Computational Chemistry and Materials Modeling
Team project 1
Topic: quantum chemistry of molecules

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

1. Explain the structural and electronic properties of linear C_nH_{n+2} (polyacetylene and its oligomers) and cyclic C_nH_n (annulenes) alkenes (use a semiempirical approach).

2. Illustrate pseudo Jahn-Teller effect in AX3 molecules.

3. Explore shapes of elemental small clusters.

4. Explain bonding in SF_6 molecule.

5. Illustrate lone-pair concept.

6. Illustrate hybridization of orbitals.

7. Where is the boundary between covalent and ionic bonding?

8. Illustrate secondary bonding.

9. Explain and illustarte duodectet rule.

10. Solve 2c2e model.

11. Solve 4c4e planar model.

12. Solve 4c4e tetrahedral model.

13. Solve 6c6e benzene model.

14. Solve 6c6e octahedral model.

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.