Syllabus, Rules and Guidelines
for
M S in Theoretical and Computational Chemistry (TCChem)
University of Dhaka
Session: 2016 – 2017 and onward

1. Course of study for M S degree in Theoretical and Computational Chemistry shall extend over a period of one academic calendar year. A student must earn a total of **32** (thirty two) credits for the award of M S degree in Theoretical and Computational Chemistry.

2. Admission into M S in Theoretical and Computational Chemistry

(i) Students who have completed/passed B S (Honors) degree in Chemistry, Biochemistry, Applied Chemistry, Pharmacy, Physics and B Sc in Chemical Engineering from the Public and Private Universities with minimum CGPA of 2.5 in the scale of 4.0 will only be eligible for admission to M S in Theoretical and Computational Chemistry under the Faculty of Science. Students from the Department of Physics must have Chemistry, both theory and practical course in their minor courses.

(ii) Academic Committee of the Department of Theoretical and Computational Chemistry will determine the criteria for admission.

3. Duration of the Program

Classes	24 weeks
Time for preparation of final examination	04 weeks
Course final examination	04 weeks
Submission of thesis	16 weeks
Publication of results	04 weeks

4. Evaluation of Students

The performance of the students will be evaluated on the basis of continuous assessment and course final examination. The marks in a course will be distributed as follows:

(a) Theory Course		
	Class Attendance	10%
	In-course assessment	30%
	Course final examination	60%
(b) Practical Course		
	Class Attendance	10%
	Class assessment	40%
	Course final examination	50%

5. Distribution of Credits

The distribution of credits will be according to the following format:

Theory	3 credits x (4+2)	= 18 credits
Practical	2 credits x 3	= 6 credits
Thesis		= 6 credits
Thesis defense		= 2 credits
Total		**= 32 credits**

6. Marks for Attendance

Attendance (%)	Marks (%)
95 to 100	10
90 to 94	08
85 to 89	06
80 to 84	04
75 to 79	02
60 to 74	01
Less than 60	00

7. In-course Assessment of Theory Courses

- The course teacher will announce the dates of in-course examinations.
- The in-course assessment will be based on tests, that is, written examinations.
- Duration of each in-course test will be of one hour and the course teacher will be responsible to assess the students sitting in his/her course.
- There will be 2 (two) tests for each 3 credits course.
- Average of the two tests should be considered to finalize the grade.
- Course teachers must announce results in 2 (two) weeks of holding the examination.
- Marks for in-course assessment must be submitted by the course teacher to the Chairman of the Examination Committee and the controller of examinations before the final examination.
- Answer scripts must be shown to the students.
- No make-up test will be arranged for a student who fails to appear or wish to re-appear in his/her in-course tests.
- Absence in any in-course test will be counted as zero for calculating the average in in-course test for that course.
- However, a student can request special permission for re-take of in-course test if recommended by the course teacher through the Academic Committee of the Department only under extraordinary circumstances (e. g., accident, death of a close relative, etc.)

8. Course Final Examination (Theory Course)

(i) The course final examination will be conducted by the Controller of Examinations as per existing rules of the university.

(ii) The course final examination will be of 3 (three) hours duration for 3 credit course.

(iii) There will be two examiners to evaluate an answer-script. One of them must be the course teacher and the second examiner may be taken from the Department of TCC. A second examiner also may be chosen from other places, inside or outside of the University of Dhaka.

9. Course Final Examination (Practical Course)

Examination of practical courses will be conducted by course teacher/teachers and one more examiner may be taken from the Department of TCC or any other places inside or outside of the University of Dhaka and this examiner may or may not be the external member of the Departmental Examination Committee.

10. Evaluation of Thesis

(i) Thesis will be evaluated as per existing rules of the university with two external examiners. One examiner may be taken from the Department of TCC other than the supervisor if suitable external examiner is not found.

(ii) Oral examination of the MS thesis students (Thesis defense) will be conducted by the members of the Examination Committee consisting of three internal and one external examiner and approved by the Academic Council of the University. Supervisor of a student will be requested to be present at the time of the presentation. He/she may participate in discussion but not in evaluation.

11. The Grading System

Marks obtained by a student in different courses will be converted to grades. A basic four point (4.00) grading scale will be followed. The following letter grade and grade point will be used to determine the student's grade point average (GPA).

Marks Obtained	Corresponding Letter Grade	Grade Point
80% or above	A+	4.00
75 to 79%	A	3.75
70 to 74%	A-	3.50
65 to 69%	B+	3.25
60 to 64%	B	3.00
55 to 59%	B-	2.75
50 to 54%	C+	2.50
45 to 49%	C	2.25
40 to less than 44%	D	2.00
Less than 40%	F	0.00

12. Improvement

(i) If a student obtains a grade C+ or lower in a theory course he/she will be allowed to repeat the term-final examination only once with the following batch for the purpose of grade improvement, but he/she will not be eligible to get a grade better than 'B+' in such a course. A student failing to improve his/her grade in a course can retain the earlier grade.

