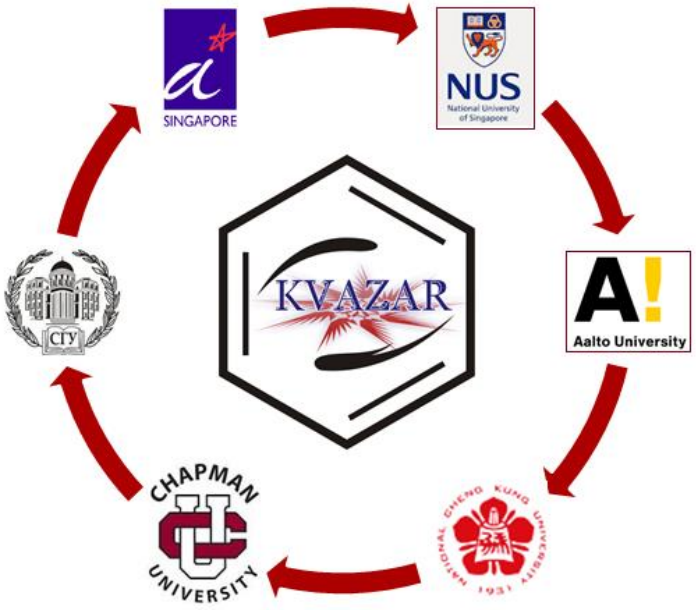
Open Cross-platform Package for Simulation Nanostructures and Biosystems



KVAZAR

http://nanokvazar.ru/

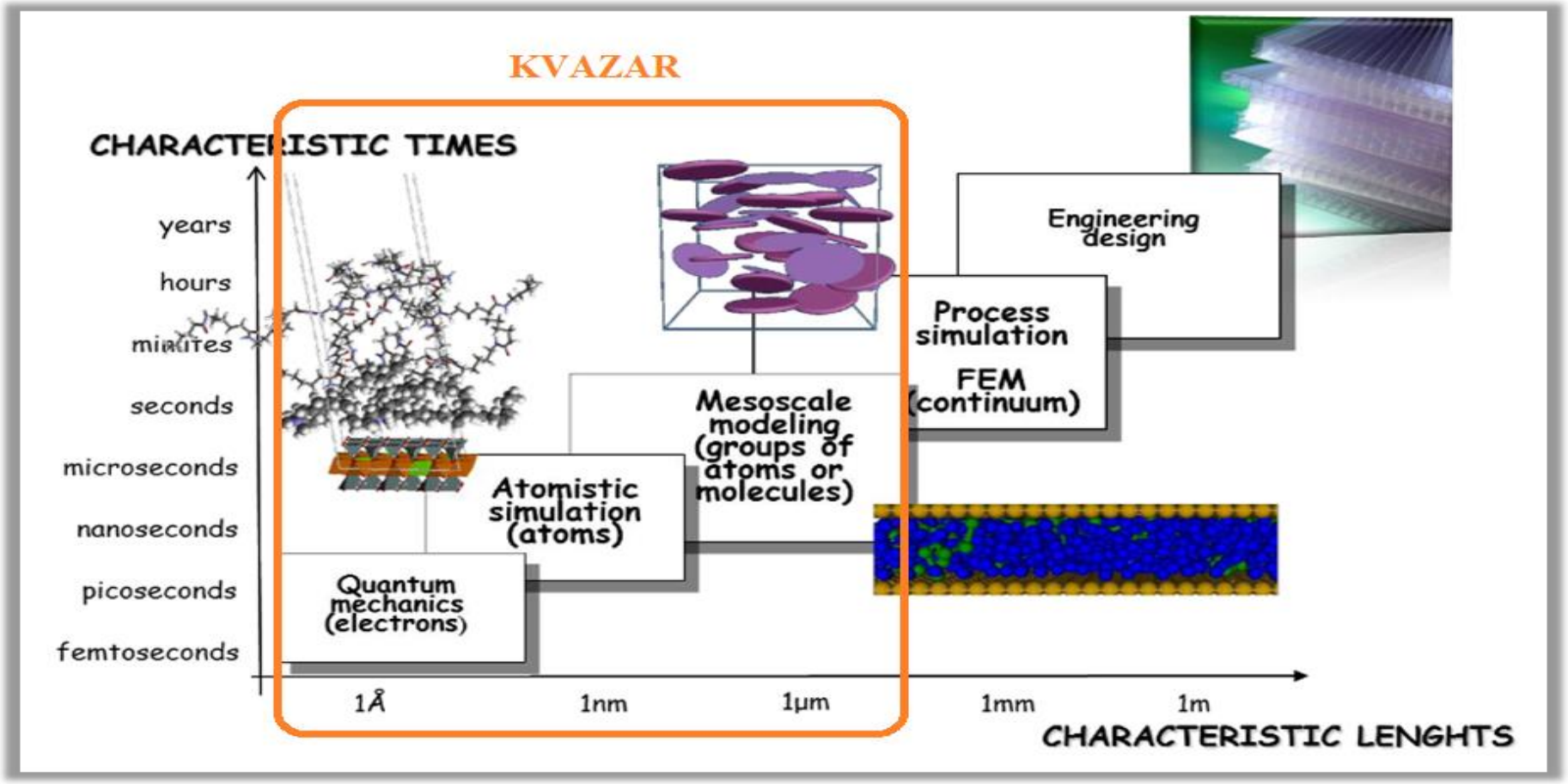
Department of Molecular Modeling,

Education and Research Institute of Nanostructures and Biosystems

Chair of Radiotechniques and Electrodynamics,

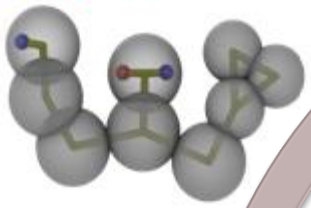
Physical Department

Hierarchy of modeling approaches: atom – molecule – mesosystem – continuous media



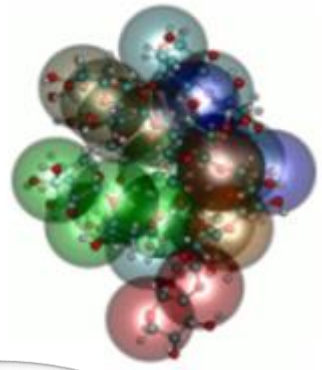
Fermeglia M., Pricl S. Prog Org Coat; 5: 187–99 (2007)

Project KVAZAR – flexible tool of multiscale computer **modeling** of nan and bioobjects and devices on its basic that is **based** on effective combination of modern approaches of quantum mechanic, molecular modeling and informational technologies



Molecular dynamics

(calculation of atoms and particles trajectories)



Quantum method

Tight-Binding

Intercore/interelectron interaction of structure atoms

Simulation of processes

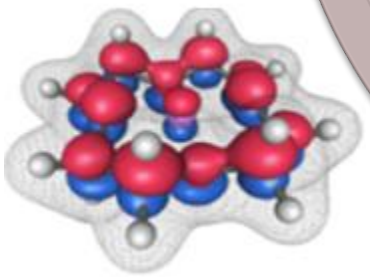
adsorption, deformation, destruction, desorption, response on external fields, defects formation

Application of:

Thermostat and barostat, water, periodic box

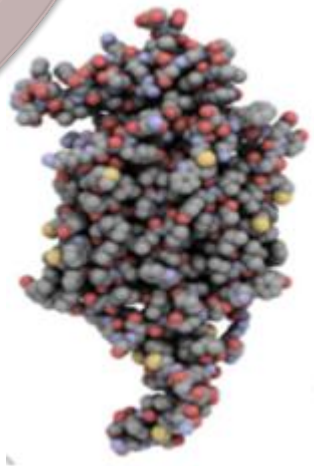
Coarse-grained method MARTINI

атомы atoms are combined in «grain» and structure has quasi-atomic mesh



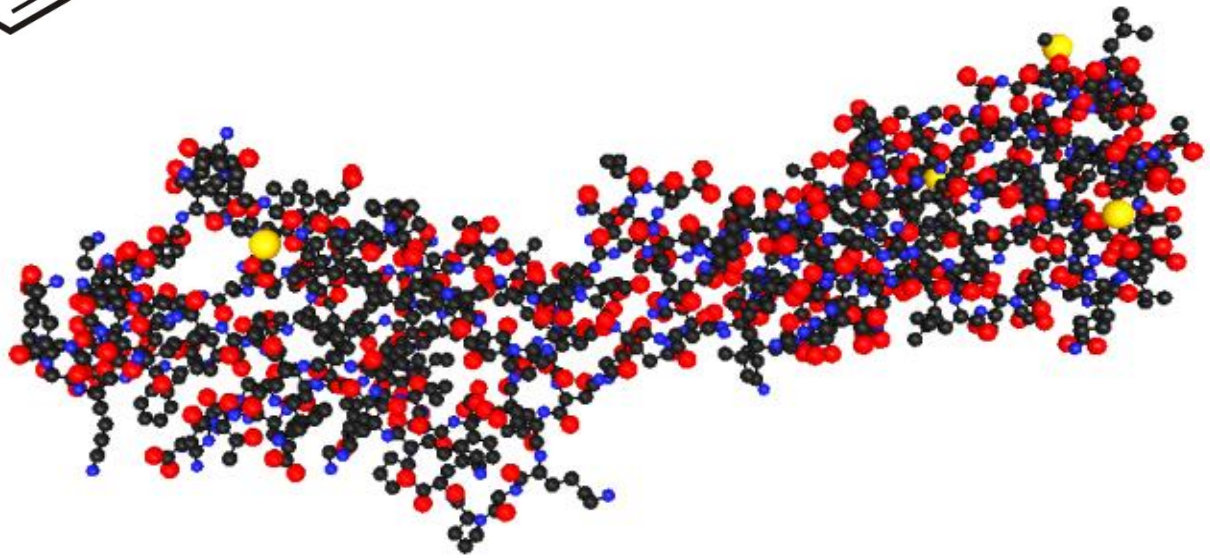
Empirical methods REBO/AIREBO –

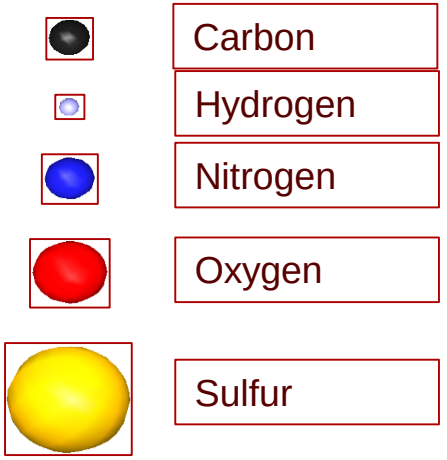
mechanical atom model



Biological Micro- and Macromolecular Systems

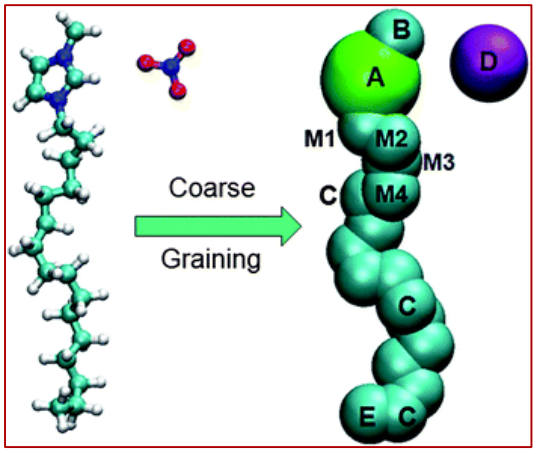
I. Problem of Overcoming the Blood-brain barrier (RSCF №14-15-00128)

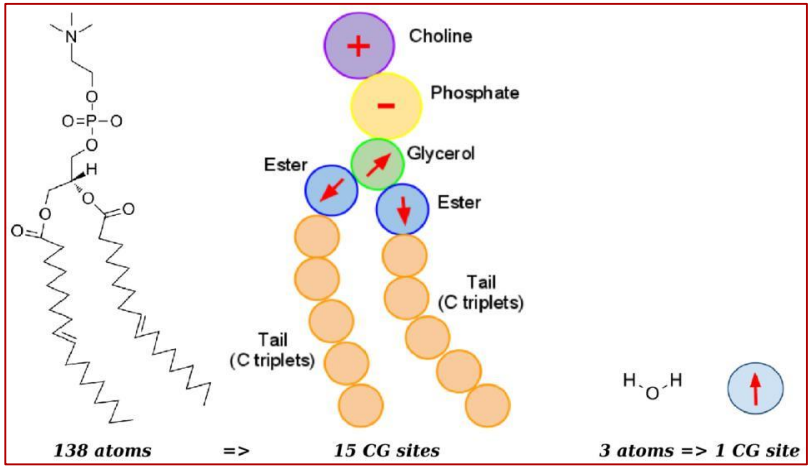




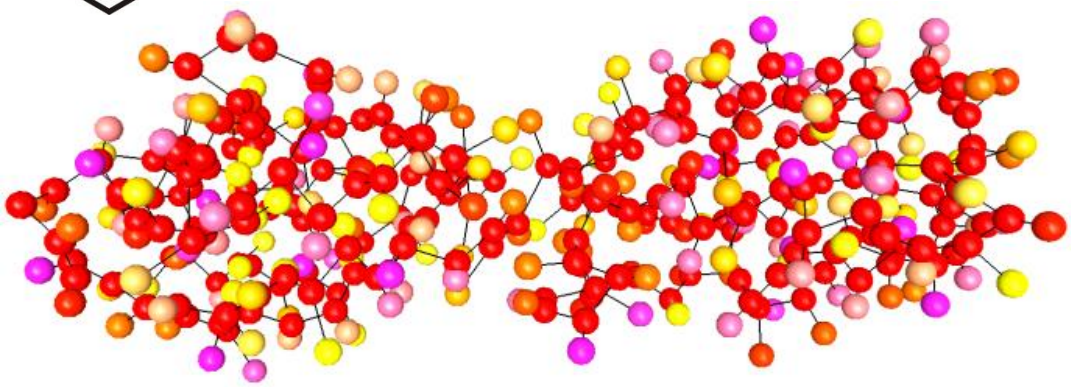
Atomistic model of endothelial receptor – **cadherin (**Protein Data Bank, PDB), on the base of which coarse-grained model in software «KVAZAR» was created

Transition from atomistic model to coarse-grained





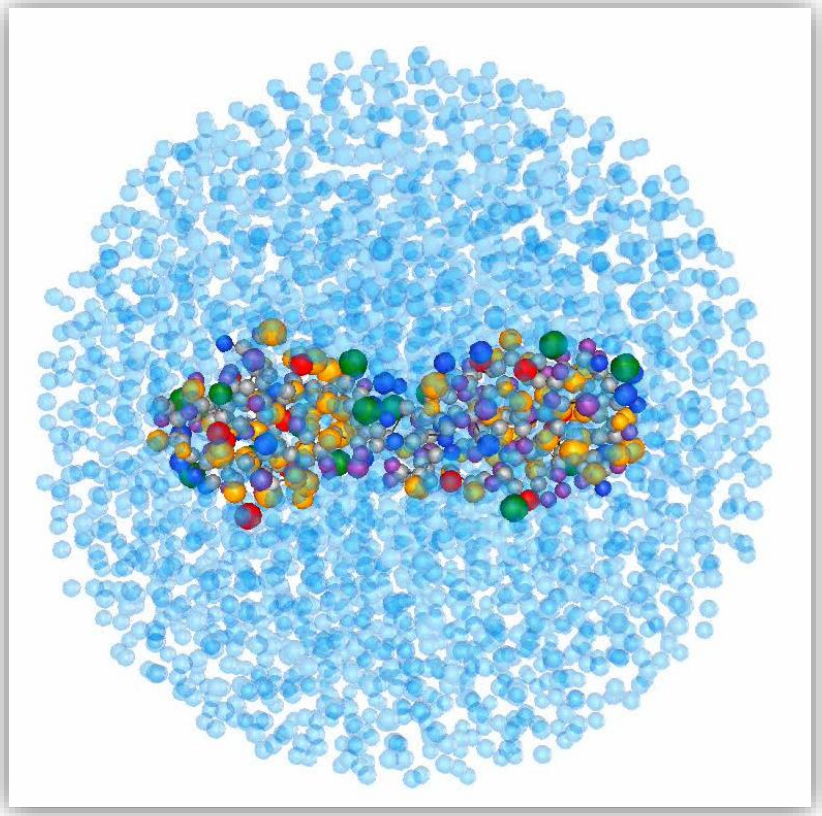
Coarse-grained model of **cadherin**.
Time of modeling – 5 ns, T=310 K.

