Computational Chemistry and Materials Modeling
Lab 2, due date is set in Storion web page
Topic: Classical molecular dynamics of molecules and solids

Notes: *Upload solution as a single file "YourName.zip". Provide absolute minimum of supporting info - no copies of work folders. Compare results with published experimental and theoretical data. Solution must be submitted as article-style report supplemented by required technical les: xyz- and cif-geometries, program run log- or out- files, extra figures etc. Be prepared to give a 5 min presentation of everything that you consider non trivial in your work.*

The Lab work is separated into three parts: *practical part*, which includes all calculations; one-minute *oral presentation* and *written report*.

Practical tasks. Take a molecule or crystal with at least two competing conformers or polymorphs. Using appropriate force field or empirical potential:

Tasks for molecules (Difficult). The maximum score can be achieved, completing part of the tasks.

- (10 %) Determine topology and create force field file mapping atomic types to a published force field.
- (25 %) Optimize geometry of important conformers including critical saddle points.
- (25 %) Estimate PES for transition between the two lowest conformers.
- (30 %) Run MD to study geometry fluctuations, accessible conformers, transition rates at normal conditions.

Tasks for solids (Easy). The maximum score can be achieved only by completing all tasks.

- (10 %) Determine topology and create force field file mapping atomic types to a published force field.
- (20 %) Optimize geometry of important polymorphs including critical saddle points.
- (30 %) Study high-barrier transitions by high-temperature MD (e.g. heat up then cool down) or some other process, such as diffusion, indentation, etc. Here, the analysis of evolution structure peculiarities with time is essential. For instance, conduct a study of mean coordination, volume per atoms, bond lengths, etc. with time.

Oral presentation. On the day of Lab report, you have to make a one-minute one-slide presentation with the main results of your work, which include the optimized structure of your selected molecule, information on stability, molecular orbitals and triplet/cation/anion state.

Lab report. Using the example of Lab report, you need to make your own, which includes all the results, their analysis and names of the input files. The following points are graded:

- (20 %) Analysis of the results.
- (5 %) Presence of input files names.
- (5 %) Appropriate grammar and vocabulary.

Total grading: Practical work (60 %) + Oral presentation (10 %) + Written report (30 %).

Sample solution: See Lab2 octane.zip.

Sample solution: See Lab2 NaCl.zip.