**Application for funding of faculty common course 2020**

**Ansökan om medel för fakultetsgemensam forskarutbildningskurs 2020**

**English course title:** Quantum Chemistry: Beyond the Black Box  
Kursnamn på engelska

**Swedish course title:** Kvantkemi: Insikt och praktik  
Kursnamn på svenska

**Extent (credits) 5**  
Omfattning (högskolepoäng)

**Language of instruction English**  
Undervisningsspråk

**Recommended prerequisites:** Basic knowledge about electronic structure methods for molecules.  
Rekommenderade förkunskaper

**General course objective/s and learning outcomes** (Also specify which PhD examination goals that are addressed/covered. Describe how.)  
Kursens syfte och mål (Beskriv vilka mål för examen på forskarnivå som beaktas och på vilket sätt.)

Modelling of molecular systems using electronic structure methods is becoming an increasingly popular tool, partly due to the emergence of fast and relatively accurate density-functional methods. However, theoretical chemistry is not converging toward an optimal method for all applications, but is rather diverging into more and more specialized methods for different applications. For many problems, e.g., in catalysis and photochemistry, the required sophisticated electronic structure methods are far from being black-box tools. This course gives the opportunity for students to understand and evaluate alternative modelling strategies, which can be applied in their own area of research. It also gives them the practical skills to design good models and carry out the required calculations.

The course specifically targets the ability to "Demonstrate the ability to identify and formulate issues with scholarly precision" and "to plan and use appropriate methods" within the context of theoretical chemistry. An important goal is to allow the students to "demonstrate the ability to identify the need for further knowledge". The course also contributed to "broad knowledge" of the research field.

**Course contents**  
Kursinnehåll

The material covers molecular systems and will specifically treat the following areas: bond dissociation and chemical reactions, reaction rate modeling, spectroscopy and excited states, transition-metal chemistry, weak interactions and computational methods for large systems (e.g., biomolecules). Regarding the electronic structure methods, it will be covered: Hartree-Fock, second order Møller–Plesset perturbation theory (MP2), density functional theory (DFT), time-dependent DFT (TDDFT), the multiconfigurational methods CASSCF and CASPT2, and the hybrid quantum mechanics/molecular mechanics (QM/MM) method. All these methods and their applications will be covered by the lectures and computer exercises. After completing this course, students should be able to discuss the validity of different theoretical approaches, and formulate problems that can be addressed by electronic structure theory.
Instruction (course structure)
Lectures and computer exercises. The illustrated points discussed in the lectures will be complemented by the computer exercises, which give the student the opportunity to get familiarity with different electronic structure methods through the computational packages Gaussian09 and/or OpenMolcas.

Assessment (form of examination)
Examination is based on the completion of computer exercises and a project based on the student’s own research interests.

Course examiner (name, e-mail): Ignacio Fernández Galván, ignacio.fernandez@kemi.uu.se
Examinator (namn, e-post)

Department with main responsibility: Department of Chemistry - Ångström
Huvudansvarig institution

Contact person/s (course responsible teacher) (name, e-mail):
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Ignacio Fernández Galván: ignacio.fernandez@kemi.uu.se
Kontaktperson/er (kursansvarig lärare) (namn, e-post)

Course dates/period: Nov-Dec 2020.
Kurs datum/period

Maximum number of participants: 10
Antal platser

Submit the application for admission to: ignacio.fernandez@kemi.uu.se
Skicka anmälan till kursen till

Submit the application not later than Nov 1, 2020.
Skicka anmälan senast