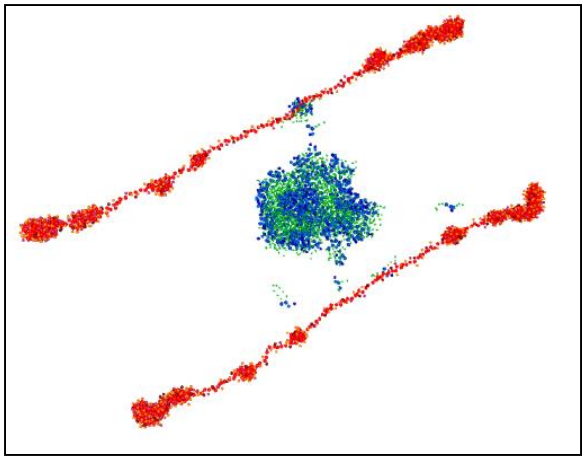


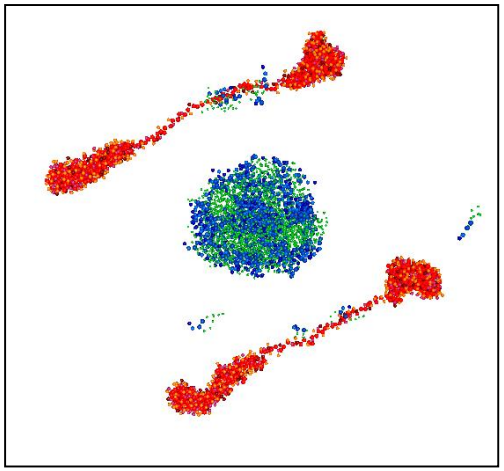


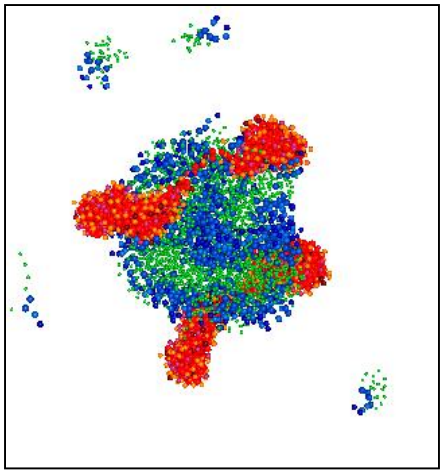


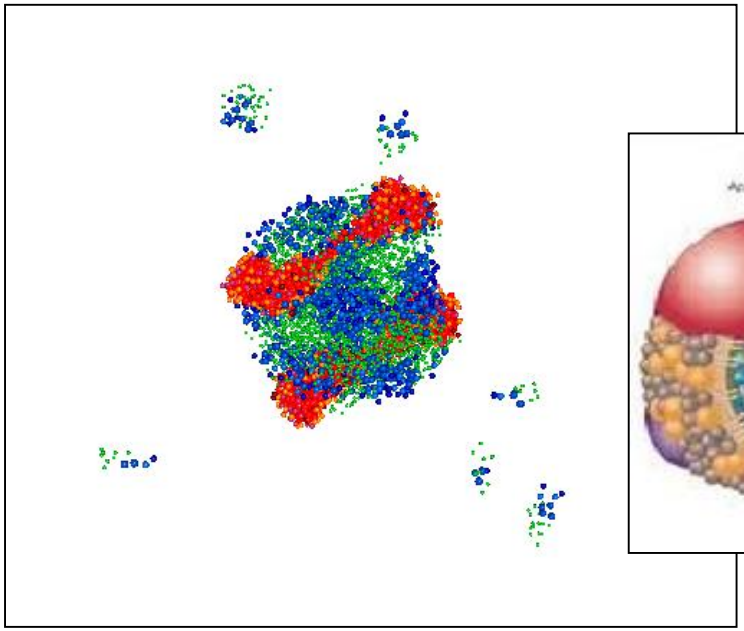