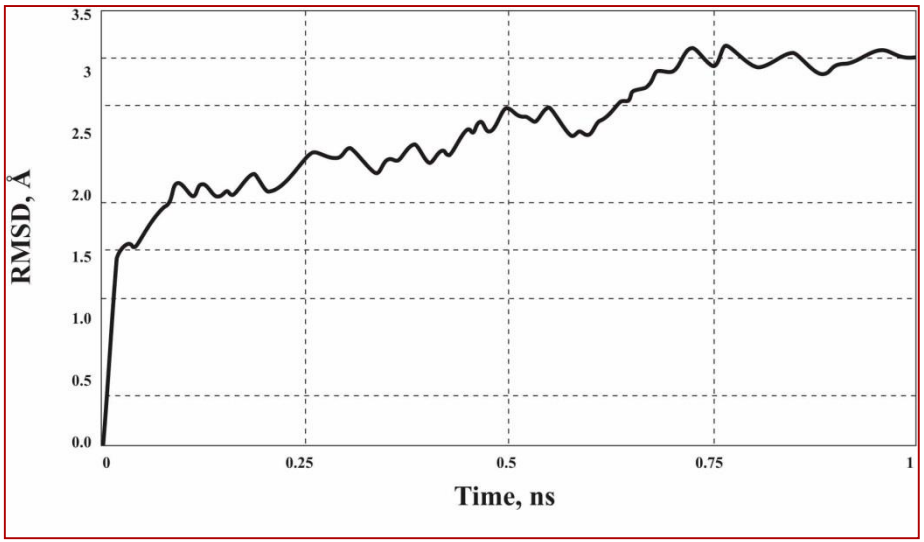


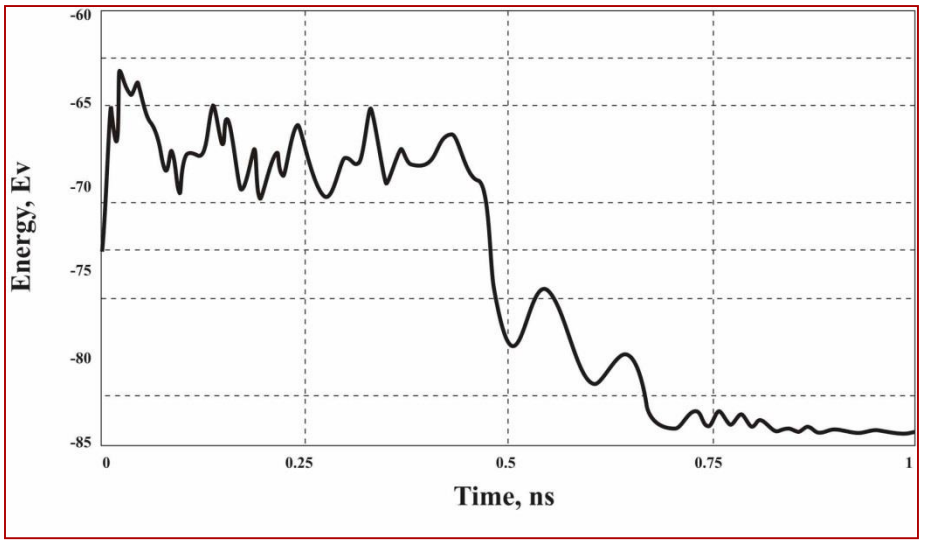
Polar non-charged under pH=7: serine, threonine, cysteine, methrionine, asparagine,

Non-polar: alanine, valine, isoleucine, leucine, proline

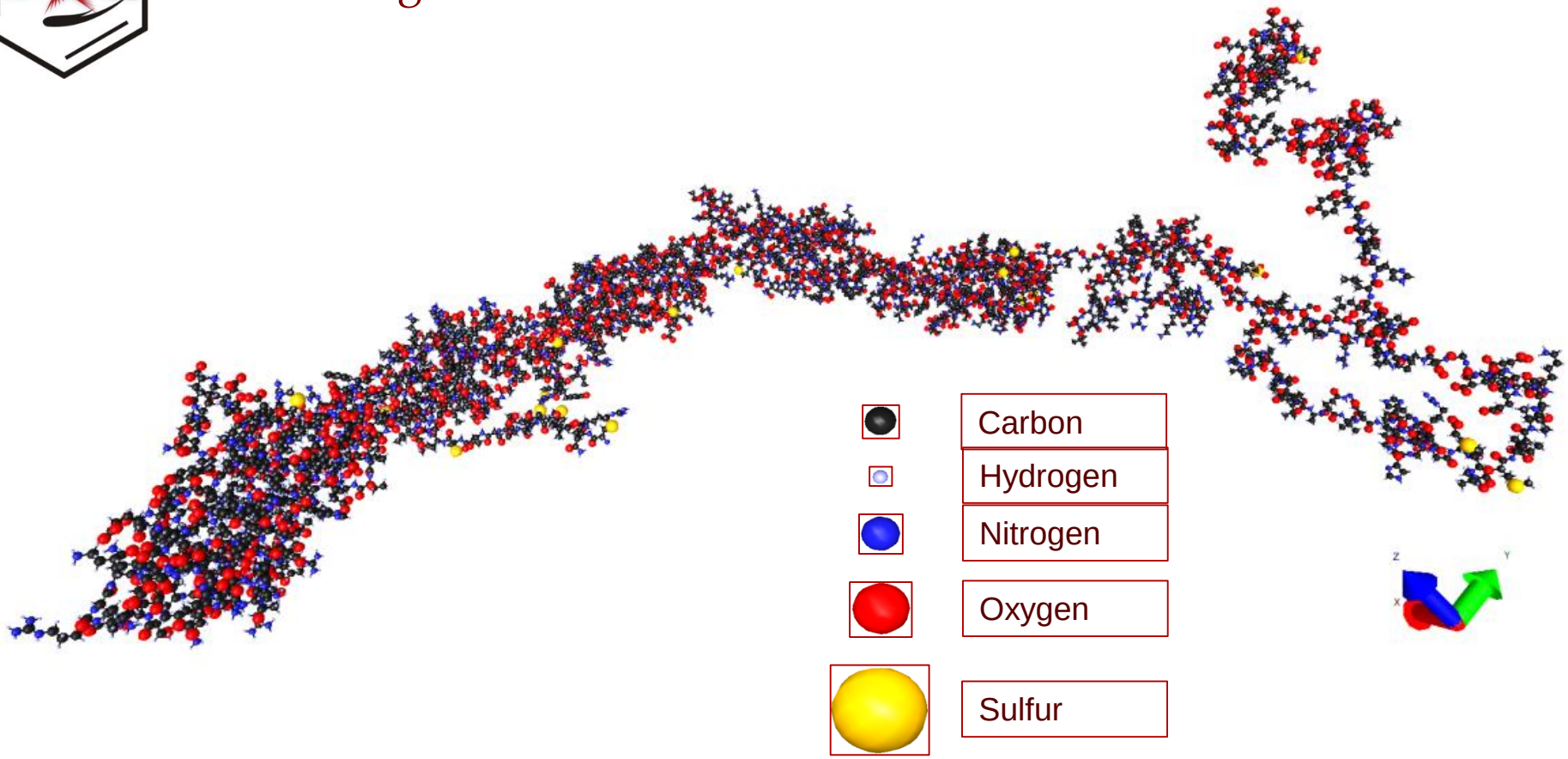
Aromatic: phenylalanine, tyrosine, tryptophan





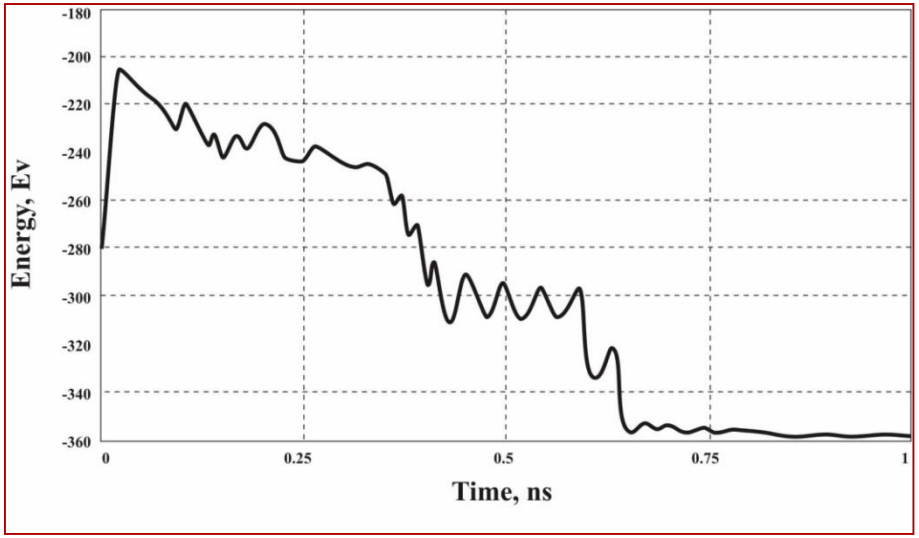


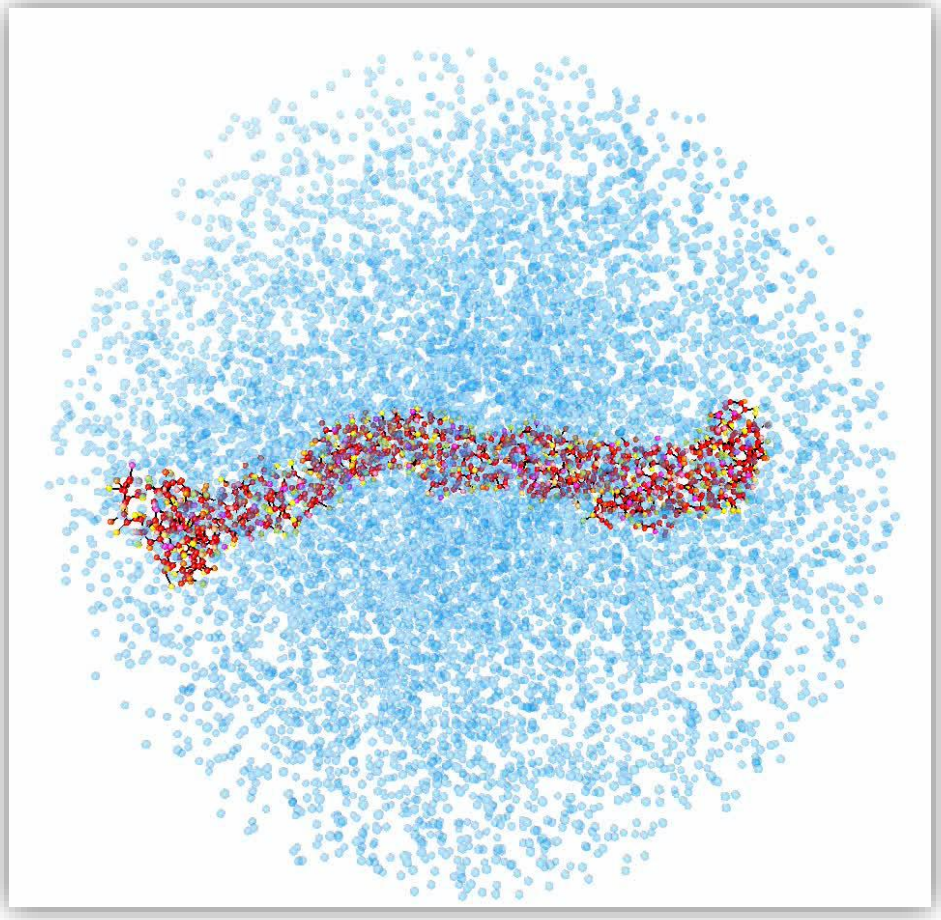
Atomistic model of cadherin antibody, on which base coarse-grained model in software «KVAZAR» was built

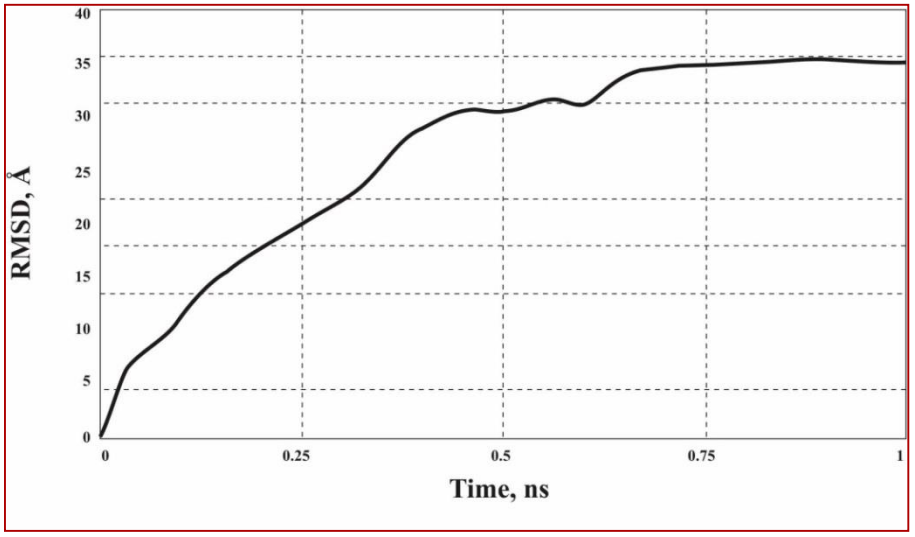


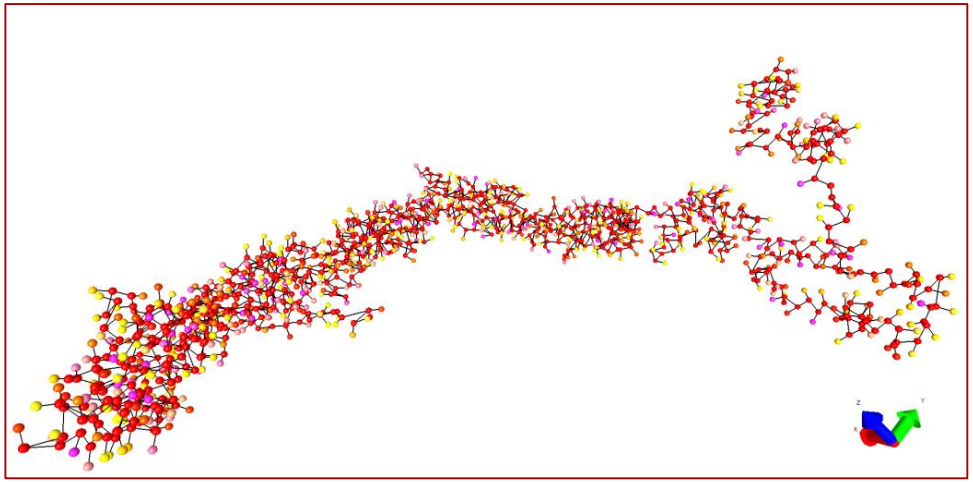
Structure: 786 amino acids (antibody)
Condition of modeling: 310 K

O.E. Glukhova, O.A. Grishina, M.M. Slepchenkov A new approach for predictive modeling of protein folding based on the natural principle of protein synthesis in living organism // Biochemistry (under review)



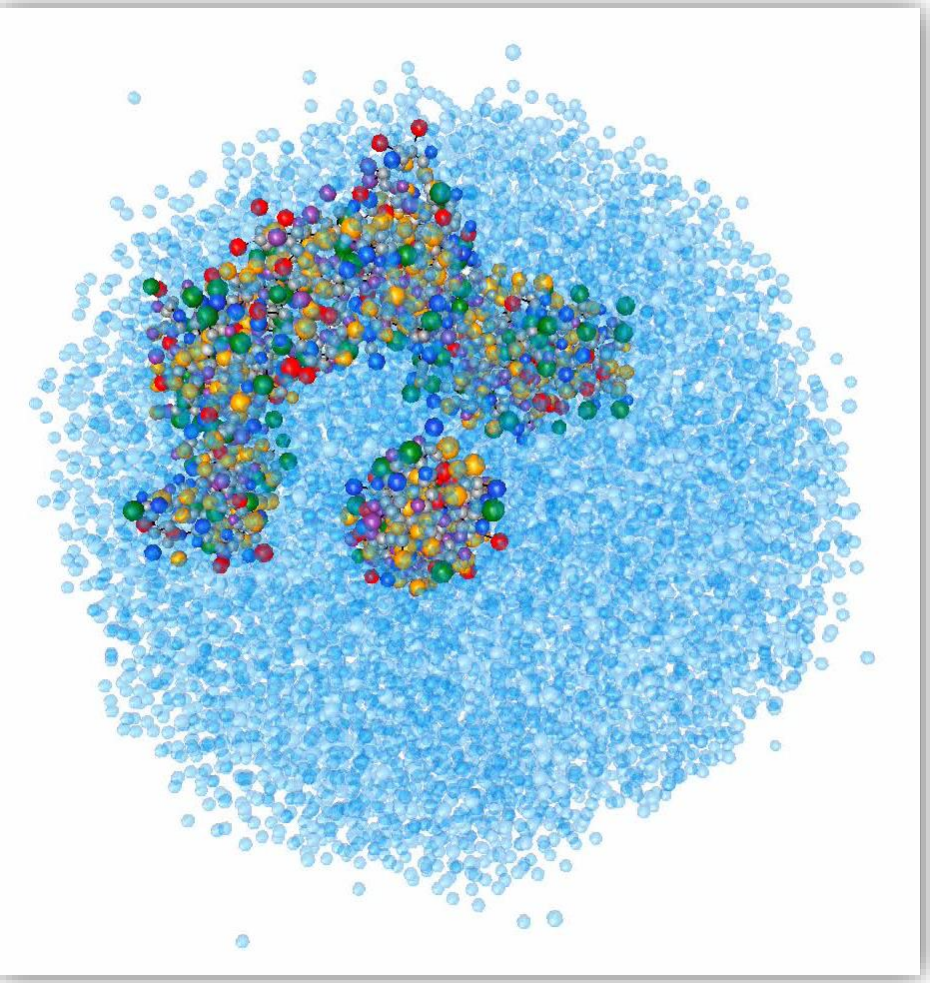




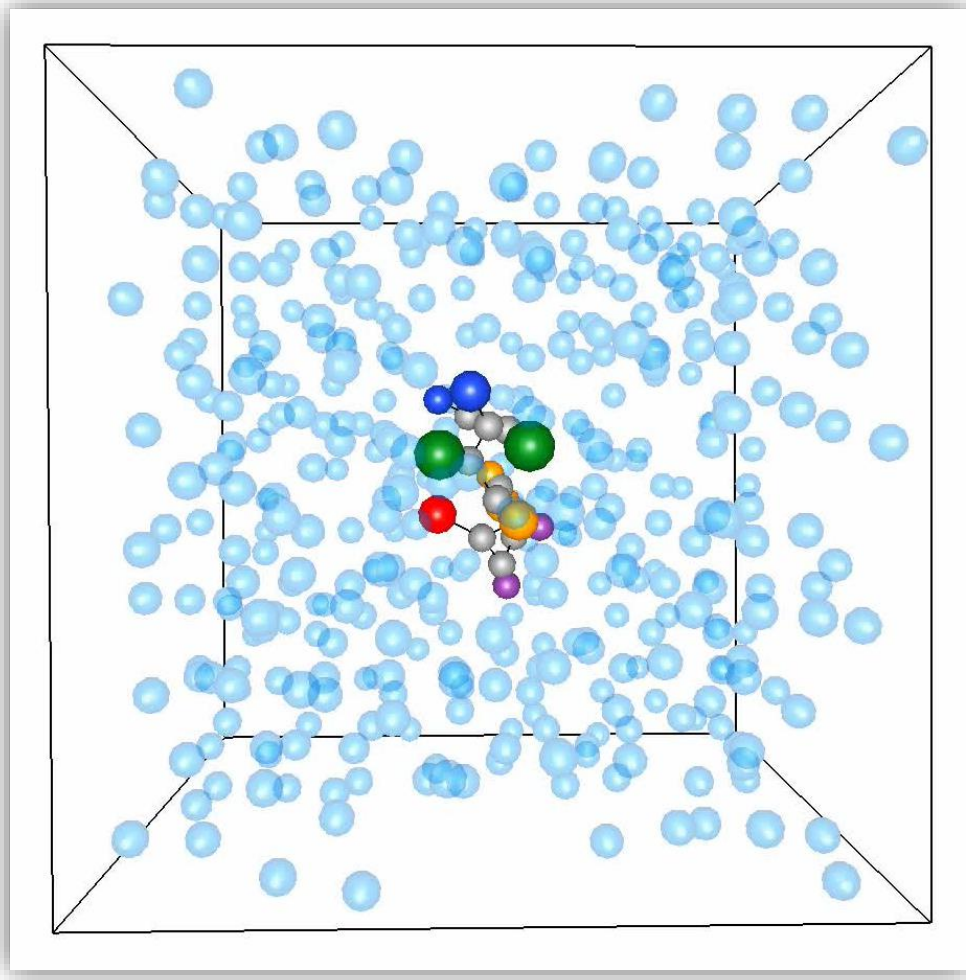


- Polar non-charged under pH=7: serine, threonine, cysteine, methrionine, asparagine,
- Non-polar: alanine, valine, isoleucine, leucine, proline
- Aromatic: phenylalanine, tyrosine, tryptophan

