Computational Chemistry and Materials Modeling
Team project 2
Topic: extended systems

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

1. Estimate the mean-square length of linear alkanes C_nH_{2n+2}.
2. Equilibrate a water box using MM3 force field.
3. Using a case study show that for sufficiently large molecules microcanonical and canonical molecular dynamics simulations are nearly equivalent.
4. Study crystallization/vitrification of SiO_2.
5. What factors determine the preference between B1 and B2 structures of ionic crystals?
6. What factors determine the preference between B3 and B4 structures of covalent crystals?
7. What factors determine the preference between fcc, hcp and bcc structures of simple metals?
8. What factors determine stability of simple cubic lattice in average valence 5 crystals?
9. Compare cohesion energies of known TiO_2 polymorphs using various methods from empirical potentials and semiempirical Hamiltonians to DFT (various functionals).
10. Study secondary bonding in halogen crystals

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.