CG-models

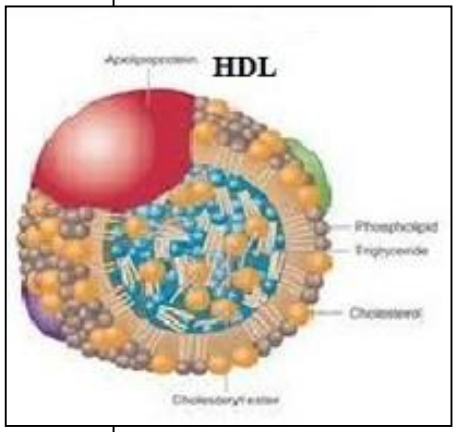
self-assembled lipoprotein HDL

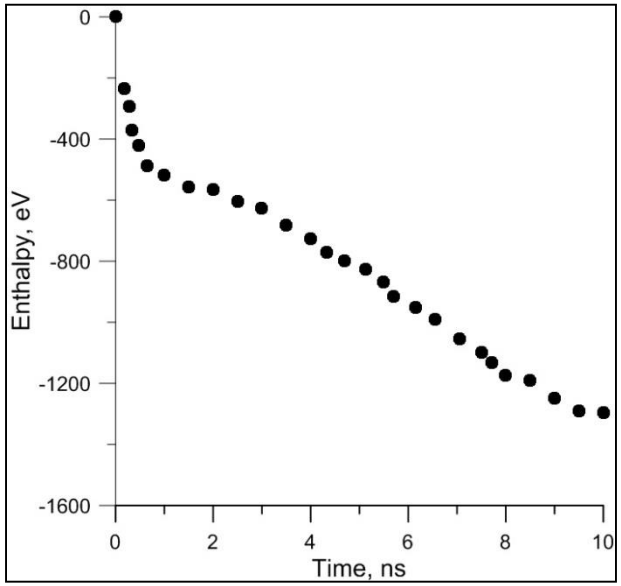