(ii) A student will be allowed to take improvement of 25% of the total theoretical credits taken.

(iii) A student obtaining 'F' grade in one or more courses (theory and practical) will not be awarded degree. However, a student obtaining 'F' grade in a course may be allowed to retake that course only once with the next batch of students in order to be awarded a degree. A student obtaining 'F' grades in more than one courses will not be allowed to repeat any course.

13. Calculation of GPA

The GPA (grade point average) will be calculated according to the following formula:

$$\text{GPA} = \frac{\sum (\text{grade points in a course} \times \text{credits for the course})}{\text{total credits taken}}$$

14. Eligibility for Sitting in Course Final Examination

(i) A student must attend at least 75% of the total classes in a course held in an academic year to be eligible for appearing in the final examination in a course.

(ii) A student attending at least 60% of classes in a course will be allowed to sit for course final examination after payment of non- collegiate fees as decided by the University.

(iii) A student attending less than 60% classes in a course will not be allowed to sit for final examination.

15. Readmission

(i) A student failing to complete the MS course in a year may seek readmission with the next available batch of students, provided he/she applies within one month of publication of the result of the concerned year.

(ii) A readmitted student will be allowed to retain his/her in-course/class assessment marks earned in previous year.

(iii) A readmitted student may be allowed to take up thesis work as decided by the Departmental Academic Committee.

(iv) The transcripts of successful readmitted student will bear the letter 'R' after GPA with a foot note explaining 'R' means Readmission.

16. Requirements for MS Degree

A minimum GPA of 2.50 on a scale of 4.00 must be obtained in order to be awarded MS degree.

17. General Regulations

(i) The Departmental Academic Committee will design courses of studies, frame syllabuses of different courses, propose examination committee and panel of examiners as per rules of the university.

(ii) The course teacher will provide the students a course outline, schedule of class assessment and relevant information in the first class of the term.

(iii) The course teacher shall announce the results of the in-course tests within two weeks of the date of holding the tests and submit the marks to the Chairman of the Examination Committee for the respective batch and also a copy to the Controller of Examinations at least two weeks before the start of the final examination. He/she should also submit a statement showing the total number of classes held and the percentage of attendance of each student in his/her course to the Chairman of the Department.

(iv) Tabulation work will be started only after all the marks of the course final examinations for the year are received by the Chairman of the Examination Committee. Marks received by the Chairman of the Examination Committee shall remain in the sealed envelope as sent by the Examiner/Examiners until tabulation work is started.

(v) The present system of conducting course final examination and publication of results by the office of the Controller of Examinations shall continue.

(vi) For any other matters not covered in these rules, the existing rules of the University of Dhaka will be applicable.

18. Courses

Core theory Courses (4):

TCC 501 Quantum Chemistry	3 credits
TCC 502 Computational Chemistry I	3 credits
TCC 503 Computational Chemistry II	3 credits
TCC 504 Molecular Spectroscopy	3 credits

Optional theory courses (any 2):

TCC 505 Statistical Thermodynamics	3 credits
TCC 506 Molecular Modeling and Drug Design	3 credits
TCC 507 Computational Methods in Reaction Mechanism	3 credits
TCC 508 Computational Biochemistry	3 credits
TCC 509 Molecular Modeling of Inorganic Compounds	3 credits
TCC 510 Computational Chemistry of Energy Materials	3 credits
TCC 511 Chemoinformatics and Computational Chemical Biology	3 credits

Practical Courses:

TCC 521L Practical Computational Chemistry I	2 credits
TCC 522L Practical Computational Chemistry II	2 credits
TCC 523L Programming and Software Development	2 credits

