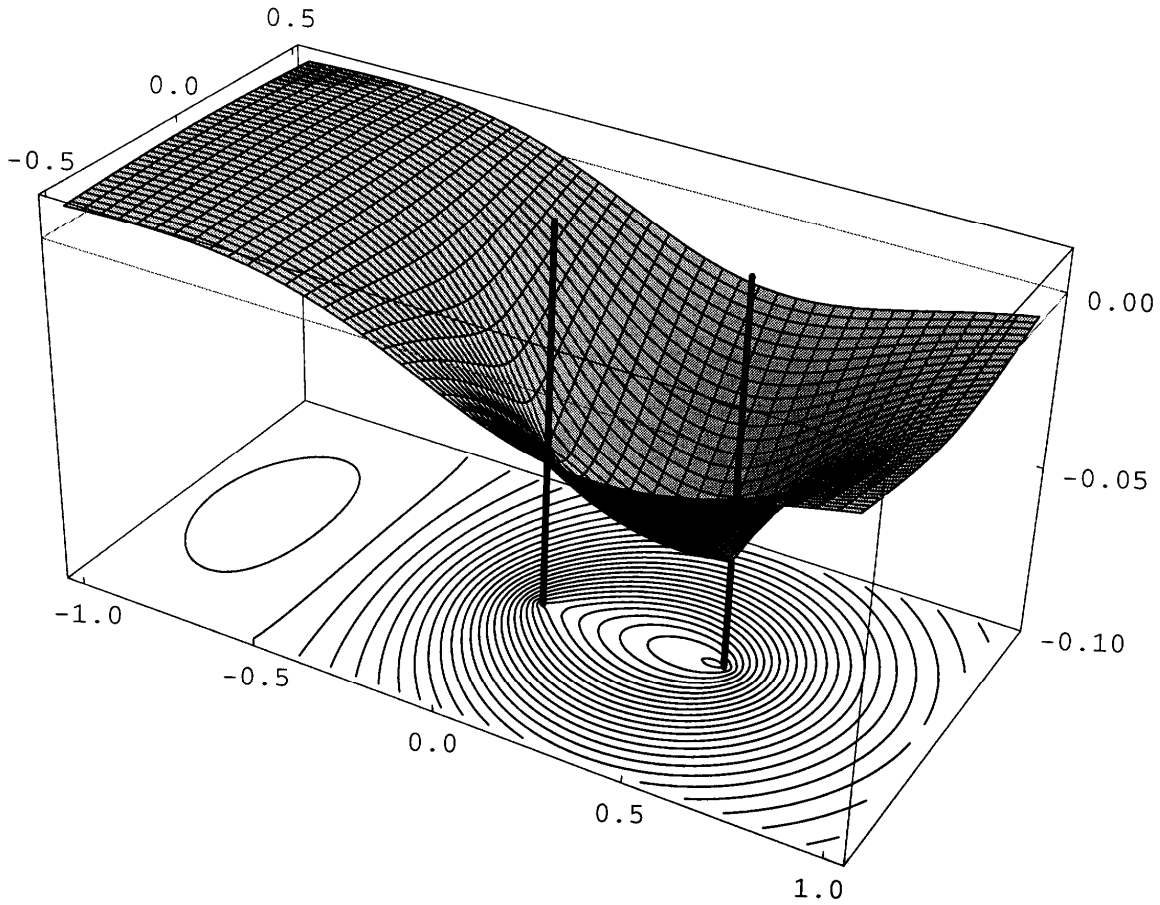
The 11th Sostrup Summer School

QUANTUM CHEMISTRY and MOLECULAR PROPERTIES

July 4 – 16, 2010



Organized by:

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Secretary to the Summer School
Hanne M. Kirkegaard

Purpose:

Quantum chemistry is changing. Theoretical calculations of energies and simple expectation values have been supplemented by calculations of static and dynamic molecular properties. Theoretical studies of NMR parameters have become standard, as have calculations of response properties such as electric polarizabilities and hyperpolarizabilities, essential to the understanding of laser-molecule interactions. Molecular systems are studied using more accurate and more advanced techniques employing, at the highest level, explicitly correlated methods. At less expensive levels, large molecular systems are studied, using for example density-functional theory combined with the techniques of linear scaling. Progress in the field relies on the introduction of new theoretical techniques as well as new computational strategies such as parallelization

Students entering the field of quantum chemistry are often confused by the apparently dissimilar techniques employed for calculating wave functions or properties from these wave functions and also about the dissimilarity with density functional theory calculations. The purpose of this summer school is to provide the participants with a thorough understanding of these topics at an advanced level, emphasizing the underlying unity of the various techniques used for calculating energies and properties. Numerical examples are extensively used to illustrate the advantages and disadvantages of the various computational techniques and approaches.