Investigation of cadherin and antibody interaction in water (T=310 K)

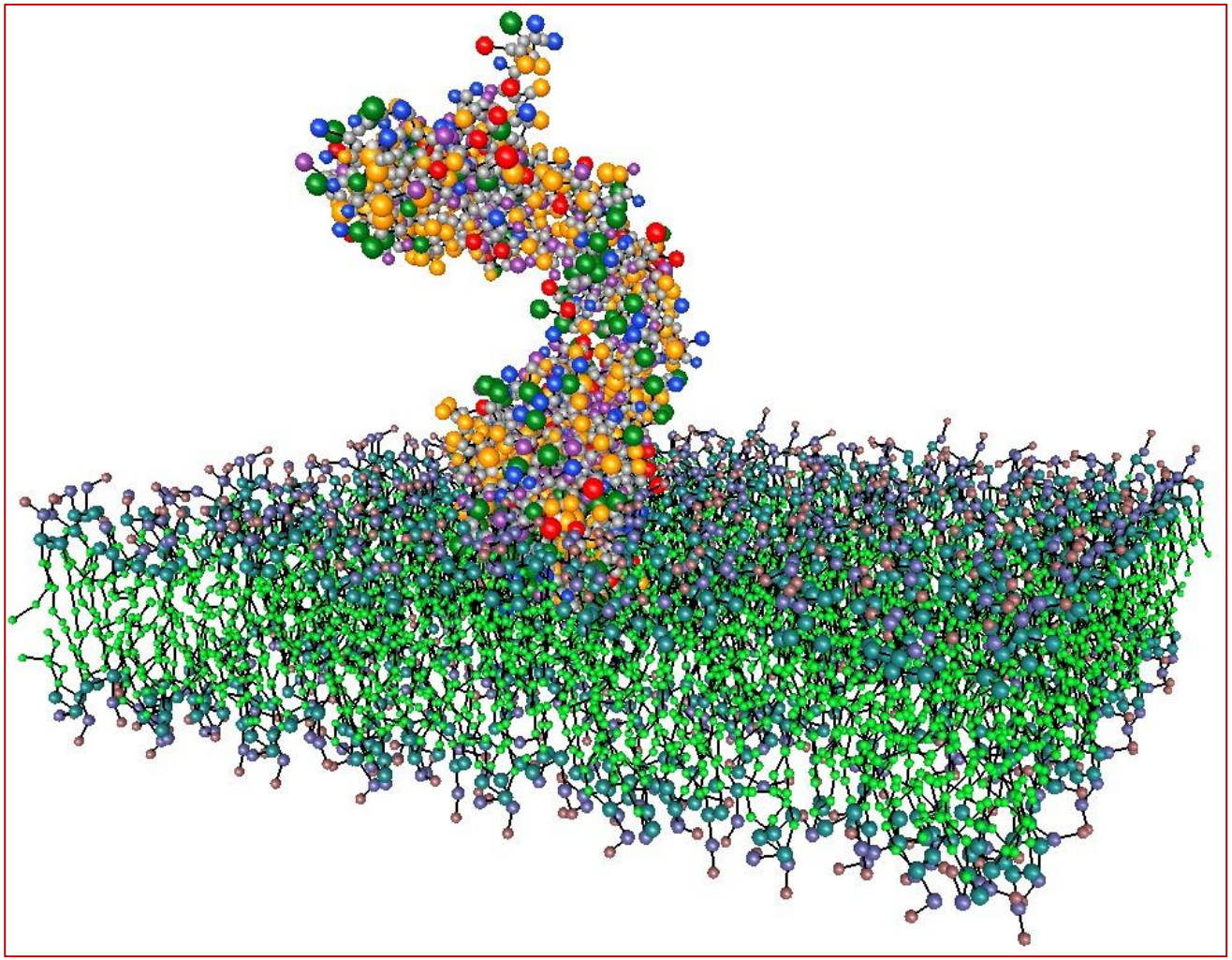


Example of periodic box application for investigation of environment influence on object



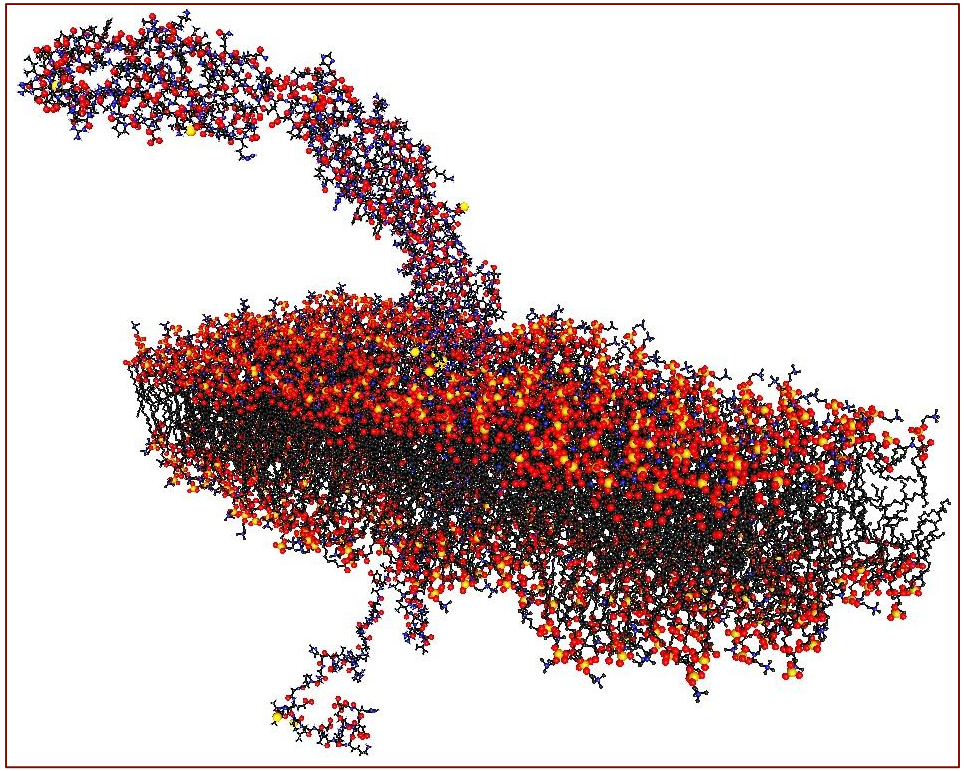
Modeling of interaction process between phospholipid bilayer (1024 DPPC) with antibody to E-cadherin (786 amino acids)

- Peptide backbone
- Polar non-charged under pH=7: serine, threonine, cysteine, methionine, asparagine, glutamine
- Non-polar: alanine, valine, isoleucine, leucine, proline
- Aromatic: fenialalanin, tyrosine, tryptophan
- Polar negatively-charged under pH-7: aspartate, glutamate
- Polar positively-charged under pH=7: lysine, arginine, histidine

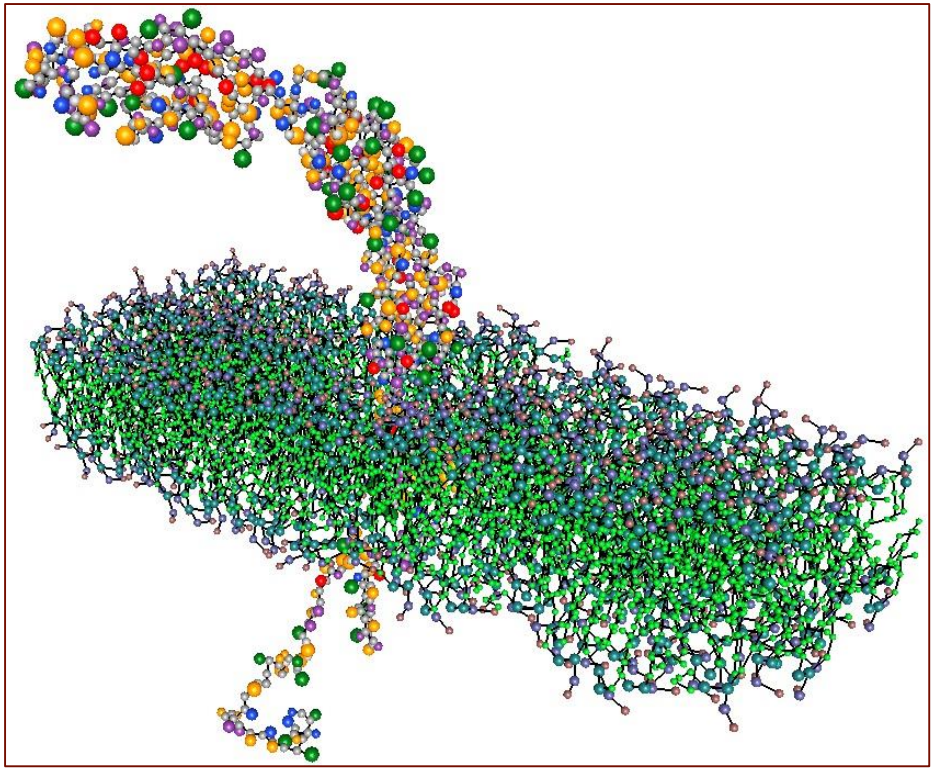


Method of formation: energetic approach for protein folding prediction
Conditions of modeling: 310 K
Method of modeling : coarse-grained model – model **Martini (KVAZAR)**
Time of modeling: 1 ns

Modeling of interaction process between phospholipid bilayer (1024 DPPC) with antibody to E-cadherin (786 amino acids). In model – extracellular, transmembrane fragment and intracellular fragment (152 amino acids)



Atomistic model of endothelial receptor (cadherin) in membrane

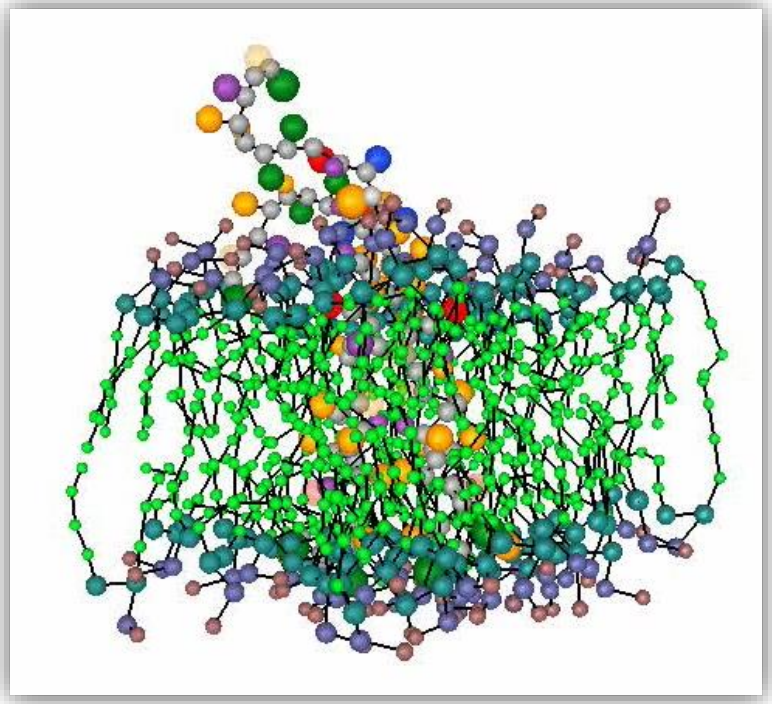


Coarse-grained model of endothelial receptor (cadherin) in membrane

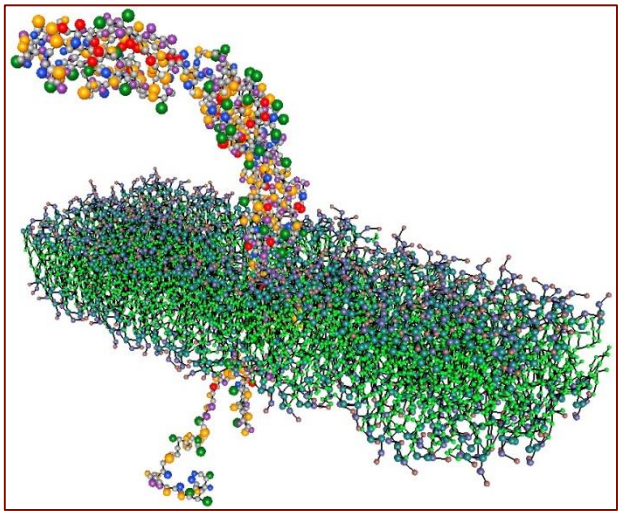
Conditions of modeling: 310 K. **Time of modeling:** 1 ns

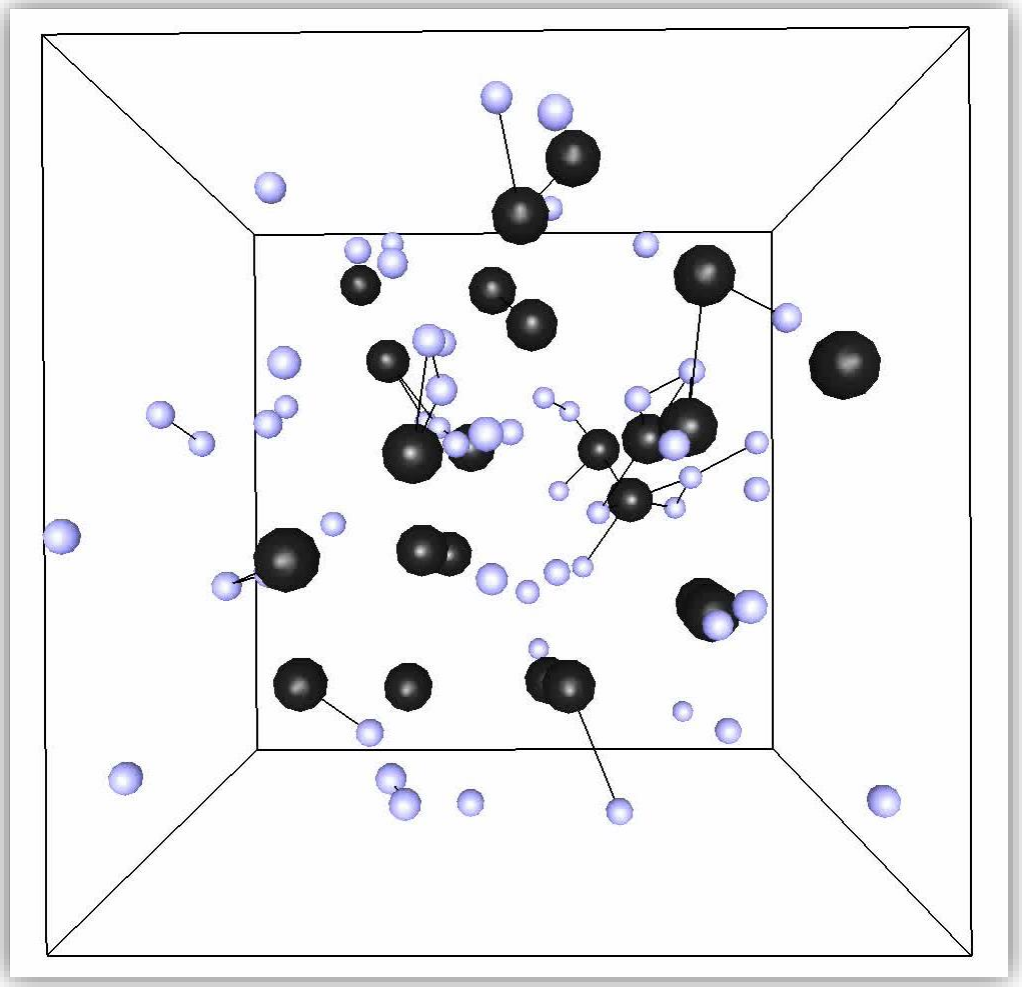
Method of modeling: coarse-grain model – model Martini (KVAZAR)

