Advanced Courses in Modern Molecular Modelling, ACM^3

We welcome you to take part in the PhD course block "Advanced courses in Modern Molecular Modelling (ACM3)", which will be given at the Albanova University Campus in Stockholm, starting November 7! The intention of the courses is to provide theoretical background and practical experience in performing molecular modelling with applications in materials science.

The courses are open for PhD students with a general background in Natural Science. Two double-hour lectures are given per day, giving the possibility for long distance students to participate. The courses are run by teachers from Theoretical Chemistry KTH, and Physical Chemistry, SU.

The following courses are given:

- Molecular Modelling: Basic Tools (8 ETCS credit points)
- Molecular Modelling: Microscopic Concepts (8 ETCS credit points)
- Molecular Modelling: Macroscopic Concepts (8 ETCS credit points)
- Molecular Modelling: Learning to Fly (8 ETCS credit points)
- Molecular Modelling: Grand Applications (8 ETCS credit points)

This course block covers a variety of aspects within Computational Modelling of Molecules and Materials. It gives a solid basis for theoretically oriented scientists to safely enter the field, as well as all for experimentalists realizing the value of modelling as a complementary tool to their measurements. The set of courses is highly comprehensive as it is given by a group of people both developing and using advanced modelling software covering the length and time scales from atomic dimensions/femtoseconds to micro meters/seconds and even beyond. Knowledge will be given to build an optimal hardware (pc-cluster), to master suitable algorithms for parallel computing of large molecular systems and to perform basic programming.

The course block comprises totally 40 ETCS points, divided to five blocks of 8 ETCS points. The two main techniques are Quantum Chemistry (QC) and Computer simulations (SIM), the QC part consists of three 8 ETCS point blocks whereas SIM part is made of two blocks of 8 ETCS points of which the first contains the basic physicochemical theory needed in simulations. A short orientation in simulations is given in the first QC block. All courses contain plenty of practical exercises and the second (more advanced) block of the SIM part ends with a project where both QC and SIM methods are combined.

This information and more will be kept updated on the course homepage,
http://www.theochem.kth.se/courses/ACM3.html

On the next page you will find a schedule for the course; the first two blocks are given in November/December 2007, the 3rd and 4th are given in March/April and the last course is given in May 2008. In the pages following you can see detailed contents of the course.

For questions or signing on to the course, please contact Peter Hammar,
hammar@theochem.kth.se 08-5537 8405.

Schedule

Part 1 and 2 run in parallel during November and December.

Two lectures per day, morning 10:00-12:30, afternoon 13:30-16:00.

Wed 7 + Thu 8 Nov
Tue 13 + Wed 14 + Thu 15 Nov
Tue 20 + Wed 21 Nov
Mon 26 + Tue 27 + Wed 28 Nov
Mon 3 + Tue 4 + Wed 5 Dec
Tue 11 + Wed 12 + Thu 13 Dec

Part 3 and 4 run in parallel during March and April;

Two lectures per day, morning 10:00-12:30, afternoon 13:30-16:00.

Tue 4 + Wed 5 Mar
Tue 11 + Wed 12 + Thu 13 Mar
Mon 17 + Tue 18 Mar
Tue 1 + Wed 2 Apr
Mon 7 + Tue 8 Apr
Wed 16 + Thu 17 Apr + Fri 18 Apr

Part 5 runs intensively during May

Two lectures per day, morning 10:00-12:30, afternoon 13:30-16:00.

Tue 6 + Wed 7 May
Tue 13 + Wed 14 + Thu 15 May

Basic tools (part 1)

(3A5711 – 8 ETCS)
Exercises solved required for passing the course.

Lecturer:
Pawel Salek, (pawsa-at-theochem.kth.se)

1L 1 - Computers

a. Overview of serial and parallel computer architectures.
b. Memory hierarchies.
c. Overview of national computer use for Computational Chemistry.

1L 2 - Algebra

a. 3-dimensional vector algebra.
b. Matrices.
c. Determinants.
d. Operators.
e. Basis sets.
f. The eigenvalue problem.
g. Orthogonal functions and Eigenfunctions.
h. The variation principle.