TCC 501 Quantum Chemistry

1. The breakdown of classical physics: Blackbody/Cavity radiation; Classical treatment of cavity radiation and the ultraviolet catastrophe; Planck's quantization hypothesis; Particle character of light; Photoelectric effect; Einstein explanation of Photoelectric effect; Compton effect; The vibration of atoms in crystals are quantized; The Hydrogen atom's spectrum; Angular momentum are quantized; De Broglie waves are observed experimentally; Heisenberg uncertainty principle. The one-dimensional classical wave equation; Separation of variables; Oscillatory solution to differential equation; Even function and odd functions.
2. The Schrödinger equation and a particle in a box; The Schrödinger equation; Linear operator in quantum mechanics; Hamiltonian operator; Eigenvalue problem in quantum mechanics; wave function and their probabilistic interpretations; Quantized energies; Normalized wave function; Average quantities in quantum mechanics; The uncertainty principle and operators; Schrödinger equation for a particle in a three dimensional box and its solution: interpretation of the solution and concept of degeneracy.
3. State functions; Quantum mechanical operators and classical variables; Observable quantities and eigenvalues; Commutators and the uncertainty principle; Hermitian operators; Hermitian operators and orthogonality; Mutual Eigen functions and time-dependent Schrödinger equation.
4. Classical harmonic oscillator; Conservation of energy of Classical harmonic oscillator; Harmonic oscillator model of a diatomic molecule; The harmonic oscillator approximation; The energy of a quantum-mechanical harmonic oscillator; Tunneling; Harmonic oscillator wave function; Parity of Hermite polynomials; Operator method of solution to the Schrödinger equation for a harmonic oscillator.
5. Spherical coordinates; The one-particle central force problem; Non interacting particles and separation of variables; Reduction of the two particle problem to one-particle problem; The two particle rigid rotor; Hamiltonian operator and Schrödinger equation of a rigid rotor; Solution of theta and phi equation; Spherical harmonics; Particle on a ring.
6. The Hamiltonian and the Schrödinger equation for the Hydrogen atom; Solution of the radial equation; Energy levels and degeneracy; The bound-state hydrogen atom wave functions; The radial factor; Ground-state wave function and energy; Wave-function for n = 2; The radial distribution function and real hydrogen like functions; System of atomic units; Radial equation of hydrogen atom as an eigenvalue equation in a.u.; Orthogonality of $1s$ and $2s$ atomic orbitals; $2p_x$, $2p_y$ and $2p_z$ orbitals have three maxima and minima value along x, y and z axes; Probability that the electrons lie between r and $r+dr$; Average distance of the electron in $1s$, $2s$ and $2p$ orbitals.

References

1. Quantum Chemistry, 2nd edition, Donald A. McQuarrie, University Science Books, 2008.
2. Quantum Chemistry, 7th edition, Ira N. Levine, Pearson, 2014.

TCC 502 Computational Chemistry I

1. The Schrödinger equation for helium atom and for many electron atoms; The molecular Hamiltonian and the Born-Oppenheimer approximation; Electronic and nuclear Schrödinger equations.
2. Principle of Perturbation theory; Perturbation theory consists of a set successive corrections to an unperturbed problem; examples are: helium atom, anharmonic oscillator and the particle in a one-dimensional box with a slanted bottom.
3. Variation method; Variational principle giving examples of the ground state of the hydrogen atom; ground state of a harmonic oscillator; Construction of trial wave functions; The LCAO basis set approach and the secular equation.
4. The basic principle of the *ab initio* method; The Hatree-Fock SCF method; The HF equation and the meaning of the HF equation; Antisymmetric of electronic wave functions; Slater determinants; Calculating the atomic and molecular energy; Minimizing the energy; Basis function and Roothaan-Hall equation.
5. Introduction of basis sets; Different types of basis set and their uses; Choice of basis sets; Basis set superposition error (BSSE); Slater and Gaussian type orbitals.
6. Introduction of electron correlation; Moller-Plesset perturbation approach to electron correlation; Configuration interaction (CI) approach to electron correlation; The coupled-cluster method; Applications of the *ab initio* method; Strength and weakness of the *ab initio* calculations.
7. The basic principles of density functional theory (DFT) and time-dependent density functional theory (TD-DFT); Hohenberg-Kohn theorem; Kohn-Sham SCF methodology; Exchange correlation function; Advantages and disadvantages of DFT compared to MO theory; General performance and overview of DFT.

References

1. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd edition, Errol G.Lewars, Springer, 2004.
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, Francis A. Carey and Richard J. Sundberg, Springer, 2007.
3. Essentials of Computational Chemistry, 2nd Edition, Christopher J. Cramer, Wiley, 2004.
4. Quantum Chemistry, 2nd Edition, Donald A. McQuarrie, University Science Books, 2008.

TCC 503 Computational Chemistry II

1. Scope of computational chemistry; Theory, computation and modeling; Computable quantities; Cost and efficiency.
2. Concept of potential energy surface (PES); Stationary point and saddle point; Geometry optimization and normal mode vibrations.
3. Basic principle of Molecular mechanics (MM) and force field; Developing a force field; Parameterizing force field; Calculation using force field; Differences in force field; Validation of force field; Advantages and limitation of force field methods.
4. Introduction of Huckel theory; Simple Huckel method; Applications of simple Huckel method; Strength and weakness of simple Huckel method.
5. Basic principles of SCF semi-empirical method; PPP, CNDO, INDO, NDDO; Applications of semi-empirical methods; Strength and weakness of semi-empirical methods.
6. Frontier molecular orbital theory (FMOT); Concept from DFT; Qualitative MOT; Woodward-Hoffman rules.
7. Simulation techniques: Monte Carlo (MC) simulations; MC integration and Markov chains; The Metropolis method; Biased MC.
8. Molecular Dynamics: Classical mechanics; Equations of motion; Finite difference methods; Verlet algorithm; Velocity verlet; The time step: practical issues and multiple time-step algorithms; Constraint Dynamics; fundamental concepts: SHAKE and RATTLE; Maxwell-Boltzmann distribution of velocities; Temperature control; velocity scaling; Andersen's method; Nose-Hoover dynamics; Calculating properties from MD trajectories.