Way of creation the models of biosystems by method of self-assembly in water



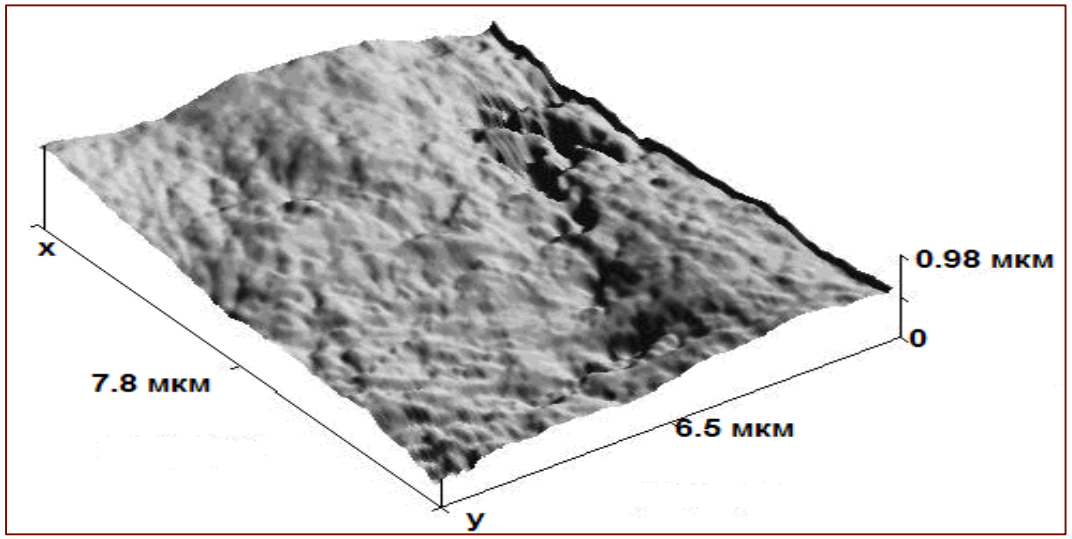
Self-assembly of system: transmembrane protein – phospholipid layer



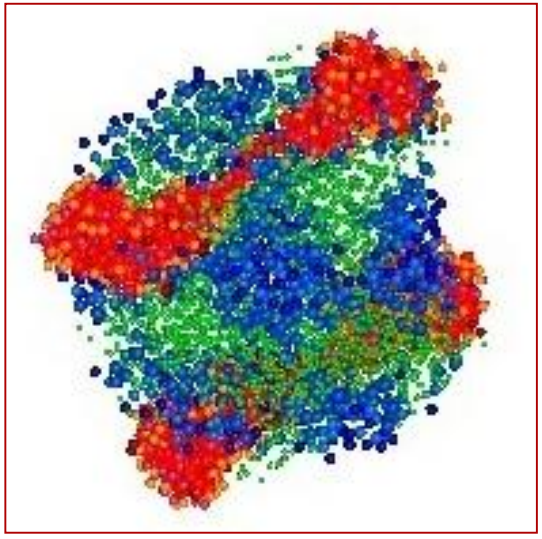


Self-assembly of propyne molecule from particular atoms of carbon and hydrogen (T=300 K, time – 5 psec, step time - 0.1 fsec)

II. Problem of atherosclerosis: construction of lipoproteins models

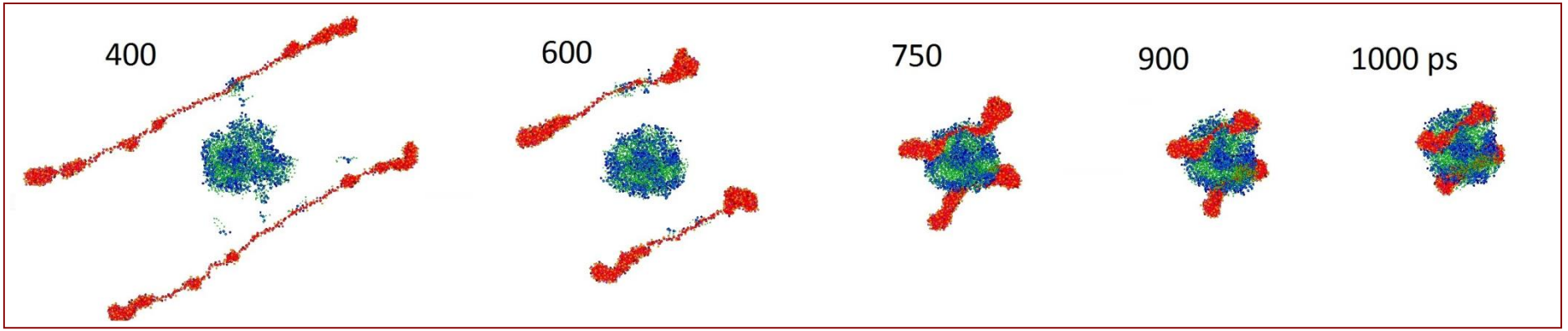


AFM-snapshot of endothelial cell surface *(Nano- and microsystem technique. 2012. № 9. P. 34 - 39)*

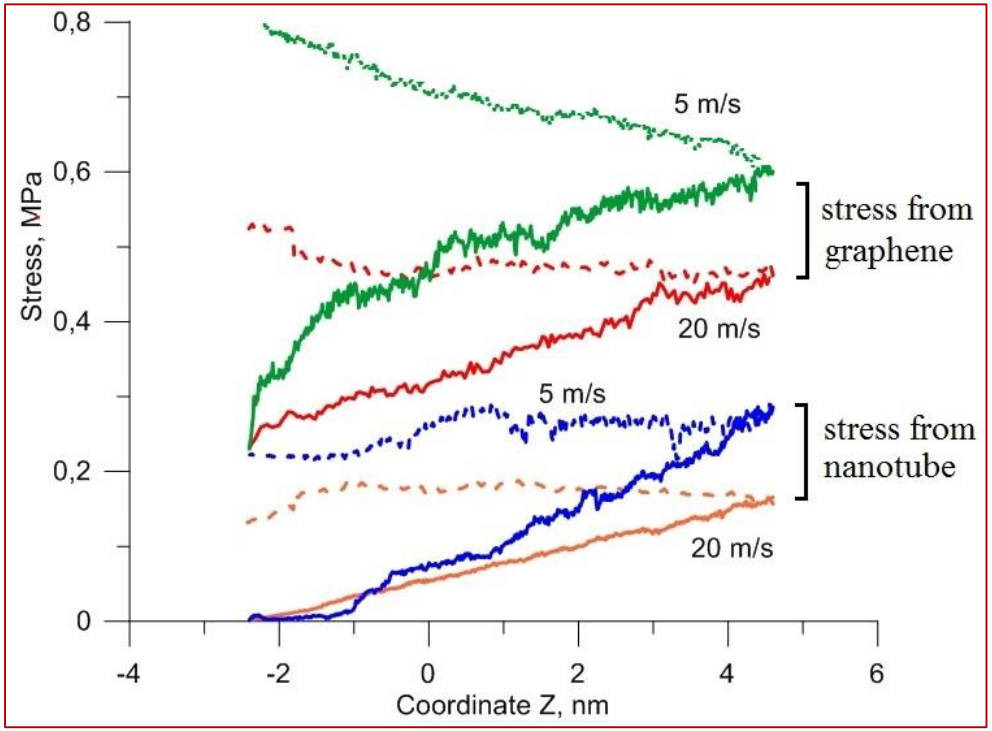


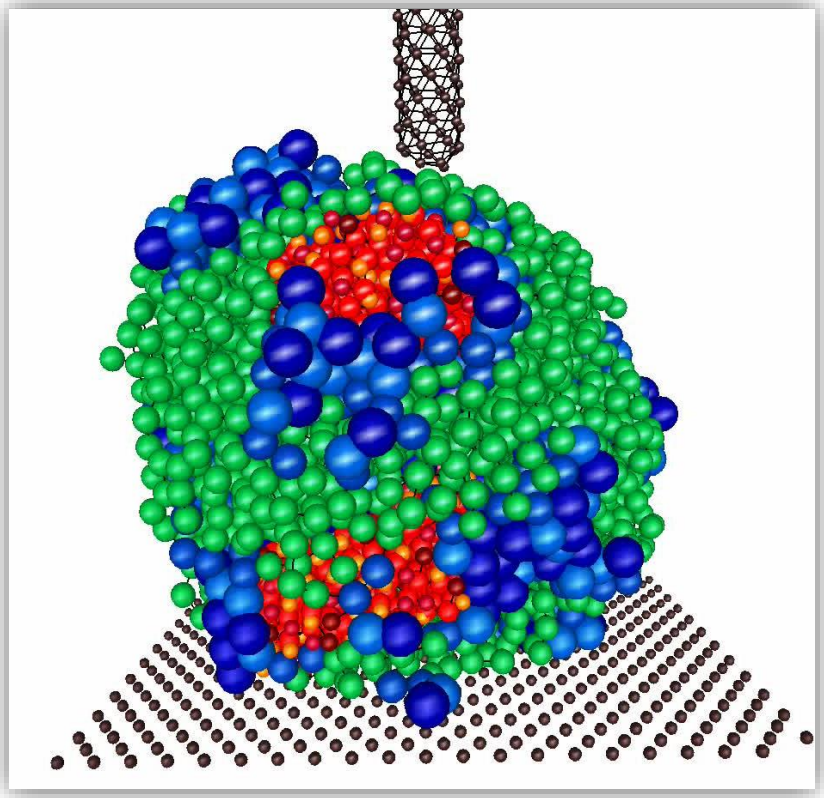
Created coarse-grained model of high-density lipoprotein (KVAZAR)

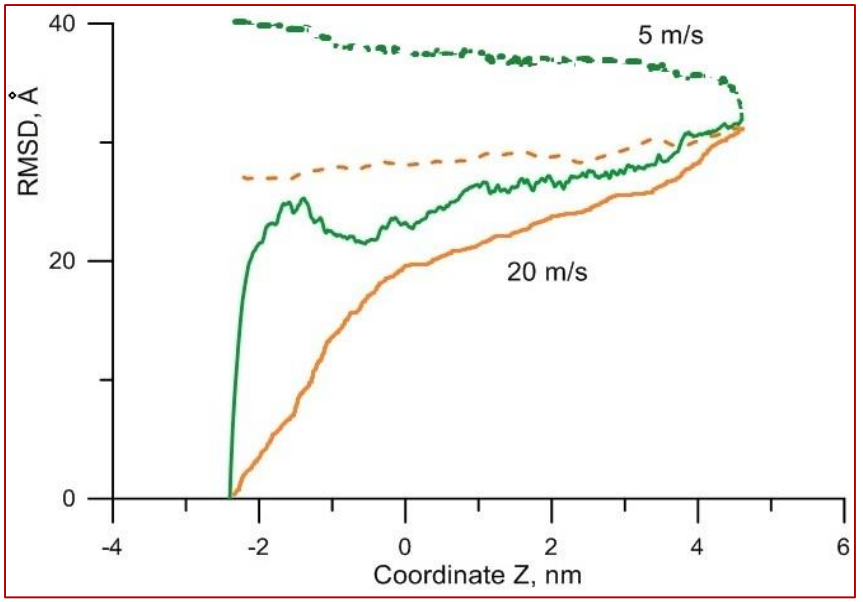
Self-assembly of high-density lipoprotein (HDL) from phospholipid molecules and two protein belts

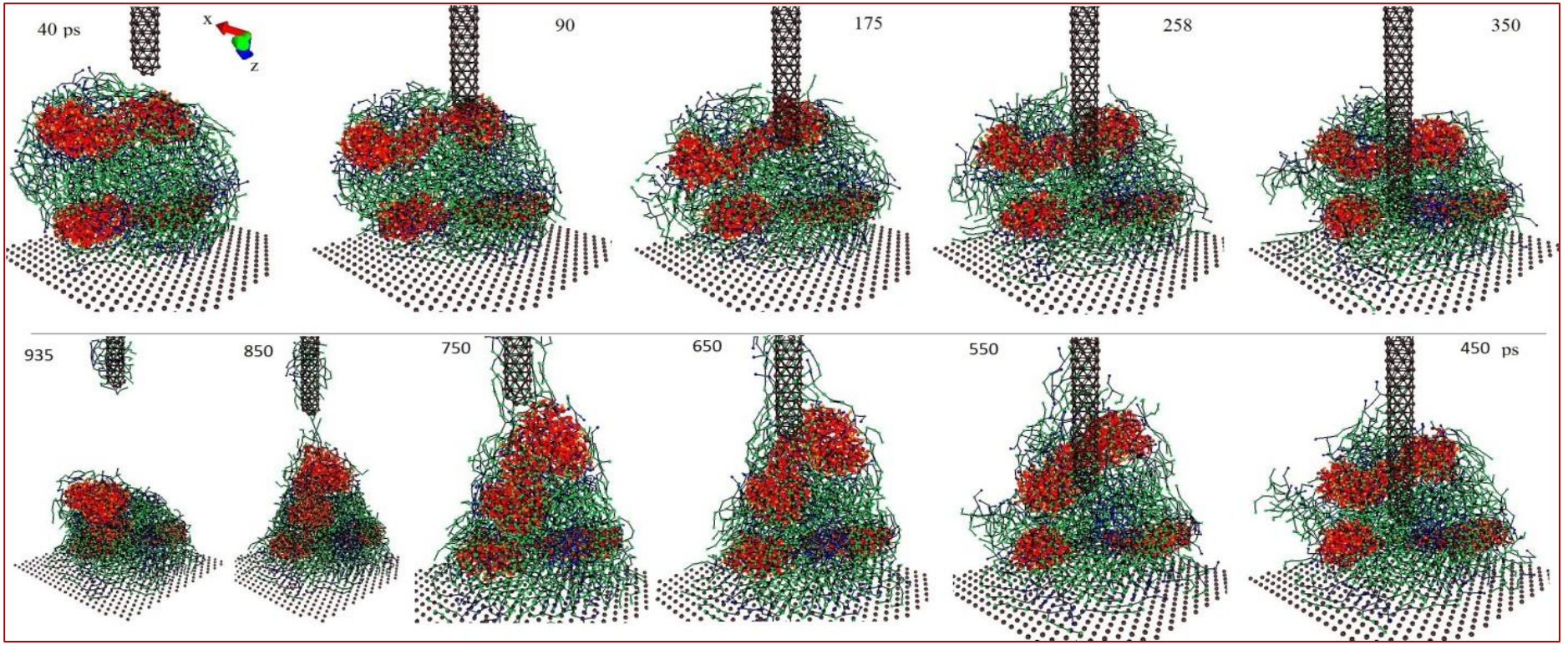


Investigation of patterns of high-density lipoprotein behavior on substrate under tip impact

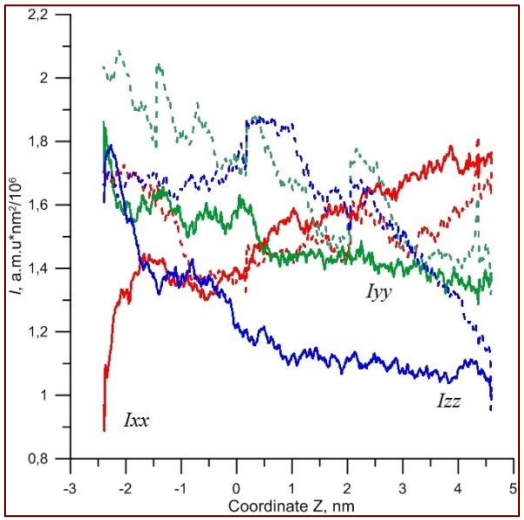


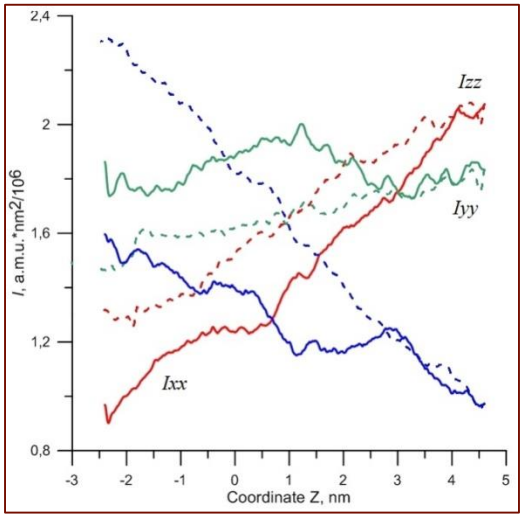


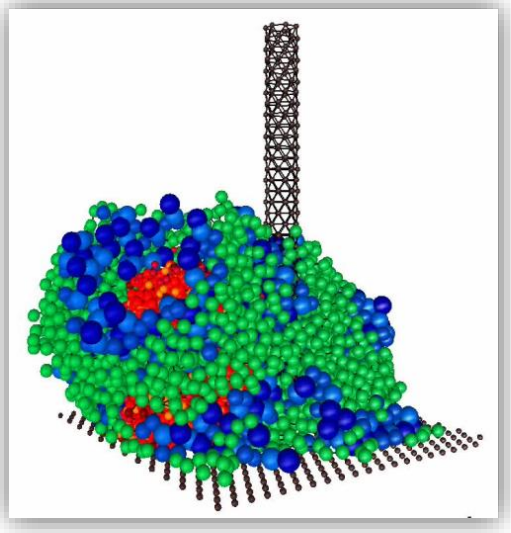




Behavior of HDL under tip impact in water under T=310 K (movement velocity 20 m/s)