1L 3 - Programming

a. On Fortran, C/C++ and scripting languages.
b. Writing efficient scientific programs.
c. Data locality.
d. Blocked algorithms.
e. Solving linear algebra problems on computers.
f. Matrix transformations.
g. Mathematical libraries.

1L 4 - Hartree-Fock theory.

a. The electronic Hamiltonian
b. Coulomb and exchange operators.
c. One- and two electron integrals
d. The total energy of the closed shell.
e. Fock equations.
f. Koopman's theorem.
g. Roothaan equations.
h. The correlation problem.

1L 5 - Basis sets

a. Basis sets: Expansion of real solutions.
b. Gaussian basis sets.
c. Contracted vs primitive. Angular dependence.

1L 6 - Density Functional Theory

a. Theoretical background
b. Hohenberg-Kohn theorems
c. Local density approximation
d. Kohn-Sham formulation of DFT
e. Comparison of HF and DFT

1L 7 - Exchange-correlation functionals

a. ρ-dependent functionals
b. Gradient corrected and hybrid functionals
c. Asymptotically corrected functional
d. Numerical integration of functionals and its derivatives

1L 8 - Calculation of Forces in Quantum Chemistry

a. Analytic gradients and Hessians
b. The Hellman-Feynman theorem
c. The potential surface
d. Geometry optimization
e. Transition state calculations

1L 9- Wave packets and ultra-fast phenomena

a. Time-dependent representation
b. The concept of wave packets
c. Comparison with classical trajectories, semiclassical Landau-Zener model
d. Representation (grids, basis functions)
e. Numerical techniques for propagation of wave packets
f. Multidimensional wave packets

1L 10 Applications of wave packets

a. Vibrational spectroscopy
b. Reaction dynamics
c. Photodissociation and photochemistry
d. Pump-probe spectroscopy

1L 11 The Monte Carlo method

a Stochastic vs deterministic processes
b Metropolis MC
c Overview of other Monte Carlo schemes
d Applications of MC in Quantum Chemistry

1L 12- The Molecular Dynamics method

a. Newtonian dynamics
b. Time scales of Newtonian MD
c. MD of simple systems
d. Some typical applications of MD

1L 13- Combining Quantum Chemistry and molecular simulations

a Hybrid QM-MM approach
b Ab-initio and Car-Parrinello molecular dynamics

1L 14- Overview of computational chemistry software

Gaussian, GAMESS, GROMACS, NAMD, DL POLY, CPMD, ESPRESSO, GOpenMol...

Microscopic Concepts (part 2)

(3A5712 - 8 ETCS)
Exercises solved required for passing the course.

Lecturers:
Boris Minaev (boris-at-theochem.kth.se,)
Olav Vahtras (olav-at-theochem.kth.se) (L15-17)

2L 1 - Wave-mechanical concepts.

a. Potential well and hydrogen atom
b. Schr¨odinger theory of hydrogen atom
c. Periodic table. SCF AO, Slater AO, Gauss AO
d. Chemical variety as a combination of few notes in music
- (s, p, d, f
instead of do, re, mi, fa, ...)

2L 2 - Angular momentum and atomic energy levels.

a. Spin of electron.
b. The Antisymmetry rule (Pauli principle). Slater determinant.
c. Spin-orbit coupling (SOC) in atoms
d. The Russell-Saunders scheme
e. Addition of Angular momentum
f. Terms of configurations 2p3p and 2p2
g. Lande interval rule
h. Slater-Condon parameters. Hund's rule
i. Transition from Russell-Saunders coupling scheme to j - j coupling
j. Mg and Fe in the ground and excited states

2L 3 - Born-Oppenheimer approximation.

a. The electronic wave function as a slowly varying function of nuclear displacements
b. Validity of BO approximation in ground and excited states
c. The Jahn-Teller effect

2L 4 - Quantum nature of the chemical bond.