References:

1. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd edition, Errol G. Lewars, Springer, 2004.
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, Francis A. Carey and Richard J. Sundberg, Springer, 2007.
3. Essentials of Computational Chemistry, 2nd Edition, Christopher J. Cramer, Wiley, 2004.
4. Introduction to Computational Chemistry, 2nd Edition, Frank Jensen, Wiley, 2007.
5. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty, University Science Books, 2006.

TCC 504 Molecular Spectroscopy

1. Molecular Symmetry and Group Theory: Symmetry elements and symmetry operations; point groups of molecules; multiplication of symmetry operations; rules for multiplications; point groups and molecular systems groups of very high and low symmetry; use of flow chart to identify a point group; optical activity and dipole moments on the basis of point group symmetry; symmetry operations and matrix representations; reducible and irreducible representations.
2. Interaction of Electromagnetic Radiation with Atoms and Molecules: Electromagnetic radiation; quantization of energy; absorption and emission of radiation; regions of spectrum; representation of spectra; signal-to-noise ratio; resolving power; width and intensity of spectral transitions.
3. Infrared (IR) spectroscopy: Solution of the Schrödinger equation for harmonic oscillator accounts for the IR spectrum for diatomic molecule; Overtones are observed in vibrational spectra; The infrared absorption process; The modes of stretching and bending; Bond properties and absorption trends; Dispersive and Fourier Transform spectrometers; Preparation of samples for infrared spectroscopy; Analysis of a spectrum; IR spectrum of compounds.
4. Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR): Nuclear spin states; Nuclear magnetic moments; Absorption of energy; The mechanism of absorption (resonance); Population densities of nuclear spin states; The chemical shift and shielding; The nuclear magnetic resonance spectrometer; The continuous-wave (CW) instrument and the Pulsed Fourier Transform (FT) instrument; Chemical equivalence, integrals and integration; Chemical environment and chemical shift; Local diamagnetic shielding, magnetic anisotropy, spin-spin splitting (n+1) rule, Pascal's triangle, the coupling constant and survey of ^{1}H NMR absorption by various types of compounds.
5. Nuclear Magnetic Resonance Spectroscopy (^{13}C NMR): The carbon-13 nucleus; carbon-13 chemical shifts; calculation of ^{13}C chemical shifts; proton-coupled ^{13}C spectra; spin-spin splitting of carbon-13 signals; proton-decoupled ^{13}C spectra; Nuclear Overhauser Enhancement (NOE); cross-polarization: origin of the Nuclear Overhauser Effect; Analysis of some spectra.
6. Ultraviolet-Visible (UV-Vis) Spectroscopy: The nature of electronic excitations; The origin of UV band structure; Principles of absorption spectroscopy; Instrumentation; Presentation of spectra; Solvents; Chromophore; The effect of conjugation; The Woodward-Fieser rules; Model compound studies; Visible spectra: color in transition metal compounds.
7. Mass Spectroscopy: The mass spectrometer; Sample introduction; Ionization methods; Mass analysis; Detection and quantization; The mass spectrum; Determination of molecular weight and molecular formula; Structural analysis and fragmentation patterns; Strategic approach to analyzing mass spectra and solving problems.
8. Combined structural problems: Solution using UV-Vis, IR, NMR and mass spectra.
9. Advanced NMR Techniques: Pulse sequences; Pulse widths; Spins and magnetization vectors; Pulsed field gradient; The DEPT experiment; Determining the number of attached hydrogen; Introduction to two dimensional spectroscopic methods and The COSY technique.

References

1. Introduction to Spectroscopy, 3rd edition, L. Pavia, G. M. Lampman and G. S. Kriz, Thomson, 2001.
2. Modern Spectroscopy, 4th edition, Michael J. Hollas, Wiley 2004.
3. Organic Spectroscopy, 2nd edition, W. Kemp, Macmillan, 1987.
4. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons, Inc.

