

### Test-exam (replacement for computational exercise report)

1) Discuss the choices of methods (HF, CCS, CCSD) for computing ground state energies. Your discussion should touch the following topics

- variational principle
- optimization condition
- electron correlation
- size consistency
- computational scaling

2) All calculations you have done are for a closed-shell state. Discuss what this means in terms of eigenvalues of the spin angular momentum operators  $S^2$  and  $S_z$ . Your discussion should touch the following topics

- allowed values of eigenvalues
- coupling of spin
- spin-symmetry of the excited states

3) [not related to computations] Discuss how time-independent non-degenerate perturbation theory is used in quantum chemistry. Your discussion should touch the following topics

- MP2 (strengths&weaknesses)
- electric molecular properties

The final exam will have tasks of this structure, but since scanning in handwritten papers will not be possible, I will have to add multiple-choice like questions which tests more explicit knowledge of equations and derivations.