Computational Chemistry and Materials Modeling
Homework 5, due date is set in Canvas LMS
Topic: Classical molecular dynamics of molecules and solids

1. Lab "Geometry optimization and molecular dynamics". For a given molecule determine the lowest energy geometry and the room temperature dynamics using an appropriate force field. Follow the algorithm given below. Part 1 (geometry optimization):

- Create initial geometry. Save that geometry as xyz-file.
- Optimize the geometry. Save the optimized geometry as xyz-file. Create a picture of the molecule. Explain the choice of the force field.
- Compare with experiment or other method.
- Determine and check symmetry. Determine a set of independent geometrical parameters, fundamental domain and generators.
- Check alternative conformations. If there is a low lying metastable state, study it.
- Explain the molecular structure.

Part 2 (molecular dynamics):

- Start with optimized geometry or other geometry of interest.
- Run MD at 300 K for the minimal time to obtain a reasonably accurate sampling.
- Save 100 snapshots to xyz-file ("movie").
- Determine all the conformations accessible by the MD and estimate transition rates between them.
- Extrapolate to a laboratory time (hours).
- Explain the observed dynamics.

The solution should be prepared in the form of a written report supplemented by the required technical files: xyz-geometries, program run log-files, figures not inserted into the report etc. Be prepared to give a 5 min presentation of everything that you consider nontrivial in your work.

List of molecules (one per student):

- any flexible molecule of your choice;
- any min-3-units oligomer of conjugated polymers: polyyne, polyacetylene, poly(p-phenylene), poly(p-phenylene vinylene), polypyrrole, polythiophene, polyaniline, PEDOT etc.;
- any "multi-flexible" part of branching alkane (e.g. isooctane) or other polymer (e.g. polybutadiene), can be cyclic;
- any "multi-flexible" part of DNA, protein, or other biomolecule;
- azobenzene, aspirine, nicotine, beta-carotene.

2. Exercise on molecular mechanics and statistical physics. Estimate the relative concentration of cis and trans conformers of butadiene molecule at the room temperature.