TCC 505 Statistical Thermodynamics

1. Introduction: Aims of statistical mechanics; various ensembles and thermodynamics; probability distributions; Stirling's approximation; binomial distribution; Lagrange multipliers; relation between partial derivatives.
2. The Boltzmann distribution; molecular partition function for an ideal gas; interpretation/physical meaning of partition function; calculation of thermodynamic properties of ideal gas using molecular partition function; translational, vibrational, rotational and electronic contributions to the thermodynamic properties of ideal gases.
3. Canonical ensemble: Distribution function; evaluation of Lagrange multipliers using second law; expressions for thermodynamic functions in terms of canonical partition function; third law and entropy; remark on microcanonical ensemble.
4. Grand canonical ensemble: Distribution function; evaluation of Lagrange multipliers; expressions for thermodynamic functions in terms of grand canonical partition function; isothermal-isobaric ensemble.
5. Various statistics: Indistinguishability of particles and Fermi-Dirac; Einstein-Bose and Boltzmann distribution functions for noninteracting particles obtained via grand canonical partition function; thermodynamic properties.
6. Noninteracting molecules: Relation of canonical partition function to molecular partition function and thermodynamic properties; monatomic, diatomic and polyatomic gases; symmetry of wave functions; ortho-para hydrogen; chemical equilibria; phase equilibria; Independent modes or particles; Fermi-Dirac system (electron gas); Einstein crystal; Debye crystal; specific heat; free electron model of metal; photon gas (black body radiation); phase space.
7. Interacting particles: Lattice statistics; Ising model for spin systems; partition function for one-dimensional system; broken symmetry; mean field theory; Curie-Weiss law; Discontinuities at the critical point; Bragg-Williams approach to "mean field" theory; Adiabatic demagnetization.
8. Crystals: The vibrational spectrum of a monatomic crystal; the Einstein theory of the specific heat of crystals; introduction to lattice dynamics; phonons.

References

1. Statistical Mechanics, Donald A. McQuarrie, University Science Books, 2003.
2. Introduction to Modern Statistical Mechanics, David Chandler, Oxford University Press, 1987.
3. Physical Chemistry, 3rd edition, R. J. Silbey and R. A. Alberty, Wiley, 2003.
4. Statistical Thermodynamics, M C Gupta, Wiley, 1990.

TCC 506 Molecular Modeling and Drug Design

1. Molecular structure of biomolecules: Amino acids and proteins; Carbohydrates; Lipids and Nucleic acids.
2. Drug discovery and drug design; Definition of drugs; Sources of drug; Modern drug design; Requirements for compounds to be drug; Stages and cost of modern drug design; Tools and teams in modern drug design; The role of computational chemistry in drug design; Drug discover-filtering out failures.
3. SAR and 2D-Quantitative Structure-Activity Relationships (2D-QSAR); Definition and QSAR methodology; Basic concepts of QSAR; Hansch analysis; Free-Wilson analysis; Molecular descriptors; Electronic parameters; Polar interactions; Steric, Biological and Topological parameters; Quantum-chemical descriptors; 2D-QSAR in drug design; Enzyme inhibition; Model system for cysteine protease; Prediction of mutagenic potencies; QSAR for antimalarial compounds; β_1- and β_2- antagonist activities; Activity-activity relationships and Validation of QSAR models.
4. Computer Assisted Drug Design (CADD); Description of CADD; Explanation of some basic terms: Pharmacophore, Lock-Key principle and Induced fit theory; Molecular Recognition; Requirements of a compound to be bioactive; The objects of CADD and Molecular Modeling; Driving forces of Receptor-Drug interactions; Solvent modeling - the role of water; The dynamic aspect of modeling; Techniques and concepts used in CADD and Molecular Modeling.
5. Introduction of molecular docking; Search algorithms; Scoring; Validation of results and the docking process.
6. Homology model building; Steps for building a homology model and reliability of results.
7. Challenges in molecular modelling; Free energy, Solvation and Reactions.

References

1. Fundamentals of Medicinal Chemistry, Gareth Thomas, Wiley, 2003.
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, Francis A. Carey and Richard J. Sundberg, Springer, 2007.
3. Computational Drug Design: A Guide for Computational and Medicinal Chemists, David C. Young, Wiley, 2009.
4. Molecular Modeling: Principles and Applications, 2nd Edition, Andrew R. Leach, Pearson Education Limited, 2001.
5. Burger's Medicinal Chemistry and Drug Discovery, 6th edition, Donald J. Abraham, Wiley, 2003.
6. Computational Organic Chemistry, 2nd Edition, Steven M. Bachrach, Willey, 2014.
7. Principles of Medicinal Chemistry, 3rd Edition, William O. Foye, Varghese Publishing Housr, 1989.