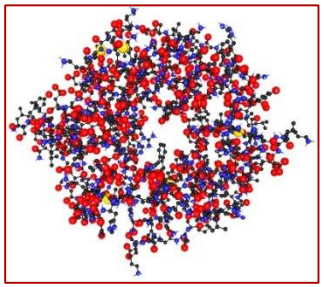




O.E. Glukhova, G.V. Savostianov // Soft Matter (under review)

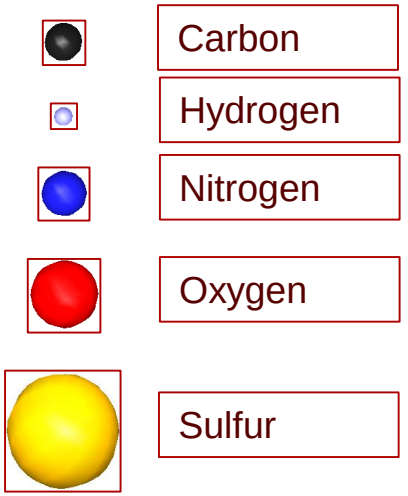
Low-density Lipoprotein: components assembly

Channel created by beta-sheets



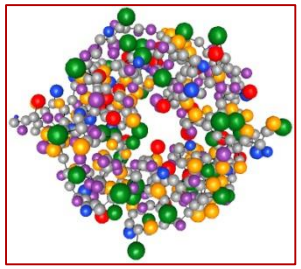
Atomistic model of **apolipoprotein B-100**

Atom types in atomistic model



Structure: 4536 amino acids
Method of construction: energetic approach for protein folding prediction
Conditions of modeling: 310 K
Time of modeling: 1 mcscec

KVAZAR

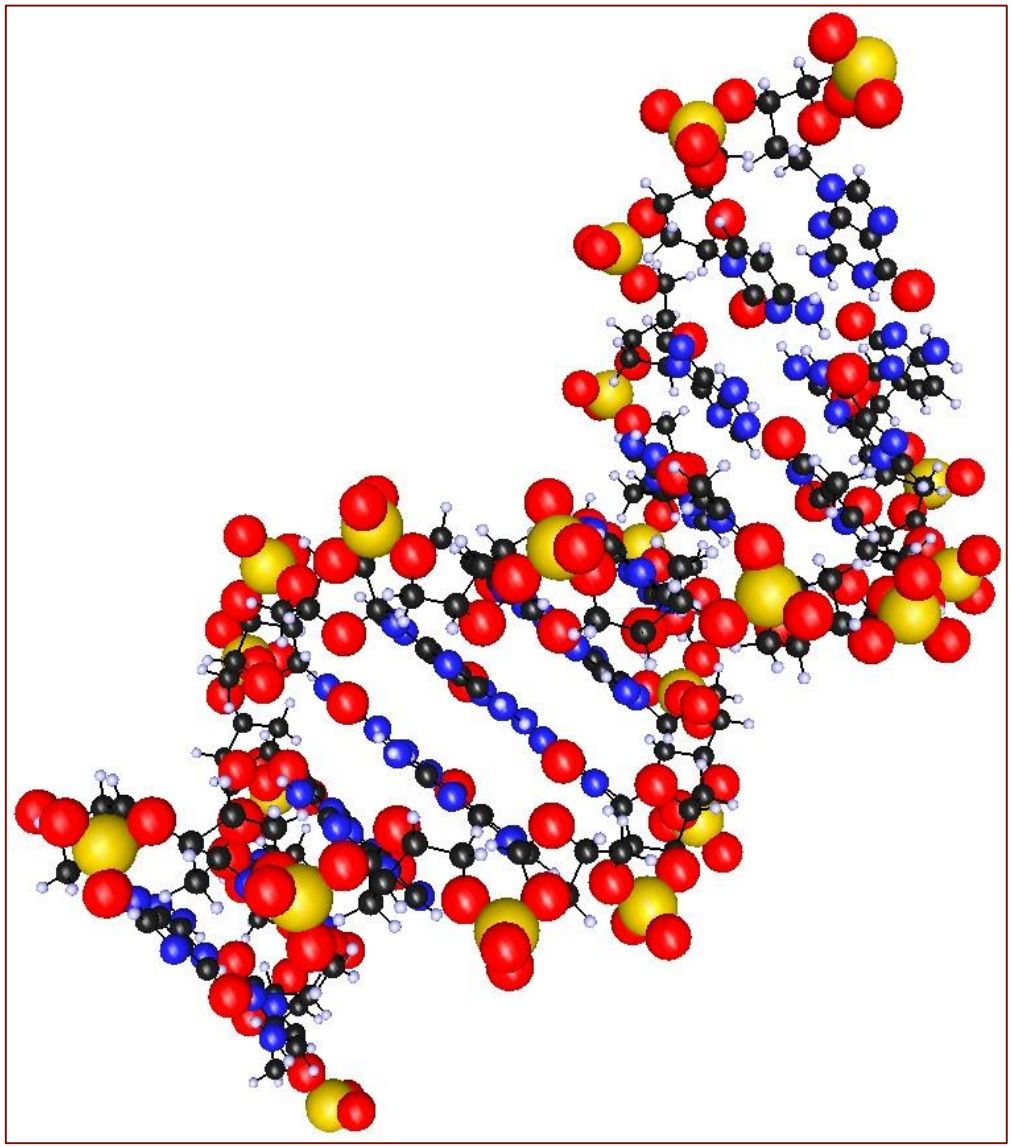


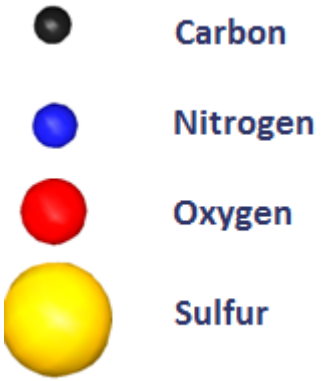
Channel created by beta-sheets

Coarse-grained model of alipoprotein B-100 (KVAZAR)

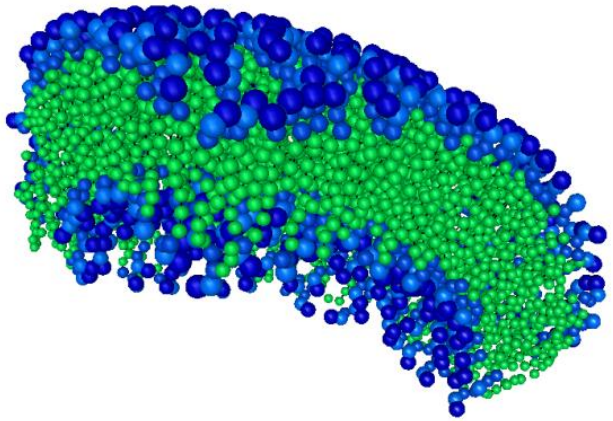
- Aromatic: fenialalanin, tyrosine, tryptophan
- Polar negatively-charged under pH-7: aspartate, glutamate
- Polar positively-charged under pH=7: lysine, arginine, histidine
- Peptide backbone
- Polar non-charged under pH=7: serine, threonine, cysteine, methionine, asparagine, glutamine
- Non-polar: alanine, valine, isoleucine, leucine, proline

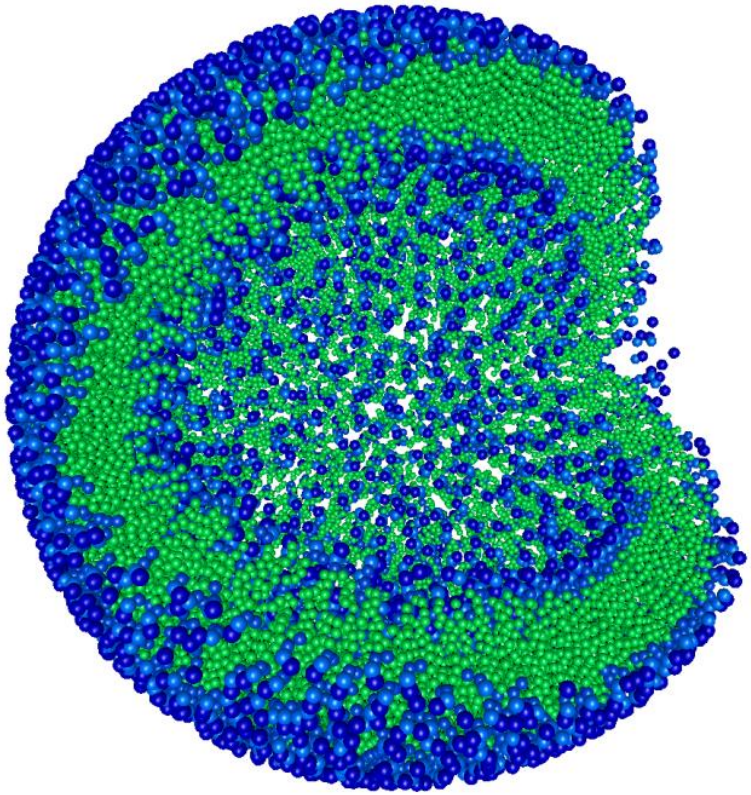
III. Examples of DNA, Viruses and Other Biosytems Coarse-grained Models

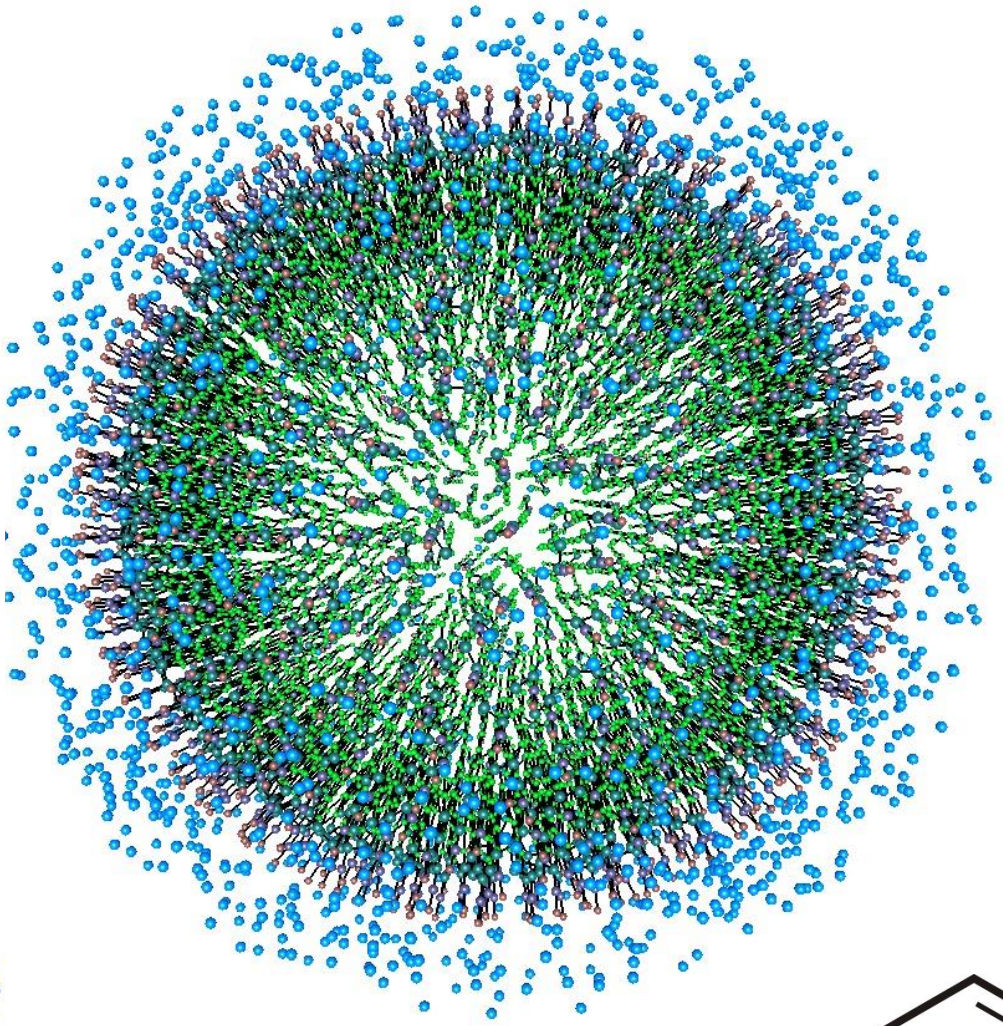




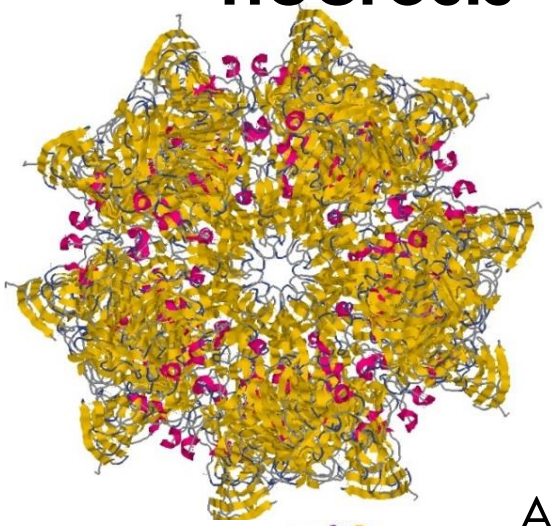
Liposome: coarse-grained modeling (KVAZAR)



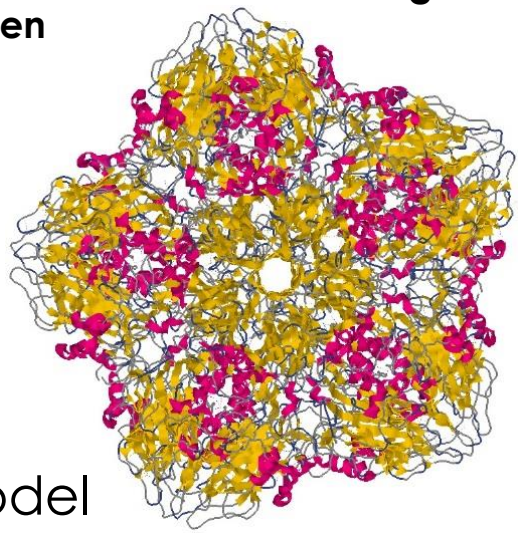




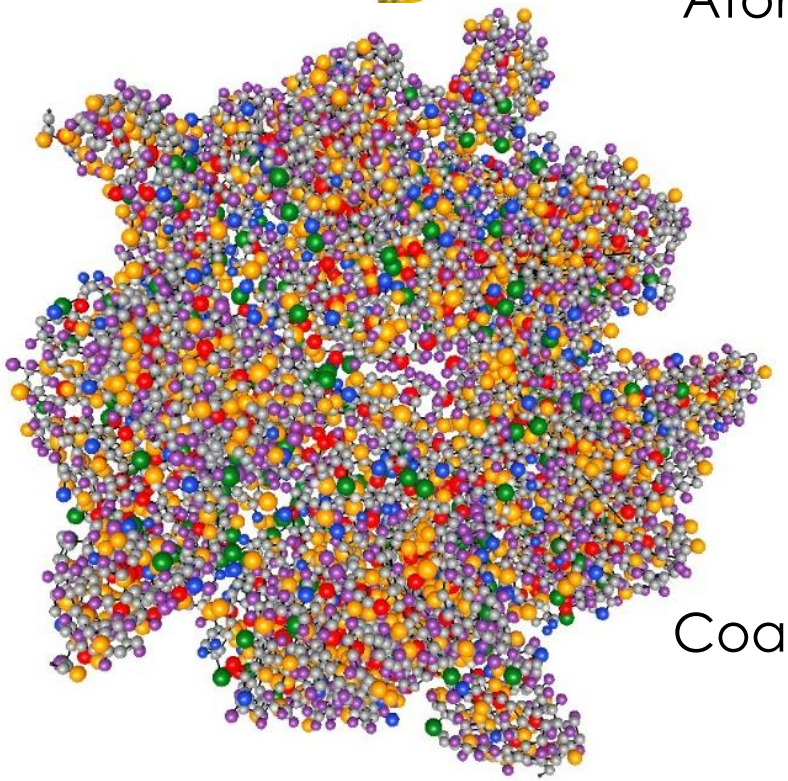
Virus of plants necrosis

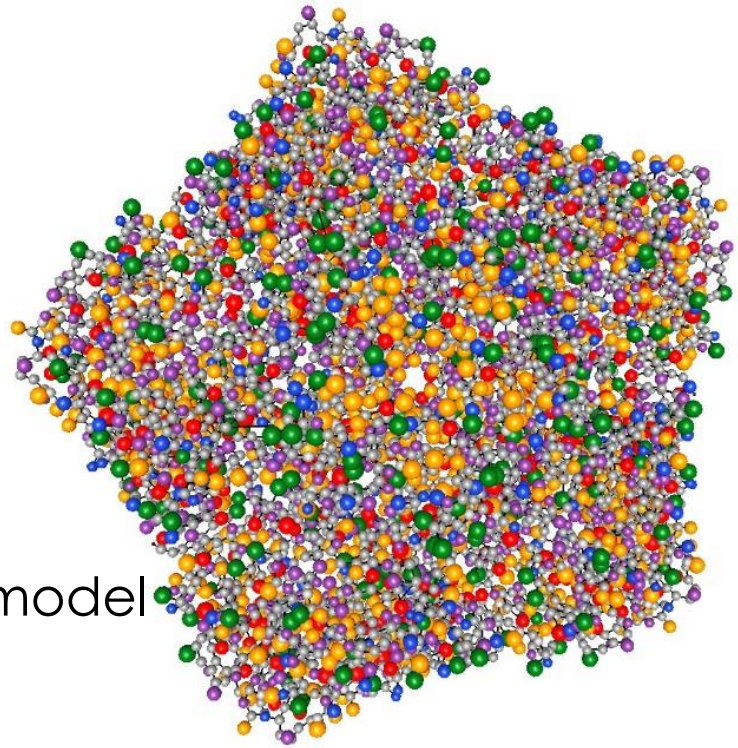


Enterovirus 71 – **virus that plays etiological role in the development of epidemic of hard neurological diseases of children**