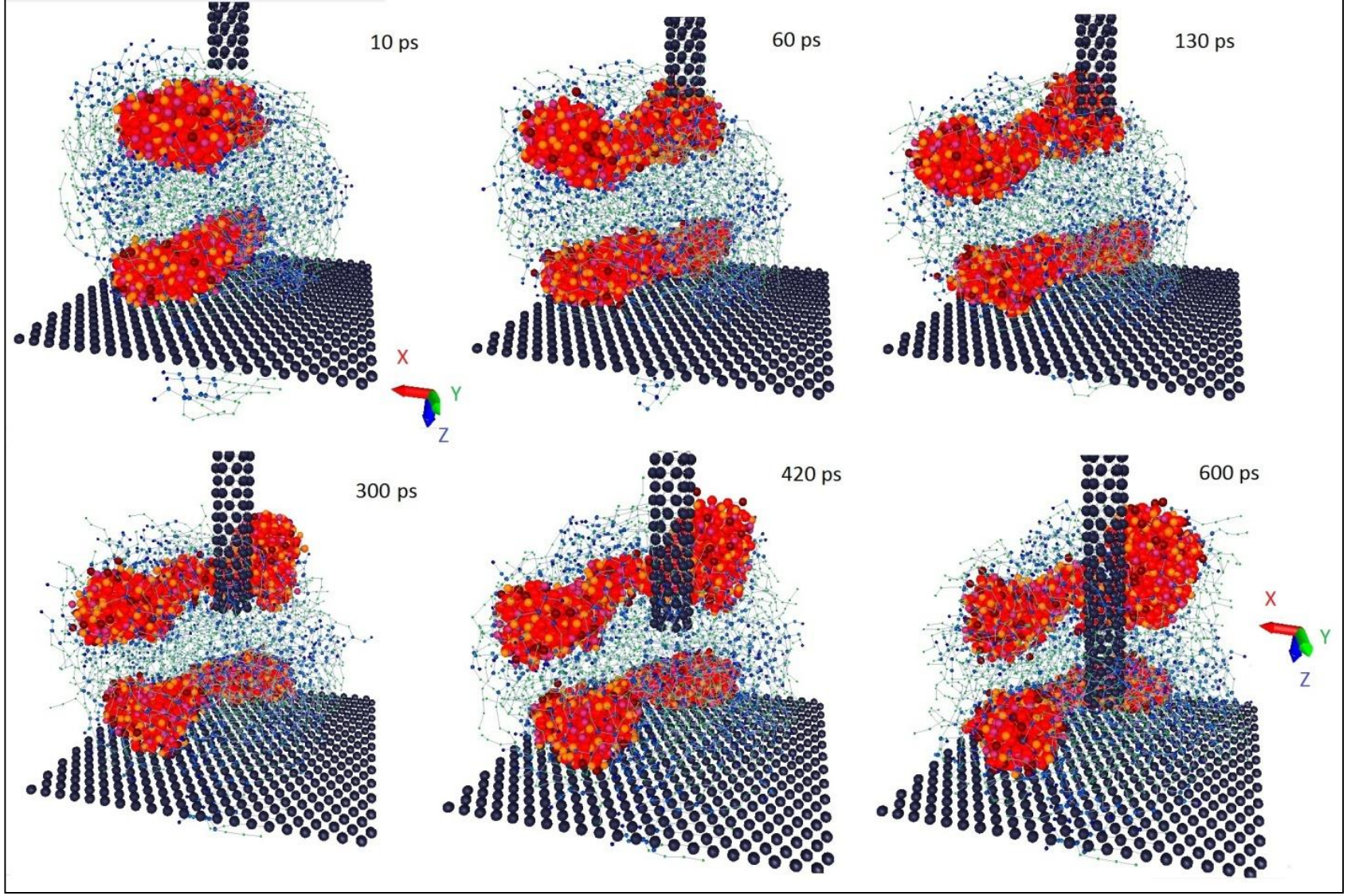






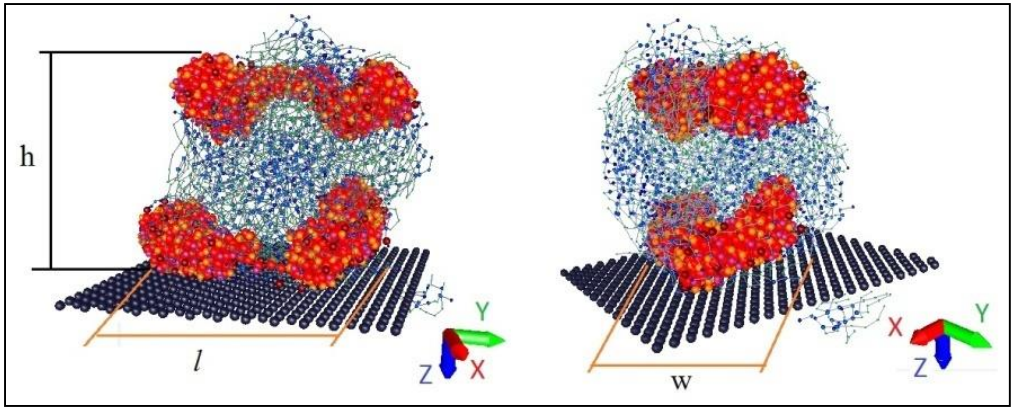


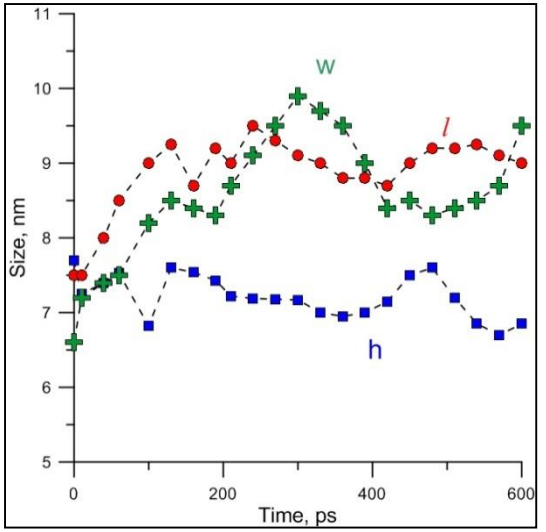


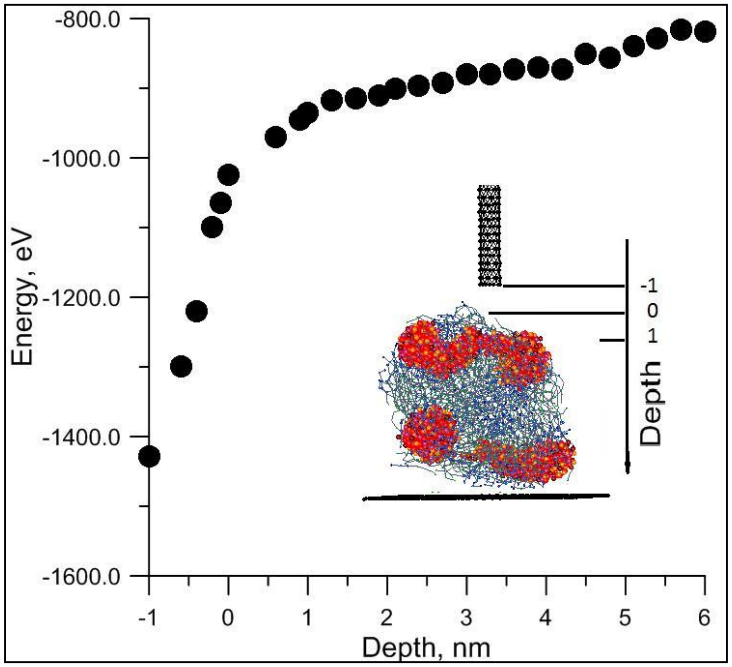


