Computational Chemistry and Materials Modeling
Team project 3a
Topic: classical molecular mechanics and statistical physics

Formulate your own project within the above defined topic or do one of the following projects.

1. Estimate the mean-square length of a linear alkane C_nH_{2n+2}.
2. Equilibrate a water box for MM3 force field.
3. Using a case study show that for sufficiently large molecules microcanonical and canonical molecular dynamics simulations are nearly equivalent.
4. Evaluate stretching, bending, torsional strength of carbon nanotubes.
5. Characterize and compare mechanical/structural parameters of at least two different carbon nanotubes in the view of their possible application in structural composites.
6. Study crystallization/vitrification of SiO_2.
7. Find and characterize SiO_2 polymorphs.
8. Simulate Si nanocrystals in SiO_2.
9. What factors determine the preference between B1 and B2 structures of ionic crystals?
10. What factors determine the preference between fcc, hcp and bcc structures of simple metals?
11. Simulate transitions in a double well potential and test a rate theory.

Reminder: This is a scientific project whose more or less complete solution has a complexity scale of a peer-reviewed publication. That is why a precise exhaustive solution is not required. But try to do your best, spending a reasonable amount of time (about 2 hours per week per team member). It is expected that you will take TA's advisory on team-projects. Prepare 10 min oral presentation (introduction, motivation, methodology, main results, conclusions) and be ready for additional 10 min of discussion. Very short written report is also required and should contain the information on participation of each team member.