a. Ionic bond in NaCl. Covalent bond
b. Heitler-London method for H2 molecule
c. Orbital and spin wave functions. Overlap integral
d. Exchange integral. The concept of Heisenberg exchange spinhamiltonian
e. The singlet ground state of the H2 molecule and its chemistry
f. The triplet state of the H2 molecule and its photochemistry
g. The role of the triplet state in chemistry and catalysis

2L 5 - Simple MO Theory of diatomic molecules.

a. Effective single-electron hamiltonian
b. Variation theorem. MO LCAO approximation
c. H2 molecule
d. Huckel approximations
e. MOs of Homo-nuclear diatomic molecules
f. United atom atom and correlation diagram. Rydberg states
g. Ground and excited states state of the O2 molecule
h. Hetero-nuclear diatomic molecules. The non-crossing rule

2L 6 - Simple polyatomic molecules.

a. H+2 ion. Mass spectrometry
b. The H2O molecule. The C2v point group. MO and valence bond description
c. The BeH2, NH3 and CH4 molecules. Hybridization

2L 7 - Huckel theory of organic chemistry.

a. Ethylene and butadiene
b. Benzene and nathtalene
c. The use of symmetry in Huckel MO theory
d. Aromaticity and 4n+2 rule
f. Problem of heteroatoms. Formaldehyde dipole moment
g. Atomic charge and electronegativity concept
h. Bond order

2L 8 - Molecular Symmetry.

a. Molecular Spectroscopy
b. Vibration-Rotation Spectra
c. Electronic Spectra
d. Symmetry elements
e. Group Theory in quantum mechanics
f. Selection rules in spectra

2L 9 - Spectroscopy and molecular orbital concept.

a. Electric dipole transition moment in ethylene and butadiene
b. Polarization of S-S transitions and symmetry selection rules
c. $\pi\pi^*$ and $n\pi$ transitions. Solvent effects
d. Photoelectron spectra as direct experimental verification of the MO concept

e. EPR spectroscopy for radicals. Anion radicals of hydrocarbons. Hyperfine coupling. Spin polarization

2L 10 - Independent Particle Models.

a. The total energy of the closed shell
b. Fock equations
c. Koopman's theorem
d. Roothaan equations

2L 11 - Electron Correlation CI

a. The concept of electronc correltion
b. Configuration Interaction
c. Configuration interaction for single excitations upon the closed shell. Ethylene spectrum
d. Configuration interaction (CI) in 3,1Σ-, 3,1Δ and 3,1Σ+ states of π3π*1 configuration in diatomics
e. CI for double excitations upon the closed shell
f. Comparison of MO CI and valence bond methods for H2 molecule

2L 12 - Perturbation Theory

a. Moller-Plesset Perturbation Theory
b. Ordinary (RS) perturbation theory
c. MP2 energy expresssions in different orders
d. Size-consistency, convergence/divergence of the expansion

2L 13 - Relativistic effects in molecules.

a. General role of relativity in molecules
a. Spin-orbit coupling
b. SOC in small molecules
c. SOC in reactions of enzymes

2L 14 - Introduction to Second quantization

a. Definition of Fock space
b. Field (creation and annihilation) operators, properties and algebra
c. Quantum mechanical operators in second quantization
d. Spin-orbital vs orbital formulation
e. Unitary transformations
f. Optimization of wave functions

2L 15 - Introduction to Response Theory

a. Derivation of response functions
b. Linear and non-linear response functions
c. Residue analysis
d. Singlet versus triplet operators

2L 16 - Calculations of molecular response properties

a. HF - response functions (TDHF, RPA)
b. DFT - response functions (TDDFT)
c. MCSCF and coupled cluster response
d. Excited state properties
e. Brief survey of applications

2L 17 - Magnetic Resonance Parameters

a. Effective spin Hamiltonians
b. Hyperfine interaction
c. g-tensors
d. Zero-field splitting

Macroscopic concepts (part 3)