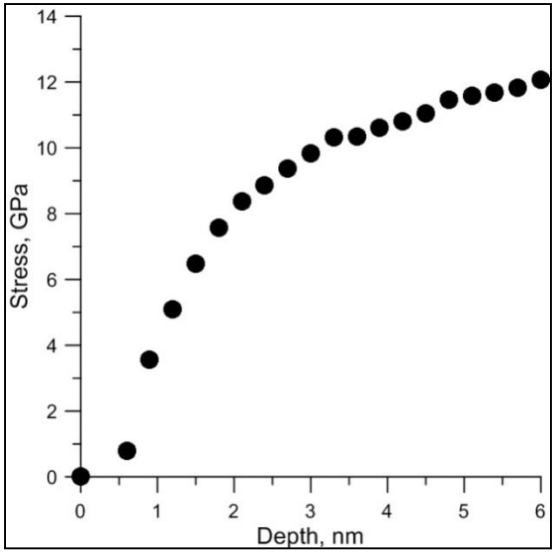
Indentation of HDL by open CNT

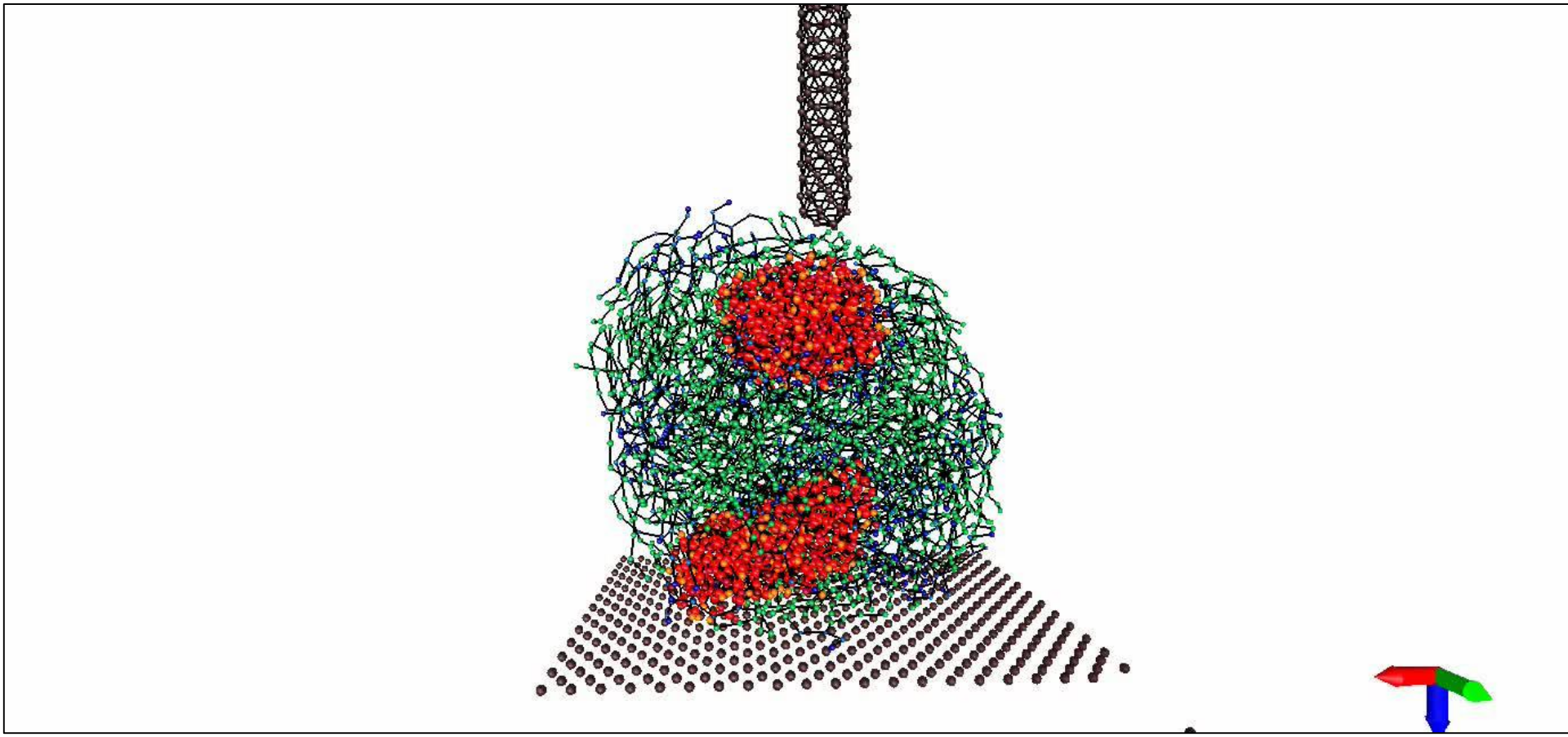
Interaction of HDL with open CNT