TCC 507 Computational Methods in Reaction Mechanism

1. Chemical Bonding and Molecular Structure: The Origin of the rotational (torsional) barrier in ethane and other small molecules, Heteroatom hyperconjugation (Anomeric Effect) in acyclic molecules, Representation of electron density by the Laplacian Function, Application of density functional theory (DFT) to chemical properties and reactivity, DFT Formulation of chemical potential, Electronegativity, Hardness and Softness, Covalent and van der Waal Radii, Formulation of reactivity—The Fukui Function, Concepts of substituent groups effects.
2. Stereochemistry, Conformation, and Stereoselectivity: Stereoselective and Stereospecific Reactions. Enantioselective Reactions.
3. Structural Effects on Stability and Reactivity: Thermodynamic stability, Relationship between structure and thermodynamic stability for hydrocarbons, Calculation of enthalpy of formation and enthalpy of reaction, Representation of potential energy changes in reactions, Reaction rate expressions, General relationships between thermodynamic stability and reaction rates, Kinetic versus thermodynamic control of product composition, Correlations between thermodynamic and kinetic aspects of reactions, Curtin-Hammett Principle, Kinetic isotope effects, Linear Free-Energy Relationships for substituent effects, Acidity of hydrocarbons.
4. Nucleophilic Substitution: S_N1 Mechanism, S_N2 mechanism, Relationship between stereochemistry and mechanism of substitution, Structural and solvation effects on reactivity, Characteristics of nucleophilicity, Effect of solvation on nucleophilicity, Leaving-group effects, Steric and strain effects on substitution and ionization rates , Effects of conjugation on reactivity, Neighboring-group participation.
5. Polar Addition and Elimination Reactions**:** Addition of hydrogen halides to alkenes, Acid-catalyzed hydration and related addition reactions, Addition of halogens, Electrophilic additions involving metal ions, Additions to alkynes and allenes, Hydrohalogenation and hydration of alkynes, Elimination reactions, The E2, E1 and E1cb mechanisms, Stereochemistry of E2 elimination reactions, Dehydration of alcohols.
6. Addition, Condensation and Substitution Reactions of Carbonyl Compounds: Reactivity of carbonyl compounds toward addition, Hydration and addition of alcohols to aldehydes and ketones, Condensation reactions of aldehydes and ketones with nitrogen nucleophiles, Substitution reactions of carboxylic acid derivatives, Ester hydrolysis and exchange, Aminolysis of esters, Amide hydrolysis, Acylation of nucleophilic oxygen and nitrogen groups, Addition of enolates and enols to carbonyl compounds: The aldol addition and condensation reactions.
7. Aromatic Substitution: Electrophilic aromatic substitution reactions, Structure-reactivity relationships for substituted benzenes, Mechanistic interpretation of the relationship between reactivity and selectivity, Reactivity of polycyclic and heteroaromatic compounds, Nucleophilic aromatic substitution by the addition-elimination mechanism, Nucleophilic aromatic substitution by the elimination-addition mechanism.
8. Concerted Pericyclic Reactions: Cycloaddition reactions: The Diels-Alder reaction, Stereochemistry of the Diels-Alder reaction, Substituent effects on reactivity, Regioselectivity and stereochemistry, Computational characterization of Diels-Alder transition structures, 1,3-Dipolar cycloaddition reactions, Cycloaddition reactions, Electrocyclic reactions, Orbital symmetry basis for the stereospecificity of electrocyclic reactions, Sigmatropic rearrangements.

Text Books

1. Advanced Organic Chemistry Part A: Structure and Mechanism, 5th Edition, Francis A. Carey, Richard J. Sundberg, Springer, 2007.
2. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. S. Richardson, Harper and Row, 1976.

TCC 508 Computational Biochemistry

1. Computational Biochemistry: Application of computer technology to biochemistry.
2. Analysis and Management of Biochemical Data: Statistical analysis of biochemical data, Biochemical data analysis with spreadsheet application, Biochemical data management with database program.
3. Visualization of Biomolecules: Representation of molecular structures, Drawing and display of molecular structures.
4. Structure and Analysis of Biochemical Compounds: Survey of biomolecules, Characterization of biomolecular structures, Fitting and search of biomolecular data and information.
5. Biomolecular Interactions**:** Biomacromolecule – ligand interaction, Receptor biochemistry and signal transduction, Fitting of binding data and search for receptor databases.
6. Enzyme Kinetics: Characterization of enzymes, Kinetics of enzymatic reactions, Search and analysis of enzyme data.
7. Metabolic Simulation: Introduction to metabolism, Metabolic control analysis, Metabolic databases and simulation.
8. Nucleotide Sequences and Recombinant DNA: Genome, DNA sequence and transmission of genetic information, Recombinant DNA technology, Nucleotide sequence analysis.
9. Protein Sequence Analysis: Information and features of protein sequence, Database search and sequence alignment.
10. Prediction of Protein Structures: Prediction of protein secondary structures from sequences, Protein folding problems and functional sites.
11. Protein Modeling: Structure similarity and overlap, Structure prediction and molecular docking, Application of protein modeling.

