Computational Chemistry and Materials Modeling
Homework 2 – additional problems

1. Lab. Take a conjugated molecule with at least one flexible single bond involved in the π-conjugation. Using semiempirical Hamiltonian of your choice:

- Optimize ground state geometry. Plot frontier orbitals (HOMO-LUMO). Calculate the energy gap. Explain electronic structure and geometry.
- Optimize geometry of the lowest energy triplet state. Calculate the relative energy of the triplet state. Plot unpaired molecular orbitals. Explain changes in electronic structure and geometry relative to the singlet state.
- Make a scan of the PES by rotating a single bond. In particular evaluate the rotational barrier and differential energies (0 vs 180, relax geometry if possible).
- Plot frontier orbitals for 90 and 180 degree of rotation. Compare with those at 0 degree. Explain the results.

The solution should be prepared in the form of a written report supplemented by the required technical files: xyz-geometries, mgf-orbitals, 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.