Computational Chemistry and Materials Modeling
Homework 4, due date is set in Canvas LMS

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. Lab. Compare cohesion energies of two TiO_2 polymorphs, rutile and anatase (or other crystal appropriate for your project), using three methods: empirical COMB3 potential, semiempirical PM7 Hamiltonian, and PBE(GGA) density functional.

3. Exercise. For silicon, determine conduction and valence band extrema in k-space and effective masses of electrons and holes, using PBE density functional.

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