Computational Chemistry and Materials Modeling
Lab 4, due date is set in Canvas LMS
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 files: 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 nontrivial in your work.*

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

- Determine topology and create force field file mapping atomic types to a published force field.
- Optimize geometry of important conformers (polymorphs) including critical saddle points.
- Estimate PES for transition between the two lowest conformers.
- Run MD to study geometry fluctuations, accessible conformers, transition rates at normal conditions.
- Study high-barrier transitions by high-temperature MD (e.g. heat up then cool down).
- Estimate phase diagram.

Sample solution: See Lab4_octane.zip
Sample solution: See Lab4_NaCl.zip