Atomistic model

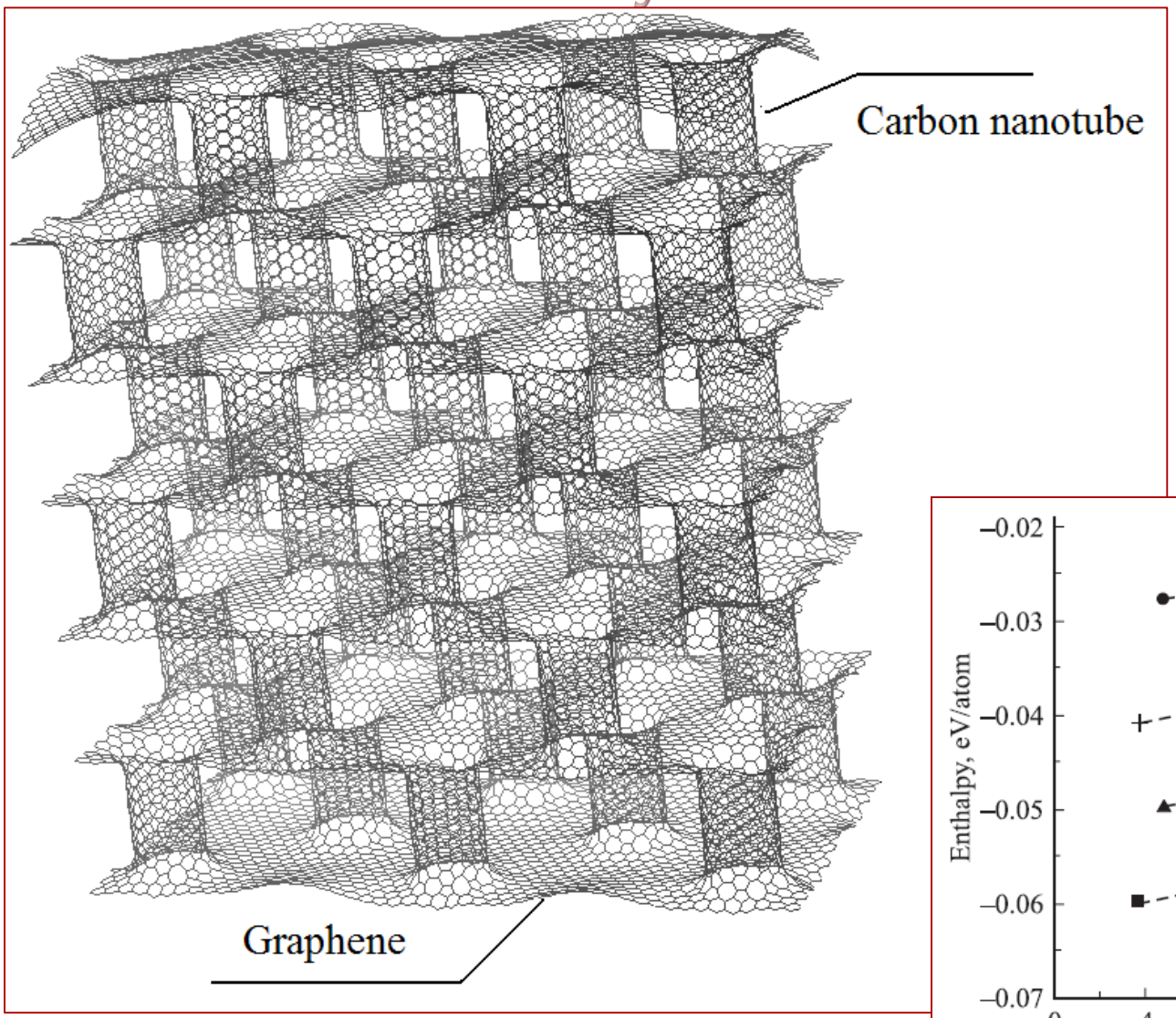




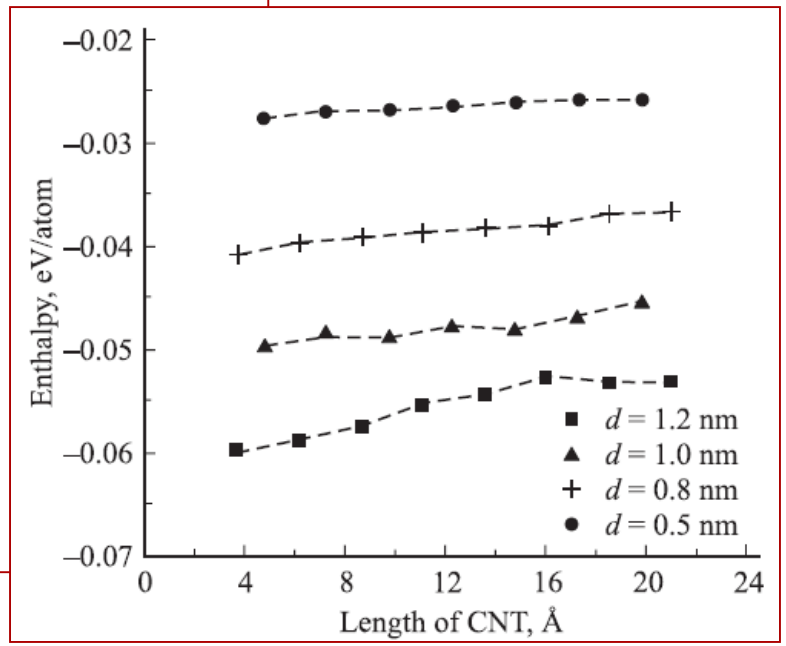
Coarse-grain model

Nanosystems: Properties and Manipulation

I. Investigation of Nanostructures Stabilities and Thermodynamics Steadiness



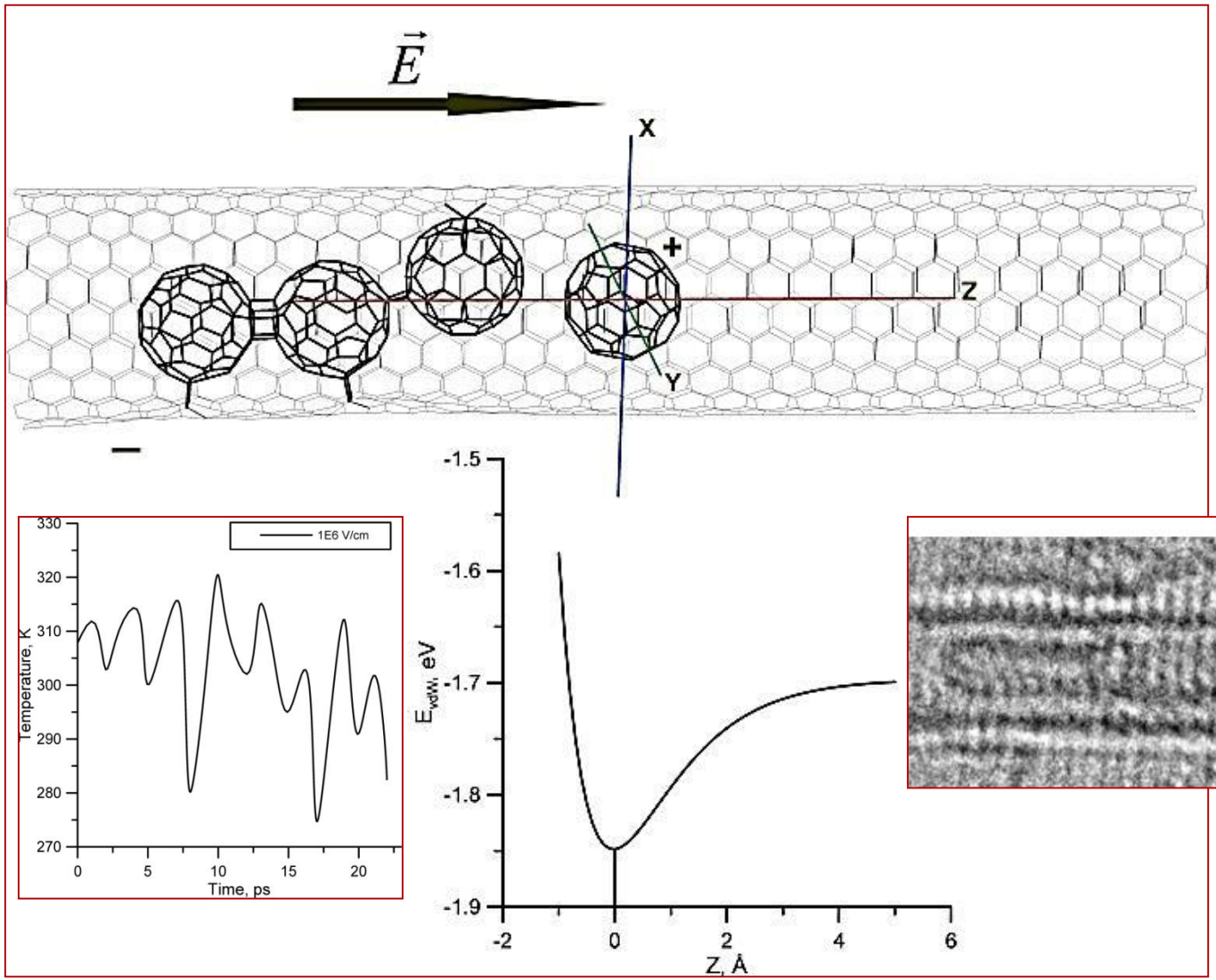
Composite material on graphene base

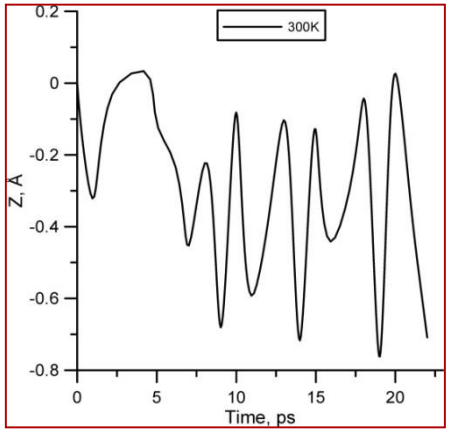


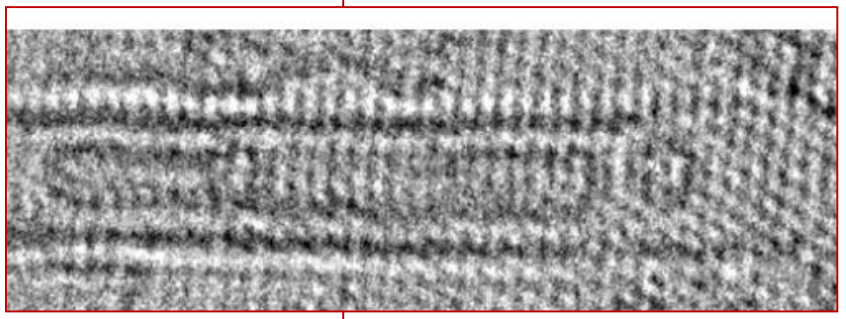
O.E. Glukhova et al., PSS 57, 994 (2015)

Grant RSCF №14-19-01308

II. Investigation of Patterns of Nanoobjects Behavior and Interaction







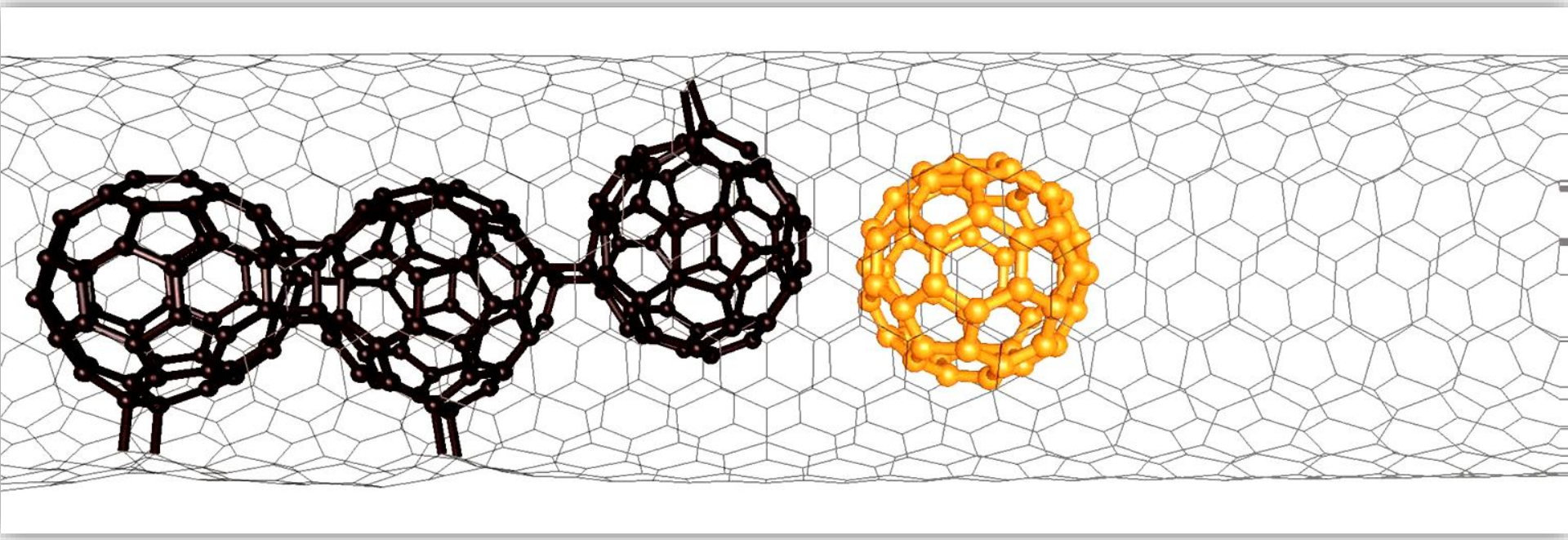
Snapshot was received in Aalto University (Finland)

Creation of molecular model of polymerized and free moleclues of C_{60} in nanotube via experiment

Model of electromagnetic waves of GHz/THz frequency range on carbon nanostructures

(molecule with +1e charge is noted by yellow):

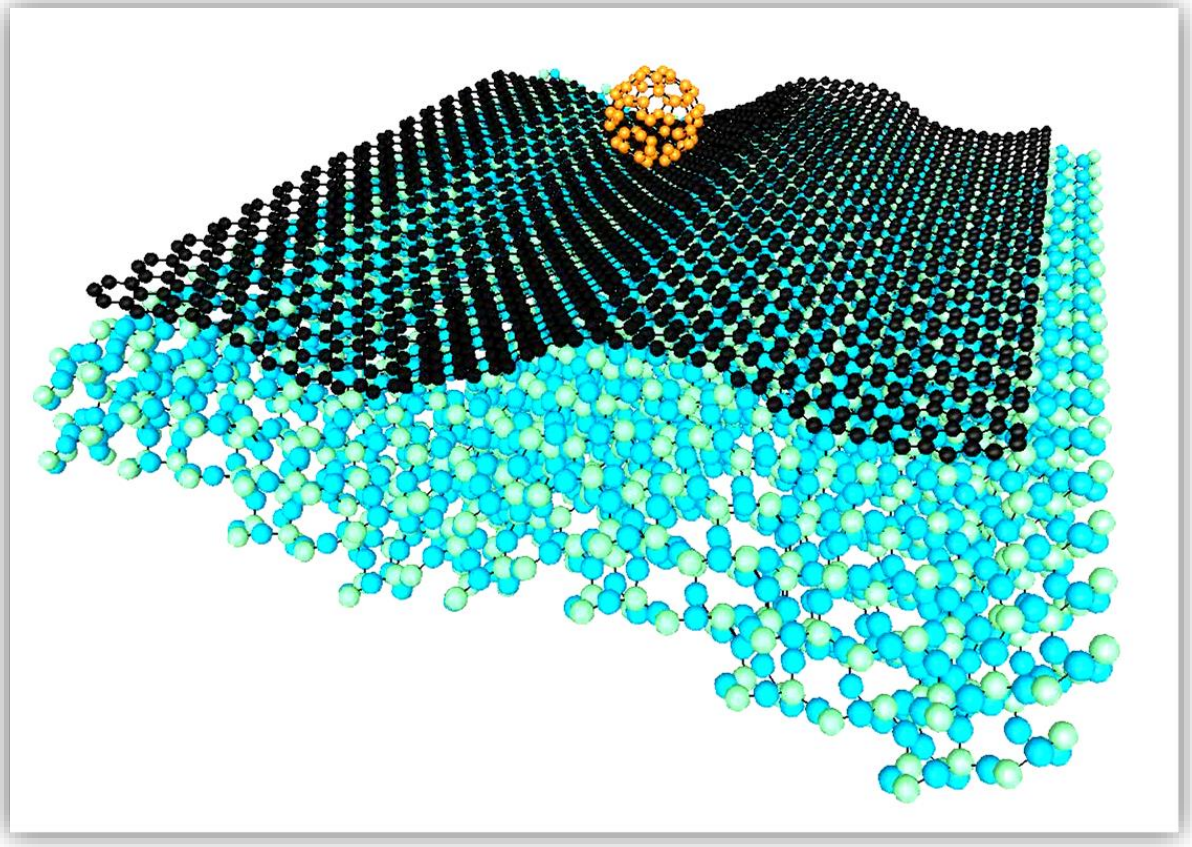
quantum method Tight-binding and molecular-mechanic method REBO/AIREBO

