Computational Chemistry and Materials Modeling
Lab 1, due date is set in Canvas LMS
Topic: basics of quantum chemistry with semiempirics

***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 with at least 10 atoms. Using semiempirical Hamiltonian of your choice:

- Optimize ground state geometry. Check its stability. Determine if it is the global minimum.
- Plot frontier orbitals (HOMO-LUMO). Calculate the energy gap.
- Calculate localized molecular orbitals and explain electronic structure and geometry.
- Optimize geometry of the lowest energy triplet state (or cation, or anion, if more appropriate for your project). Calculate the relative energy of the triplet state. Plot unpaired molecular orbitals. Explain changes in electronic structure and geometry relative to the singlet state.

Sample solution: See Lab1_benzene.zip