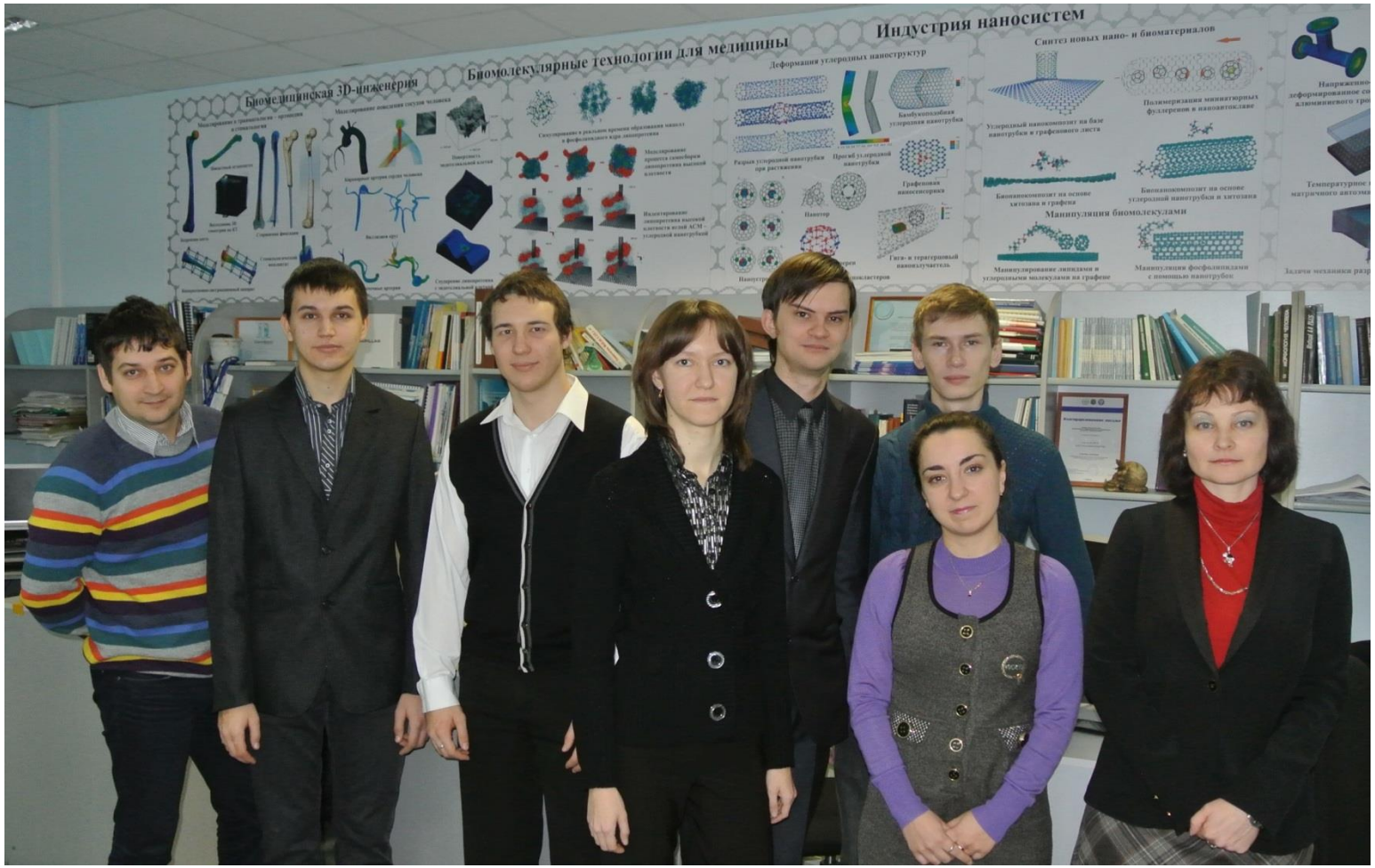






Interaction of HDL with closed CNT


Thank you for your attention!



Thank you for attention!