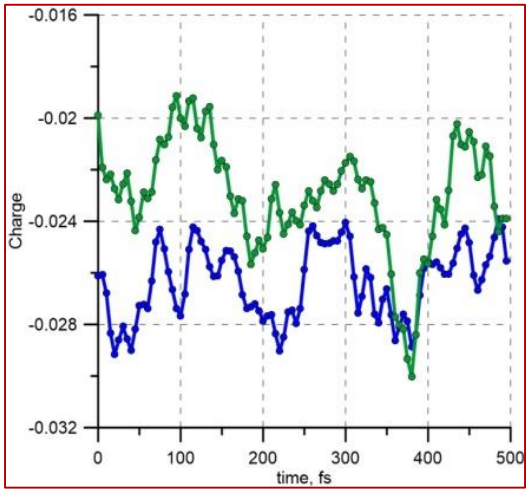


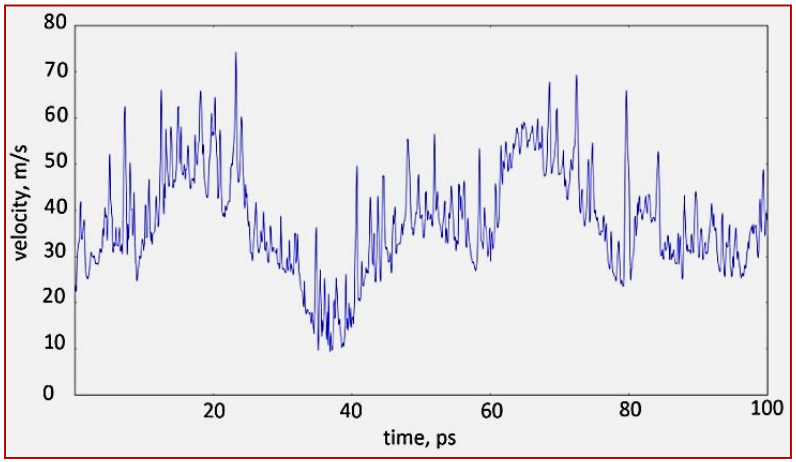
M.M. Slepchenkov, A.S. Kolesnikova, G.V. Savostyanov, I.S. Nefedov, I.V. Anoshkin, A.G. Nasibulin and O.E. Glukhova *Giga- and terahertz range nanoemitter based on a peapod structure* // Nano Research. 2015 (in press) – publishing house Springer.

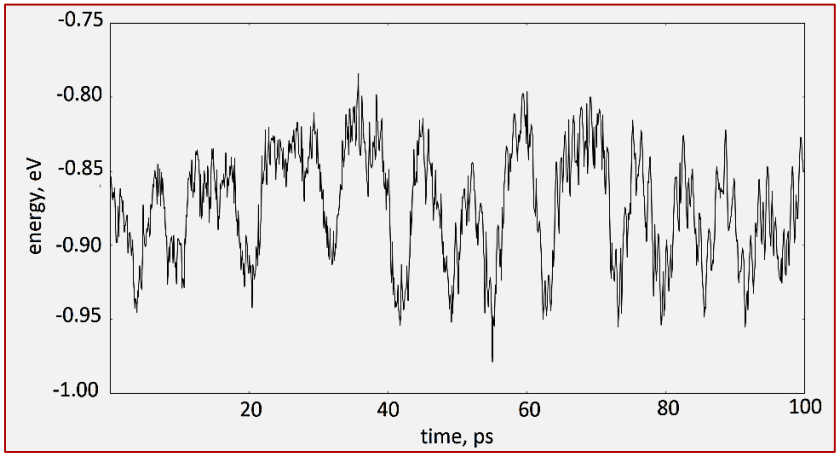
Patent for invention «*The way of obtaining electromagnetic radiation of giga- and terahertz frequency range*». Certificate of state registration №2013151936 от 14.01.2015. Authors: O.E. Glukhova, A.S. Kolesnikova, M.M. Slepchenkov,

Investigation of patterns of molecule C_{60} behavior supported by curvilinear graphene (substrate SiO_2, T=300 K): quantum method Tight-binding

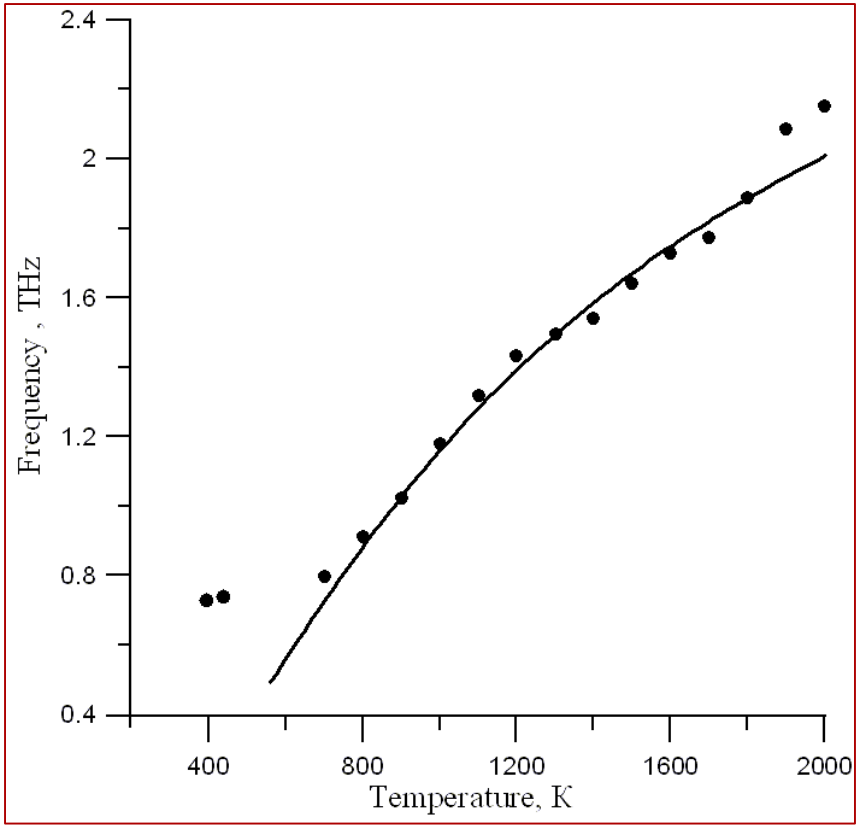


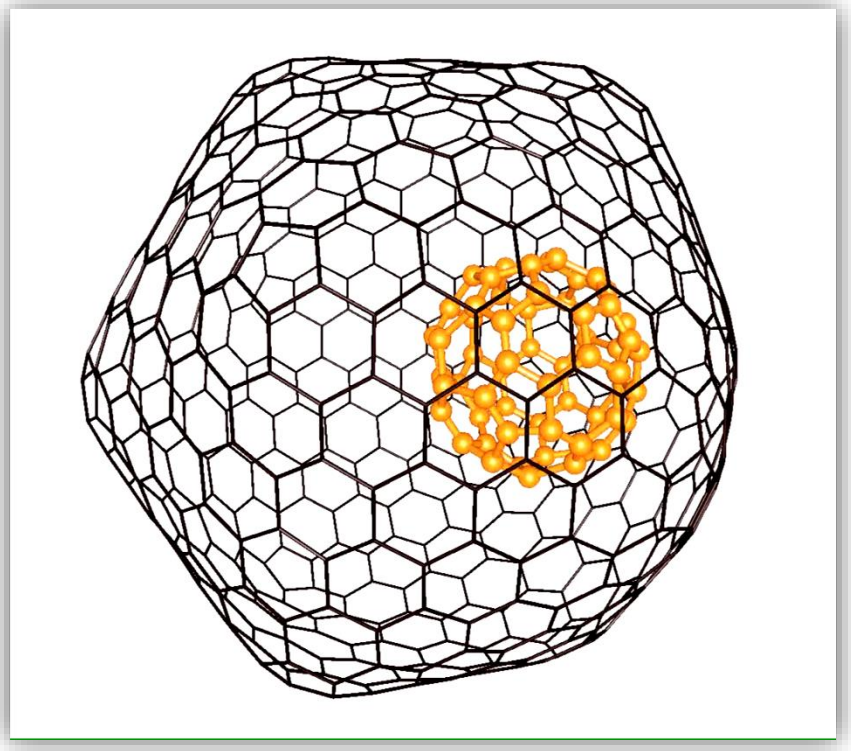


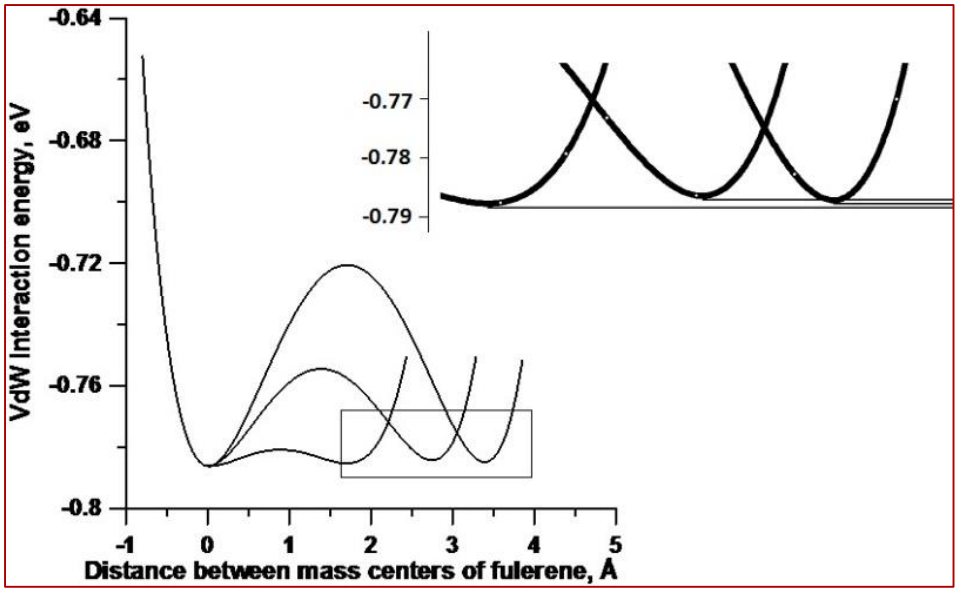




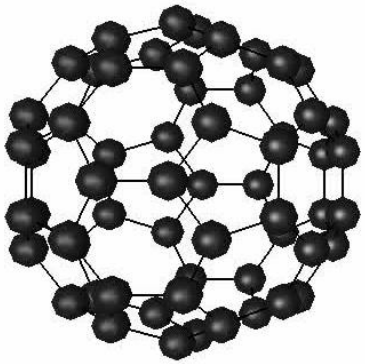
Investigation of molecule movement inside nanostructure shell (molecular and mechanic REBO/AIREBO)

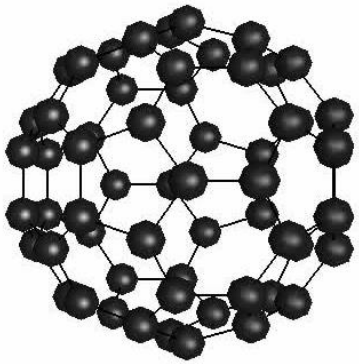


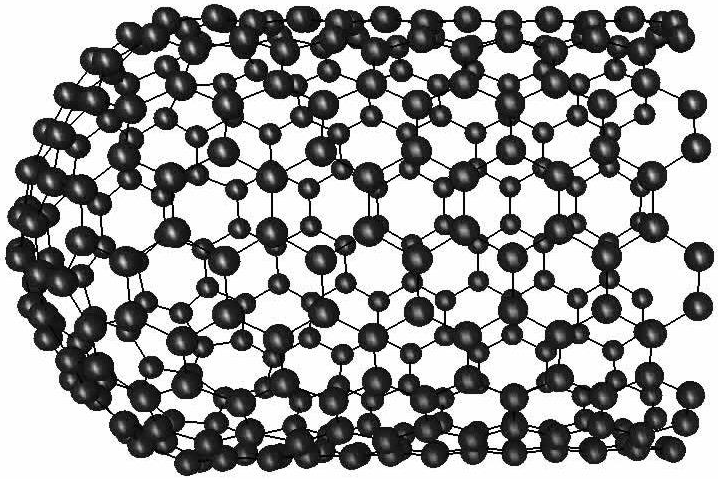


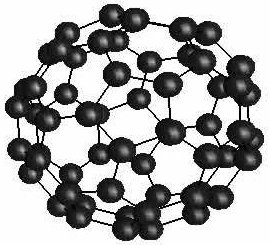


Modeling of collisions, formation and destruction of chemical bonds: molecular and mechanical method REBO/AIREBO

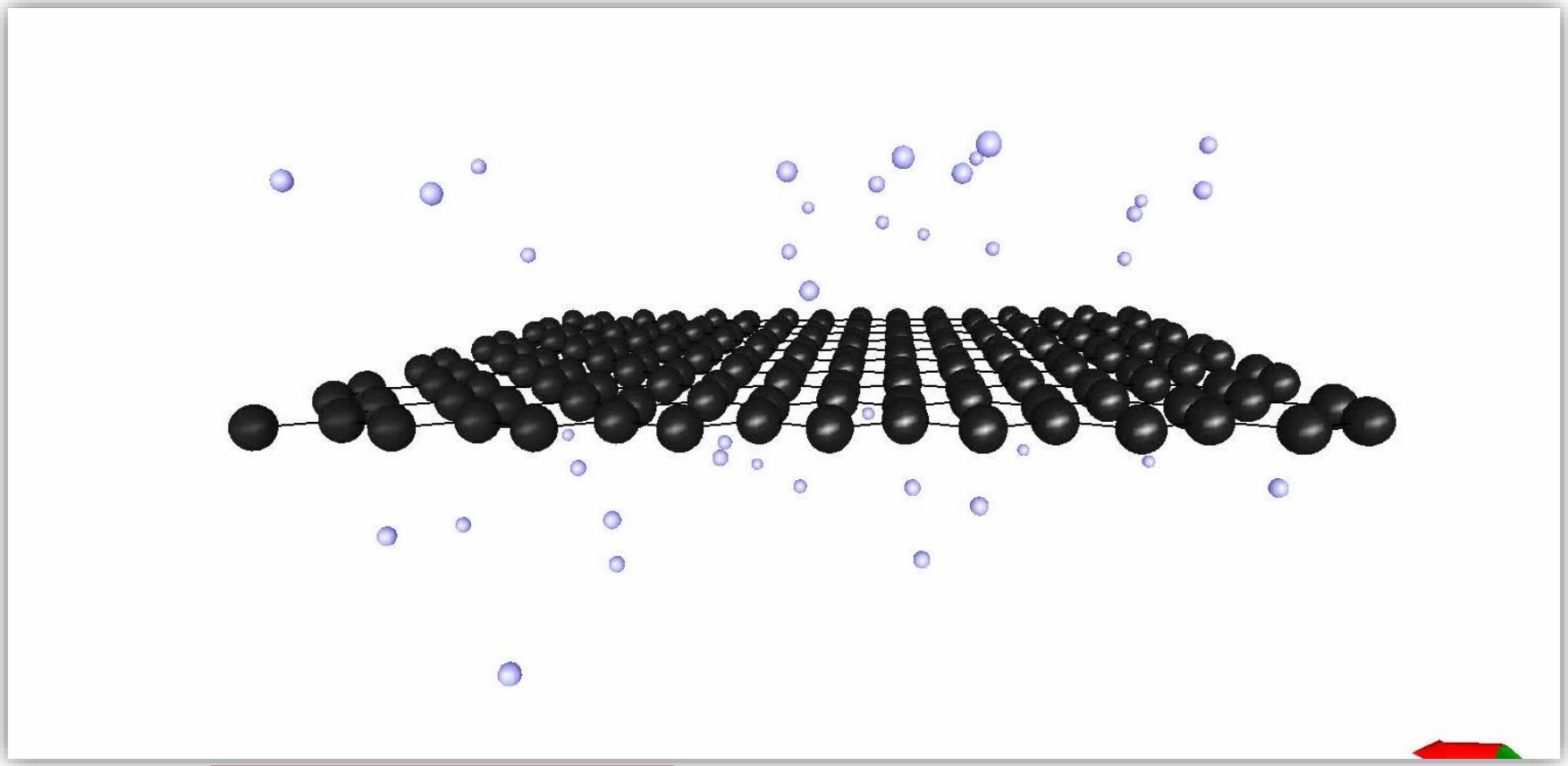


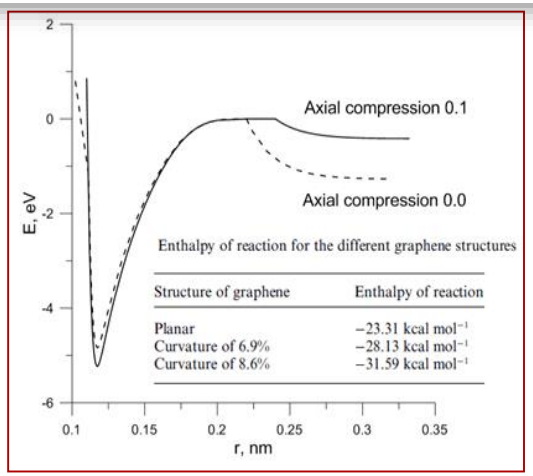






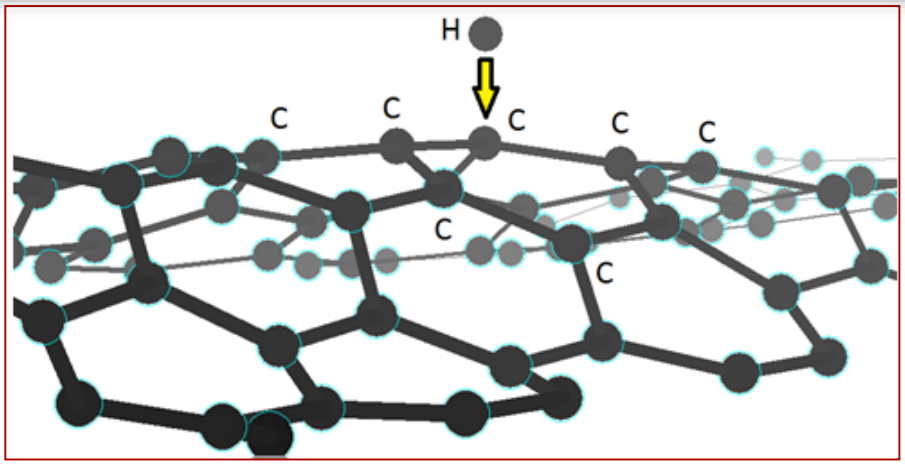
Modeling of graphene hydrogenation process



