Metody Symulacji w Nanotechologii" NANO12

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Tutorial. Part IV. Modeling of electrical and mechanical properties of bionanosytems

Ex wn#1 (2h) ***PDB i VMD – computer visualisation of nanosystems***

1. Protein Data Band database - basics.
   1.1. Open the WWW page of theProtein Data Bank and answer (in your report) the following questions:
      1.1.1 How many structures are available in the PDB today?
      1.1.2 How many structures of nanotubes may be found in the PDB?
      1.1.3 Enlist at least 3 living organisms for which 3-D structures of hemoglobin proteins are stored in the PDB. Register PDB codes of these hemoglobins.
      1.1.4 How many proteins are linked to the word: „biotechnology" in PDB?
      1.1.5 What molecule was nominated „A molecule of the months" in PDB as of the day of our exercises?
      1.1.6 Download from the PDB (to a local folder) a file in a PDF format having 2AHJ structure (or any structure related to fibroin).
2. VMD graphical environment – an introduction.
   2.1 Find in the Internet the Visual Molecular Dynamics code for Windows. Get acquainted with a manual of this code. Determine the current version number and hardware requirements.
   2.2 Run the vmd code (it should be installed on PKV computer). If you prefer to work with your own notebook, register to the VMD code as academic user and install it on your computer.
   2.3 Use the command „Load molecule" to load a protein written before on a local HD (point 1.1.6). Learn how to navigate the molecule model using a computer mouse (R, T, S, keys, scroll). Measure a distance between selected atoms.

3. Protein visualization.

   3.1 Check at least 4 options for a protein representation and colouring available in the VMD.
   3.2 Learn how to select amino acids and display them in a selected colour.
   3.3 Select all tryptophans (Trp) and display tham in "red" using a licorice representation.
   3.4 Learn how to save a graphical representation ("save state" command). Learn how to load the saved state.
   3.5 Learn how to change the background colour in the Main display window.

4. Modeling of a nanotube using VMD.

   1.1 Use an Internet to review possible graphical representations of carbon nanotubes.
   1.2 Find in the Internet coordinates of any nanotube that may be loaded into VMD (or ArgusLab). Download these coordinates.

1.3 Use VMD or ArgusLab (Pymol??) to create your own the most beautiful picture of a nanotube. The points will be awarded for the clarity, originality, and effectiveness in structural information display technique. Save this Picture and send it to your email mailbox. This Picture should be inserted into a report from this exercise (formats *.doc , *docx or pdf are accepted).

1.4 Hints:

(a) Nanotube Quicktime movies: see.: http://www.ipt.arc.nasa.gov/gallery.html

(b) Nanotube generator, use notepad to copy data, write down the output with the name having extention *.pdb,

Read in this file into VMD or Arguslab code (version 1.0 is ok)

http://www.ugr.es/~gmdm/java/contub/contub.html

(c _) Learn how to use a plugin to VMD - nanotube builder:

http://www.ks.uiuc.edu/Research/vmd/plugins/nanotube/

5. Your short report (1-2 pages) from this exercise wn#1 should contain:

A. Answers to questions 1.1.1-1.1.5

B. A nice Picture (your own!) of a carbon nanotube (SW or MWNT) prepared using (preferably) the VMD code. You may pretend that this graphics will be used for a book cover. Give some information explaining what features of a nanotube are presented in this particular graphical model.

CW wn#2. (2h) Quantum modeling of drugs – structures and electrostatic potentials

1. Learning the ArgusLab.
   1.1 Dig out in the Internet the newest version of ArgusLab (academic licence is free). Instal the code on your computer (it has been already installed on PKV PCs)
   1.2 Learn „nuts-and-bolds" of pull-down Menu and „Builder" options. Learn how to measure interatomic distances and bond angles in a molecule.
   1.3 Built a model of water.
   1.4 Optimize the structure of water molecule. Use AM1, PM3, MNDO Hamiltonians. In a separate calculation find an optimal (the lowest energy) geometry using molecular mechanics („pliers icon"). Write down H-O-H angles and O-H distances into a table. Compare your results with experimental data (Wiki). Decide which computer method would you recommend for that type of calculations. Select visualization of orbitals HOMO and LUMO for water , for example, in the AM1 method. Select an option: calculate the electron density. Calculate an electrostatic potential (AM1) for H20 molecule. Project the electrostatic potential on that surface. Note how positive and negative regions of MEP are graphically represented. Do you see that water molecule has a dipole moment?
2. Building a model of a drug molecule.
   2.1 Find a structural formula of Aspirin (wiki).
   2.2 Built a model of aspirin (ArgusLab)
   2.3 Optimize a geometry of aspirin using MM and AM1 methods, find in the output a value of heat of formation (kcal/mol) by the AM1 method.
   2.4 Calculate MEP (charge distribution) in aspirin.
3. Calculation of torsional potential in aspirin (Arguslab).
   3.1 Select amino-acetyl group and measure a torsional angle of this group with respect to phenyl ring plane. Sample this angle entry 30 deg, in the range of 0-360 deg, Please make 12 calculations of Total energy. (Here only a single point (one conformation) energy evaluation will be performed, don't make geometry optimization.
   3.2 Prepare a plot: Energy (kcal/mol) vs. torsional angle (deg.) Where a minimum on this plot is located? Compare your result with those obtained by classmates. Are the results identical. Explain possibile differences.
4. Have a glimpse on NAMD Internet tutorial and local tutorial (separate instruction will be provided by WN).
5. The report (1 page.) from Ex. wn#2 contains:
   A. A Table with results of geometry optimization of water (MM, AM1.PM3, MNDO, exp)
   B. The torsional potential plot (aspirin)
   C. The energy of the lowest conformer of aspirin.

EX wn#3 (2h) ***A study of nanomechanics of nanocompsite biomaterial***

Students prepare inputs, perform simulations (MD – locally, SMD on a designated cluster) using molecular dynamics simulation, it is a part of a real scientific practical project. They analyze results of simulations as well. Students construct a model of a *Caddisfly* fibroin fragment (2 beta strands). They learn how to study a strength of nanomaterial. They study the effect of phosphorylation and the presence of Ca^{+2} ions. They have to prepare own inputs and scripts. They optimize geometry of a protein (programs used: VMD i NAMD).

1. On a local PC (PKV, Windows): Using a separate instruction prepare *bat files and input files. Ask instructor for hints what velocity of pulling should be used and what force constant of a virtual spring is recommended.
2. On a local PC (PKV, Windows): Perform D0 step of MD simulations (minimization, optimization of a water shell). Perform D1 step (MD – equillibration of the whole system).
3. Learn details how to log in into a remote Linux luster. Transfer appropriate input files, note that sometimes conversion of formats may be needed (Small/big Endian problem etc..). Learn how to submit computational job to a cluster. Submit D2 (SMD) job to the queue. Please, control validity of k_SMD and Vel, and frequency of storing trajectory frames and writing out data into the output file. (wrong parameters will lead to a fast Cash of your tests). Monitor an output file (*.out). Sometime one have to repeat D2 calculations several times before decent results are obtained. Learn how to transfer output file into a local computer. Learn how to check the state of a Job on a cluster (qstat –b).
4. Write your own scripts (or use the scripts prepared by dr L. Peplowski) to extract from *.out data on a value of applied virtual force and protein extension induced by this SMD force.
5. Prepare a plot (from D2) force – time (or better (force – extension). Check what units on these plots should be inserted.
6. The final report (1-2 pages, EX wn#3) should contain information on parameters used in the simulation (a copy of an input file is ok) and the plot force-time (or extension). The e-mail address for sending the PDF report file will be given during exercises.