Mock Exam
Introduction to Electronic Structure Methods
(Autumn Semester 2023)

Family Name: **First Name:**

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1. What is meant by the term correlation hole?

2. Name two ways of how to reduce the number Slater determinants in configuration interaction when treating a) dynamic correlation and b) static correlation.

3. Which methods do have a possible self-interaction (i.e. an electron interacting with itself) error: a) CISD; b) MP2; c) CCCSD(T) and d) KS-DFT with approximate exchange-correlation functional.

4. a) What is the energy correction due to electron correlation at a) first-order (MP1)? b) Derive the expression for the energy correction at 2nd order (MP2).

5. What is the wavefunction Ansatz in coupled cluster theory? Using the same one-electron basis set e.g. 6-3111+G**, which method is more accurate: CISD or CCSD? Why?

6. Write down the relation between the many-electron wavefunction and the electron density. Can you determine the ground state electron density via a variational principle in a) exact DFT? b) DFT with an approximate exchange-correlation functional? Why? Is the resulting ground state energy above or below the exact value?

Bonus: What are generalized gradient approximations (GGAs)? Why are they called ‘generalized’? Give a few examples of frequently used GGA.