(3A5713 - 8 ETCS)
Project work required for passing the course.
Lecturers:
Aatto Laaksonen (aatto -at- physc.su.se) Phone: 08-162372
Alexander Lyubartsev (sasha -at- physc.su.se) Phone: 08-161193

3L 1 - Thermodynamics

a. States of matter
b. Systems and surrounding
c. Energy and structure
d. Temperature, pressure and intermolecular interactions

3L 2 - Thermodynamics

a. State functions and thermodynamical variables
b. Enthalpy, entropy and free energy
c. The laws of thermodynamics
d. The machinery of thermodynamics

3L 3 Statistical thermodynamics - Boltzmann distribution

a. Quantum mechanics - statistical thermodynamics - thermodynamics
b. The statistical method
c. Principle of equal probabilities
d. Boltzmann distribution
e. Molecular partition function

3L 4 Statistical thermodynamics - Canonical ensemble

a. Canonical ensemble
b. Qauntum and classical canonical partition function
c. Derivation of thermodynamic quantities
d. Statistical interpretation of the 2-nd law of thermodynamics

3L 5 Statistical thermodynamics - other ensembles

a. Microcanonical ensemble
b. Grandcanonical ensemble. Chemical potential.
c. Constant-Temperature – Constant-Pressure ensemble
d. Fluctuations

3L 6 Statistical thermodynamics - Ideal systems

a. Polyatomic molecules in a gas phase
b. Factorization of the partition function
c. Translation, rotation and vibration
d. Spectroscopy and thermodynamics

3L 7 Statistical thermodynamics - non-ideal systems

a. Non-ideal systems
b. Virial expansion
c. Van der Waals equation

3L 8 Statistical thermodynamics - Lattice systems

a. Lattice statistics
b. Ising model and spin systems
c. Lattice polymer models. Flory-Huggins theory

3L 9 Quantum statistical thermodynamics

a. Quantum statistics, Bosons and fermions.
b. Bose-gas. Bose condensation.
c. Fermi-gas. Electrons in metals

3L 10 Kinetics

a. Chemical reactions
b. Chemical kinetics (elementary reactions)
c. Equilibrium
d. Reaction order and molecularity
e. Chemical kinetics (complex reactions)

3L 11 Kinetics

a. How reaction rates can be affected
b. Arrhenius law
c. catalysis
d. homogeneous and heterogeneous catalysis
e. transition state theory (part I)

3L 12 Kinetics

a. Biological reactions and processes
b. Proteins and enzymes
c. Enzyme catalysis

3L 13 Liquid theories

a. Intermolecular interactions
b. Correlation function and Radial distribution function
c. Analytic liquid theories

3L 14 Electrolytes and polyelectrolytes

a. Electrochemical models.
b. Coulomb systems and continuum models. Debye-Huckel theory.
c. Strong non-ideality and correlations
d. Poly-electrolytes
e. Poisson-Boltzmann equation

Learning to Fly (part 4)

(3A5714 - 8 ETCS)
Project work required for passing the course.
Lecturers:
Aatto - Aatto Laaksonen (aatto -at-physc.su.se) Phone: 162372
Sasha - Alexander Lyubartsev (sasha -at-physc.su.se) Phone: 161193

4L 1 Simulation methods. Molecular Mechanics

a. Force fields (FF) - intro
b. Parameterisation of FFs
c. Molecular mechanics (MM)
d. Energy minimization (EM) techniques
e. Conformational analysis
f. Introduction to some MM software for EM

4L 2 Monte Carlo method: background

a. Stochastic processes. Simple Monte Carlo methods.
b. Importance sampling
c. Markovian master equation
d. Phase space sampling
e. Various Monte Carlo techniques
f. Time in MC?