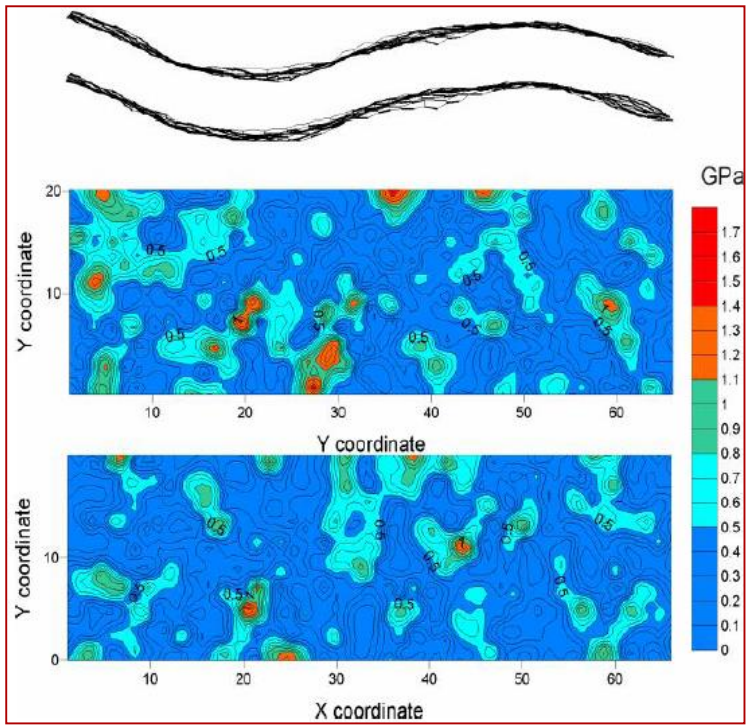


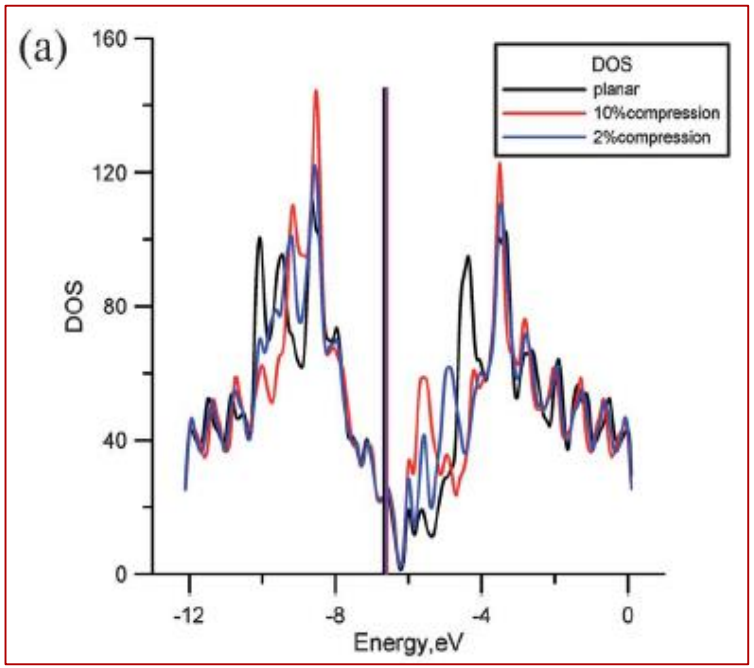
Enthalpy of reaction for the different graphene structures

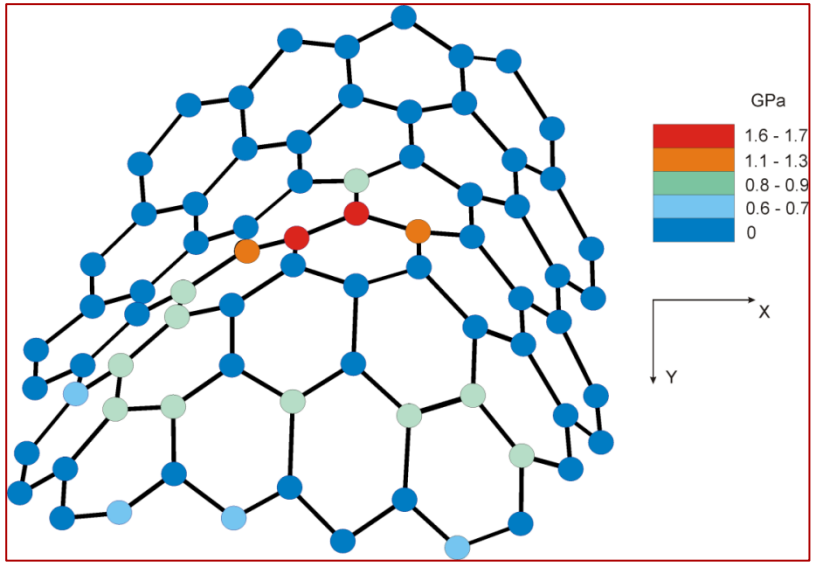
Structure of graphene	Enthalpy of reaction
Planar	−23.31 kcal mol^{-1}
Curvature of 6.9%	−28.13 kcal mol^{-1}
Curvature of 8.6%	−31.59 kcal mol^{-1}

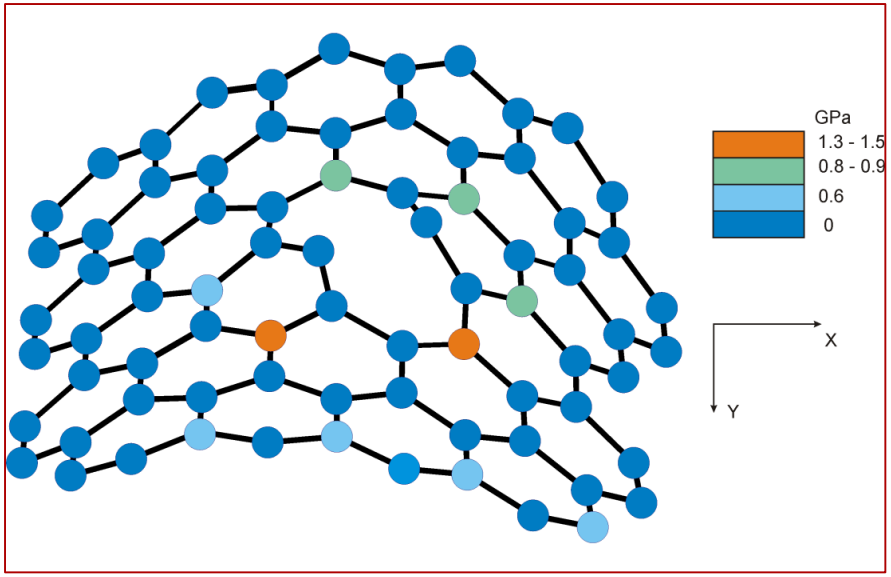


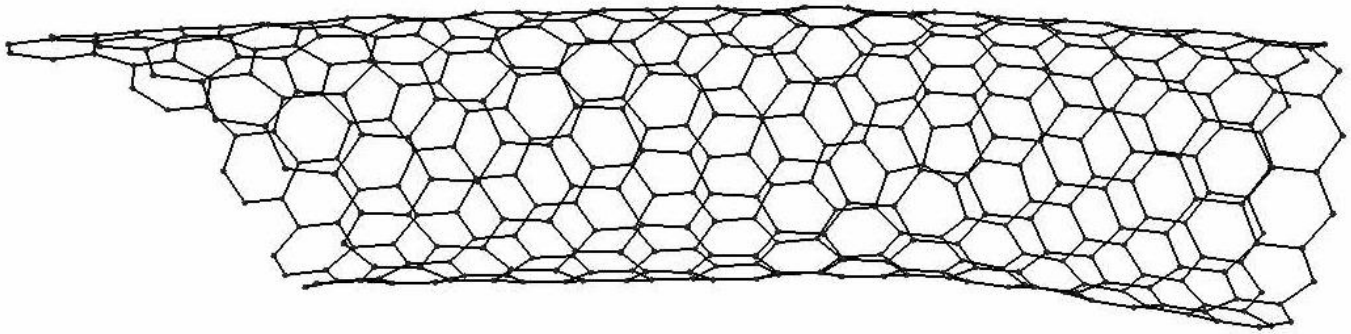
III. Modeling of deformation and destruction processes

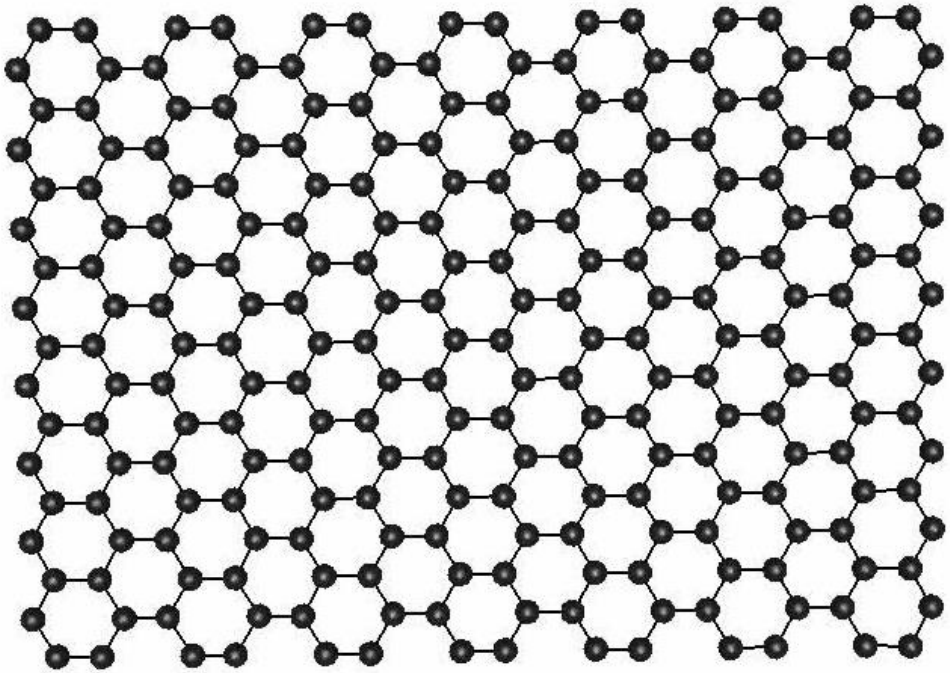




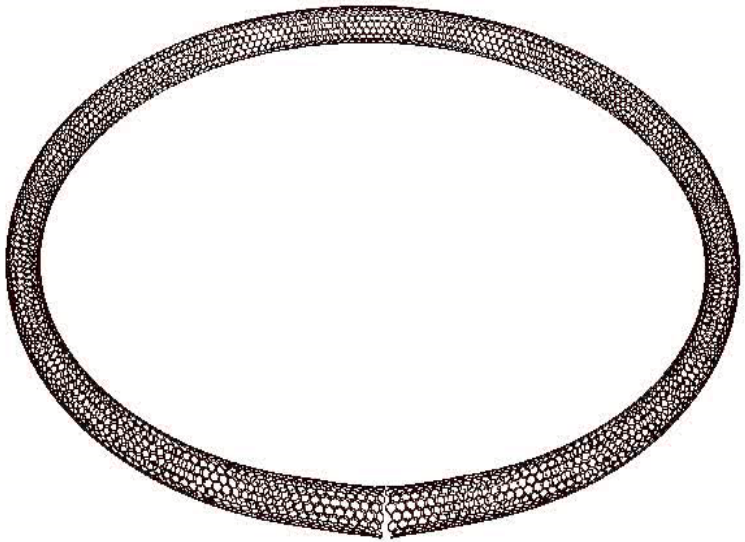








Unfolding of nanotorus into tube after disruption. Velocity of deformation wave 250 m/s



Capabilities of software KVAZAR

Construction of atomistic and coarse-grained models of biomacromolecules
Prediction of protein folding
Simulation of chemical reactions (*association*, *isomerization*, *dissociation*)
Prediction of nano- and biostructures mechanical properties
Simulation of deformation and destruction processes
Simulation of biomacromolecules self-assembly
Prediction of behavior and properties in external electrical and magnetic fields
Prediction of nano- and microobjects behavior under impact of pressure and temperature

Certificates for software

1. «***Multiprocessor software for modeling molecular systems for supercomputers» KVAZAR***». №2014610217, 09.01.2014 (G.V. Savostianov, R.A. Safonov)
2. «***The program for designing and 3D-visualization of nano-objects (Atolib3d)***». №2011619402, 9.12.2011 (OE. Glukhova, SN Limanskii)
3. «***Program for nanomodeling (Ring)***». Certificate of state registration of computer program №2010612881, 28.04.2010 (O.E. Glukhova, O.A. Terentiev)
4. «***Training program of design, passive microwave devices (GOE-MV-09)***». №2010612336, 30.03.2010 (O.E. Glukhova, I.N. Saliy)

Patents

1. «***A method for producing electromagnetic radiation giga- and terahertz frequency range***», №2013151936 от 14.01.2015 (O.E. Glukhova, A.S.Kolesnikova, M.M. Slepchenkov)
2. «***A process for preparing low molecular weight polymers dimers C20 fullerene***». №2360864 от 10.07.2009 (O.E. Glukhova)

International space KVAZAR

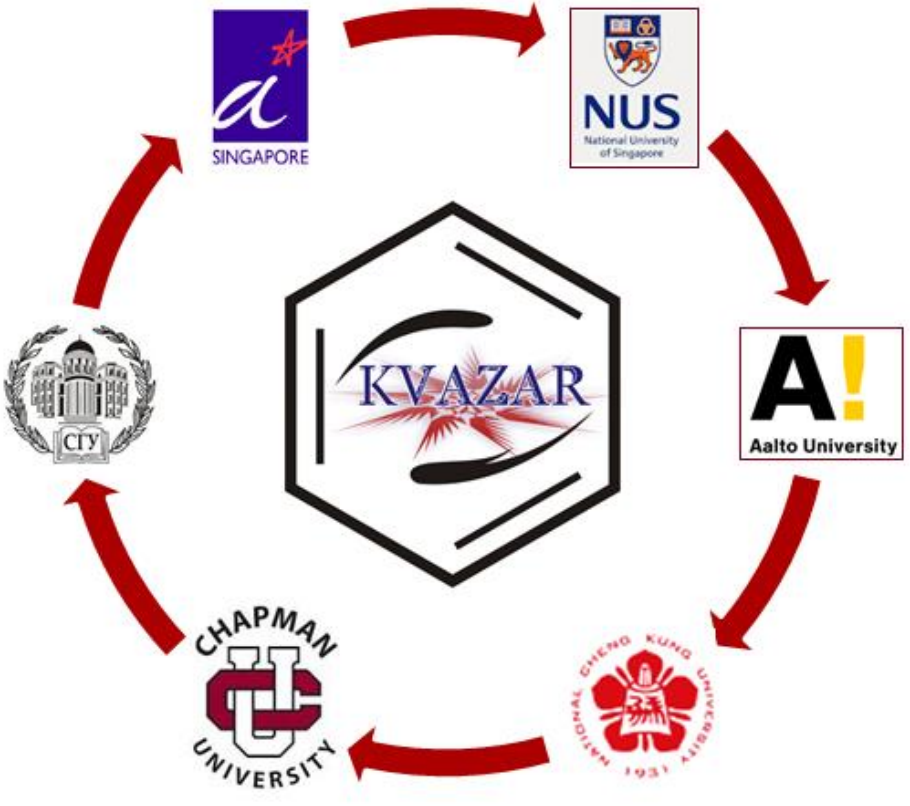
1) *Nanyang Technological University*, Singapore

2) A*STAR, *Institute of High Perfomance Computing*, Singapore

3) *Schmid College of Science & Technology, Chapman University*,Orange, CA

4) *National Cheng Kung University*, Taiwan

5) *Aalto University*, Finland



Young scientists (PhD)

Руководитель проекта
д.ф.-м.н. О.Е.Глухова

A.S.Kolenikova

M.M.Slepchenkov

O.A.Grishina

Post-graduated students

G.Savostianov

D.Shmygin

V.Mitrofanov

V.Shunaev

Students and masters

A.Fadeev

M.Shubin

K.Asanov

A.Zyktin

A.Kuryleva

D.Melnikov