Text Books

1. An Introduction to Computational Biochemistry, C. Stan Tsai, Wiley-Liss, 2002.
2. Computational Biochemistry and Biophysics, Oren M. Becker, Alexander D. MacKerell, Jr., Benoit Roux and Masakatsu Watanabe, Marcel Dekker, 2001.

TCC 509 Molecular Modeling of Inorganic Compounds

1. Structural Aspects: Accuracy of structure prediction, Molecular visualization, Isomer analysis, Analysis of structural trends, Prediction of complex polymerization, Unraveling crystallographic disorder, Comparison with solution properties.
2. Stereoselectivities: Conformational analysis, Enantioselectivities, Racemate separation, Stereoselective synthesis, Structure evaluation, Mechanistic information.
3. Metal Ion Selectivity: Chelate ring size, Macrocycle hole size, Preorganization.
4. Spectroscopy of Inorganic Compounds: Vibrational spectroscopy, Electronic spectroscopy, EPR spectroscopy, NMR spectroscopy.
5. Electronic Effects: *d*-orbital directionality, The trans influence, Jahn-Teller distortions.
6. Bioinorganic Chemistry: Complexes of amino acids and peptides, Metalloproteins, Metalloporphyrins, Metal-Nucleotide and Metal-DNA interactions, Other systems.
7. Organometallics: Metallocenes, Transition metal-allyl systems, Transition metal phosphine compounds, Metal-metal bonding, Carbonyl cluster compounds.
8. Compounds with *s*-. *p*- and *f*-block elements: Alkali and alkaline earth metals, Crown ethers, Cryptands, Spherands, Biologically relevant ligands, Main group elements, Lanthanoids and Actinoids.

Text Book

1. Molecular Modeling of Inorganic Compounds, Peter Comba, Trevor W. Hambley.

TCC 510 Computational Chemistry of Energy Materials

1. Energy Storage materials: (i) *Rechargeable Lithium Batteries:* Introduction, Overview of computational approaches, Li–ion batteries, Cell voltages and structural phase stability, Li–ion diffusion and defect properties, Surfaces and horphology, Layered cathode materials for Li- ion and Mg-ion batteries. (ii) *Hydrogen:* Introduction, Computational approach in hydrogen storage research, Chemisorption approach, Physisorption approach, Spillover approach, Kubas-Type approach.
2. Energy Conversion in Solid Oxide Fuel Cells: Introduction, Computational details, Cathode materials and reactions, Surfaces: $LaMnO_3$ and $(La,Sr)MnO_3$ Perovskites, Surface termination, Surface point defects, Oxygen adsorption and diffusion, Rate-determining step of the surface reaction, Bulk properties of multicomponent perovskites, Oxygen vacancy formation and migrarion in $(Ba,Sr)(Co,Fe)O_{3-\delta}$, Disorder and cation rearrangement in $(Ba,Sr)(Co,Fe)O_{3-\delta}$, Defects in $(La,Sr)(Co,Fe)O_{3-\delta}$, Ion transport in electrolytes, Reactions at SOFC anodes.
3. Heterogeneous Catalysis for Energy Conversion: Introduction, Particle size dependence of catalytic reactivity, Activity and selectivity as a function of the metal type, Reactivity as a function of state of the surface, Mechanism of acid catalysis: Single site versus dual site, Basic concepts of heterogeneous catalysis, Surface sensitivity in CH activation, Homolytic activation of CH Bonds, Heterolytic activation of CH bonds, Brønsted acid catalysis, Lewis acid catalysis, Surface sensitivity for the C−C bond formation, Transition metal catalyzed FT reaction, C−C bond formation catalyzed by zeolitic Brønsted acids, Structure and surface composition sensitivity: Oxygen insertion versus CH bond cleavage, Silver-catalyzed ethylene epoxidation, Benzene oxidation by iron-modified zeolite.
4. Solar Energy materials: Introduction, Thin-film photovoltaics, First-Principles methods for electronic excitations, Hedin's equations and the GW approximation, Hybrid functionals, Bethe–Salpeter Equation, Model Kernels for TDDFT, Examples of Applications, Cu-Based Thin-Film absorbers, Delafossite transparent conductive oxides.
5. Toward the Nanoscale: Introduction, Review of simulation methods, established computational methods, Evolutionary methods, GM methods, Amorphization and recrystallization, Nanoclusters (ZnO, ZnS, MnO_2, TiO_2) Nanoarchitectures (MnO_2) Nanoparticle (Nucleation and Crystallization), Properties of nanoporous materials (MnO_2, TiO_2 ZnS and ZnO).