4L 3 Monte Carlo method: techniques

a. Optimizing MC runs
b. MC averages
c. Simple MC algorithms
d. Write your own MC code

4L 4 Molecular dynamics: background

a. Classical mechanics: Newtonian, Lagrangian and Hamiltonian equations
b. Basic molecular dynamics algorithms
c. Constant-Pressure and Constant-temperature molecular dynamics
d. Molecular dynamics (MD) : rigid molecules

e. Molecular dynamics : flexible molecules
f. MD vs MC

4L 5 Molecular dynamics: HowTo

a. Planning a simulation study for MD
b. Start, equilibration and production phases
c. Trajectory: what is it?
d. Averages from trajectories
e. Static and dynamical properties from MD
f. Visualization of simulation results
g. How do I know to trust the results?
h. Write your own MD code from short modules

4L 6 Molecular dynamics: techniques

a. Calculating electrostatic forces
b. Time scales and motional modes
c. Extending/restricting the phase space
d. Rare events
e. Parallel computational strategies for MD
f. Examples of large-scale or tricky simulations

4L 7 Free energy computations

a. Free energy from simulations
b. Various free energy simulation schemes
c. A closer look: The expanded ensemble method
d. Applications: solubility, protein folding

4L 8 Mesoscale Simulation methods 1

a. Non-equilibrium MD
b. Stochastic (Brownian and Langevin) dynamics
c. Dissipative particle dynamics
d. Coarse-graining techniques

4L 9 Mesoscale Simulation methods 2

a. Boltzmann eqation
b. Lattice gas models
c. Cellular automata
d. Lattice Boltzmann method

4L 10 Mesoscale Simulation methods 3

a. Kinetic Monte Carlo (kMC) method
b. Hydrodynamics
c. Multi-scale modeling (bridging the scales)

4L 11 Simulation methods

a. How can QC and simulation studies combined.
b. Simulations and property surfaces
c. MD simulations and spectroscopy

4L 12 Simulations and computers

a. Hardware aspects to speed up simulations.
b. Strategies and advices to build and maintain a pc-cluster
c. National HPC resources for various types of simulations

Grand Applications (part 5)

(3A5715 - 8 ETCS)
Exercises solved required for passing the course.
Lecturers:
Fahmi Himo (himo-at-theochem.kth.se) (L 1-2),
X (…) (L 3-7)
Ying Fu (fyg-at-theochem.kth.se) (L8-9)

5L 1 – Modelling chemical reactions

a. Solvation models and solvation effects
b. Basis set effects.
c. Zero point and isotope effects
d. Accuracy of DFT methods.
e. Calculation and interpretation of potential energy surfaces
f. Modeling reaction pathways

5L 2 – Modelling enzymatic reactions

Characterization techniques 1
5L 3 - Magnetic Resonance Spectroscopy

a. Spin relaxation
b. NMR
c. EPR
d. Related spectroscopies (ODMR, ENDOR)
e. Paramagnetic systems
f. NMR and EPR as tools in biochemistry

Characterization techniques 2
5L 4 - Vibrational Spectroscopy

a. Force fields and normal modes
b. Calculation of Infrared spectra
c. Calculation of Raman spectra

Characterization techniques 3
5L 5 - Optical / UV spectra

a. Fundamental optical excitations
b. Oscillator strengths
c. Polarization and Dichroism
d. Vibronic spectra
e. Franck Condon principle
f. Optical/UV spectroscopy as a diagnostic tool

Characterization techniques 4
5L 6 - X-ray spectroscopy

a. Photoelectron spectra
b. X-ray absorption
c. X-ray emission

d. Auger spectroscopy
e. Resonant X-ray spectroscopies

Characterization techniques 5
5L 7 - Non-linear phenomena

a. Polarizabilities and hyperpolarizabilities
b. Harmonic generation
c. Many-photon excitation
d. Few-state models
e. Vibrational contributions
f. NLO as application tool

Computational Nanoscience
5L 8 - Electronic and Optical properties of nanoparticles

a. Scale consideration v.s. molecular and solid-state systems
b. Electronic properties of individual nanoparticle
c. Optical properties of individual nanoparticle
d. Nanoparticle assembly/network: electronic and photonic crystals

Computational Nanoscience
5L 9 - Applications of nanoparticles in bio and medical fields

a. Multiphoton quantum dots for confocal microscopy
b. Medical/biochemical diagnostic using nanoparticles
c. Future nano devices