Topics:

At the summer school, the following topics are discussed:

1) Second quantization.
2) HF, CI, MCSCF, CC, MP and explicitly correlated methods. Each method is described in depth, including its computational scaling and performance in comparison with other methods.
3) Density-functional theory: Hohenberg–Kohn theory, the Levy–Lieb and Lieb density functionals, ensembles, Thomas-Fermi theory, the adiabatic connection and Kohn–Sham theory, LDA, GGA and hybrid methods
4) Time-independent response theory: geometrical derivatives and force constants, vibrational frequencies and intensities, electric and magnetic susceptibilities, NMR shielding constants and spin–spin coupling constant.
5) Time-dependent response theory: dynamic polarizabilities and hyperpolarizabilities, one- and two-photon transition moments and electronic excitation energies.
6) Atomic orbitals, molecular basis sets, and molecular integral evaluation.

7) Convergence in *N*- and one-electron spaces, calibration and benchmarking.

8) Large molecular systems and linear-scaling techniques.

9) The molecular electronic Hamiltonian: external electromagnetic fields, electron spin, relativistic corrections, and gauge transformations

These topics will be covered in exercises as well as in lectures. Each day comprises three to five lectures given by the organizers as well as three hours of problem solving. The students will be divided into smaller groups in the exercise sessions. Each group will have a tutor associated.

The monograph "Molecular Electronic-Structure Theory" (Wiley, Chichester, 2000), written by the organizers, will be distributed to the participants. This monograph will be followed closely in the lectures and exercise sessions. In addition, preliminary chapters for a second edition of the monograph will be handed out for the topics not covered in the first edition.

Who can participate?
The summer school is intended for advanced graduate students and research workers in related fields. The participants should have a basic knowledge of quantum mechanics and quantum chemistry. The number of participants is restricted to 60.

Location:
The summer school is held at a boarding school (Himmelbjergegnens Natur- og Idrætsefterskole) situated in the Danish countryside 3 km from Himmelbjerget and 30 km west of Aarhus.

Cost:
The cost of the summer school is DKK 9,000.- which includes food and lodging (double rooms) and a nominal tuition fee. It also includes the cost of the monograph. No funds are available for stipends.

Applications:
Applications should be received before April 1 2010. Participants will be accepted on a first come basis. The maximum number of participants is 70. After receipt of your application, we will submit an invoice for DKK 9,000.- to you. As soon as this invoice has been paid by you, you will receive a letter of acceptance.

Oslo and Aarhus, December 2009

Trygve Helgaker Poul Jørgensen Jeppe Olsen

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Please use BLOCK LETTERS and return as soon as possible, and no later than April 1, 2010.

Surname _____

First name _____

Affiliation _____

Female ☐ Male ☐

Address [☐ Institution ☐ Home]

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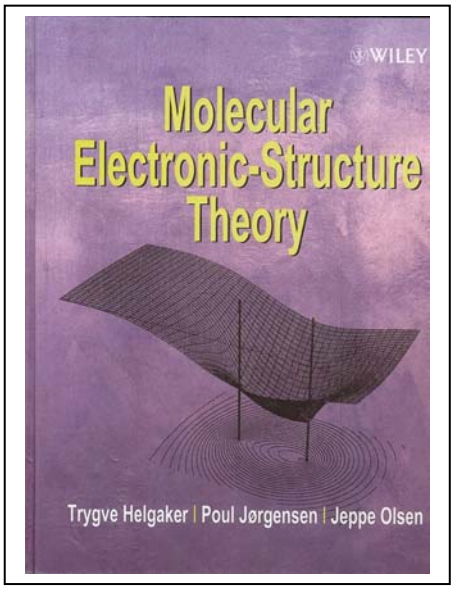
Electronic mail _____



Please return before April 1, 2010
to

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