Text Books

1. Computational Approaches to Energy Materials, Aron Walsh, Alexey A. Sokol, C. Richard and A. Catlow, John Wiley & Sons, Ltd, 2013.
2. Introduction to Fuel Cell Technology, Chris Rayment and Scott Sherwin, Department of Aerospace and Mechanical Engineering, University of Notre Dame, USA, 2003.

TCC 511 Chemoinformatics and Computational Chemical Biology

1. Chemoinformatics: Some trends in chemoinformatics. Molecular similarity measures. Similarity searching using 2D structural fingerprints. Predicting the performance of fingerprint similarity searching. Bayesian methods in virtual screening and chemical biology. Reduced graphs and their applications in chemoinformatics. Fragment descriptors in structure-property modeling and virtual screening. Pharmacore based virtual screening. Virtual ligand screening against comparative protein structure models. AMMOS software: method and application. Chemoinformatics processing of enzymatic transformations. The interweaving of chemoinformatics and HTS. Computational systems chemical biology.
2. Drug binding site prediction: A molecular dynamics ensemble-based approach for the mapping of druggable binding sites, Analysis of protein binding sites by computational solvent mapping.
3. Prediction of protein-Protein Docking and Interactions: AGGRESCAN: method, application and perspectives for chemical biology. ATTRACT and PTOOLS: open source programs for protein-protein docking.
4. Entropy, Solvent and Protonation: Estimation of conformational entropy in protein-ligand interactions: A computational perspective. Explicit treatment of water molecules in data-driven protein-protein docking: The solvated HADDOCKing approach. Protein-water interactions in MD simulations. Assignment of protonation states in proteins and ligands: combining pKa prediction with hydrogen bonding network optimization.
5. Toward the use of Robust Free Energy Methods in Chemical Biology: Best practices in free energy calculations. A practical guide to protein-drug binding free energy calculations. Free energy calculations from one step perturbations.

Text Books

1. Chemoinformatics and Computational Chemical Biology, Jürgen Bajorath (editor), Humana Press, Springer Science+Business Media, 2011.
2. Computational Drug Discovery and Design, Riccardo Baron (editor), Humana Press, Springer Science+Business Media, 2012.

TCC 521L Practical Computational Chemistry I

Computational study of the following topics will be done on PC using Gaussian and/or other software:

- Potential energy surface (PES).
- Ion-ion interactions, Ion-dipole interactions, dipole-dipole interactions, ion-induced dipole interactions, hydrogen bonding, temporary dipole-induced dipole interactions (dispersion force).
- Metal- ligand interations.
- UV-Vis, IR, Raman, NMR and CD spectra of some organic compounds.
- Solvation of ions.
- Structure, chemical composition and property relationship of crystalline solids

References

1. Exploring chemistry with electronic structure methods, 2nd edition, James B. Foresman and Aeleen Frisch, Gaussian Inc.
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, Francis A. Carey and Richard J. Sundberg, Springer, 2007.
3. Introduction to Spectroscopy, 3rd edition, L. Pavia, G. M. Lampman and G. S. Kriz, Thomson, 2001.
4. Modern Spectroscopy, 4th edition, Michael J. Hollas, Wiley 2004.
5. Inorganic Chemistry, G. L. Miessler and D. A. Tarr,Pearson Education Pvt. Ltd.
6. Fundamentals of Material Science and Engineering, W.D. Callister, John Wiley & Sons Inc.
   The Organometallic Chemistry of the Transition Metals,R. H. Crabtree, Wiley Interscience.

TCC 522L Practical Computational Chemistry II

Computational study of the following topics will be done on PC using Gaussian and/or other software:

- Homolytic and heterolytic fission
- Free radical substitution
- Electrophilic substitution
- Unimolecular and bimolecular nucleophilic substitution
- Electrophilic and nucleophilic addition
- Elimination reactions (E1 and E2)
- Hydrolysis of esters and amides
- Reaction mechanism of some specific reactions

References

1. Exploring chemistry with electronic structure methods, 2nd edition, James B. Foresman and Aeleen Frisch, Gaussian Inc.
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, Francis A. Carey and Richard J. Sundberg, Springer, 2007.
3. Organic Chemistry, 8th Edition, T. W. G. Solomons and C. B. Fryhle- John Wiley & Sons.
4. Organic Chemistry, 7th edition, William H. Brown, Brent L. Iverson, Eric V. Anslyn, Christopher S. Foote.
5. Frontier Orbital Theory: I. Fleming

TCC 523L Programming and software development

One or more programming language will be taught to develop software for solving problems in Chemistry.