Department / Institute	Department of Theoretical and Computa
Program	MS in Theoretical and Computational Ch
Syllabus	(2017-2018)
Followed Admission Year	2019-2020, 2018-2019, 2017-2018

SL	Course Type *	Course Prefix *	Course Code *
1	Lecturing	TCC	501

2	Lecturing	TCC	502

3	Lecturing	TCC	503

4	Lecturing	TCC	504

5	Lecturing	TCC	505

6	Lecturing	TCC	506

7	Lecturing	TCC	507

8	Lecturing	TCC	508

9	Lecturing	TCC	509

10	Lecturing	TCC	510

11	Lecturing	TCC	511

12	Laboratory	TCC	521L

13	Laboratory	TCC	522L

14	Laboratory	TCC	523L
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Course Title *	Year *	Semester *	Course Credit *
Quantum Chemistry	1st Year	N/A (Yearly)	3

Computational Chemistry I	1st Year	N/A (Yearly)	3

Computational Chemistry II	1st Year	N/A (Yearly)	3

Molecular Spectroscopy	1st Year	N/A (Yearly)	3

Statistical Thermodynamics	1st Year	N/A (Yearly)	3

Molecular Modeling and Drug Design	1st Year	N/A (Yearly)	3

Computational Methods in Reaction Mechanism	1st Year	N/A (Yearly)	3

Computational Biochemistry	1st Year	N/A (Yearly)	3

Molecular Modeling of Inorganic Compounds	1st Year	N/A (Yearly)	3

Computational Chemistry of Energy Materials	1st Year	N/A (Yearly)	3

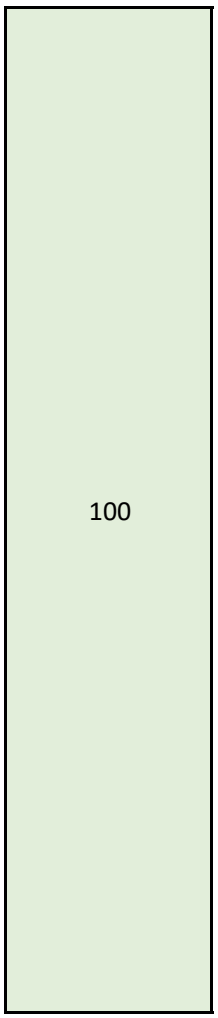
emoinformatics and Computational Chemical Biol	1st Year	N/A (Yearly)	3

Practical Computational Chemistry I	1st Year	N/A (Yearly)	3

Practical Computational Chemistry II	1st Year	N/A (Yearly)	3

Programming and Software Development	1st Year	N/A (Yearly)	3

Total Marks *
100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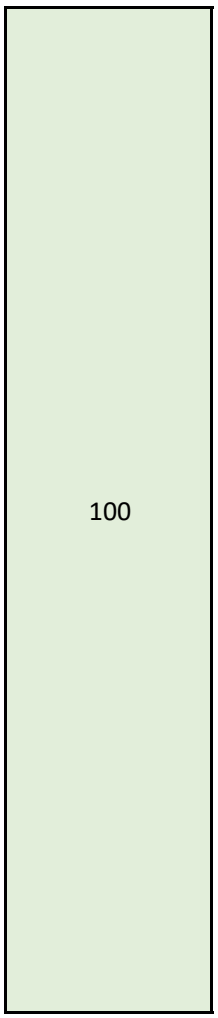
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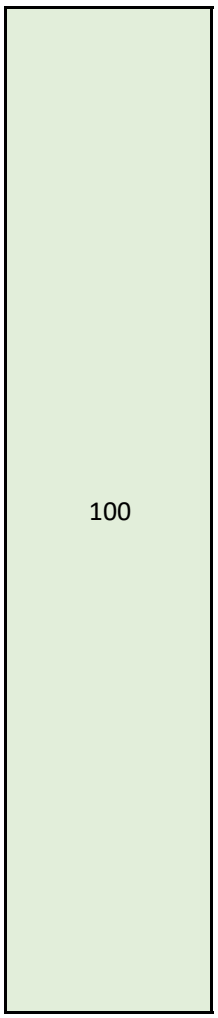
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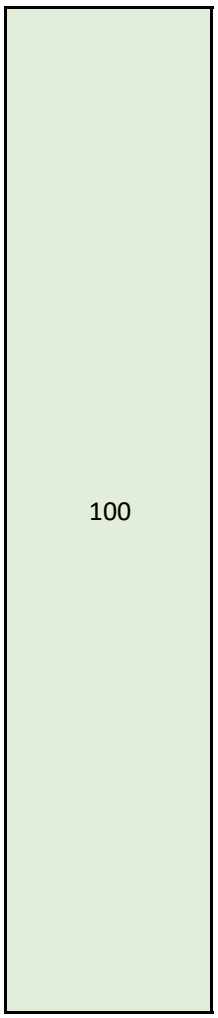
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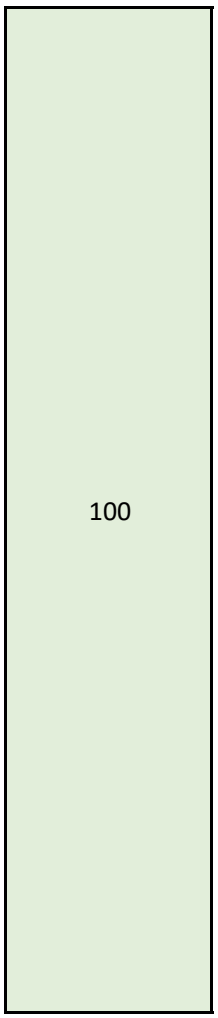
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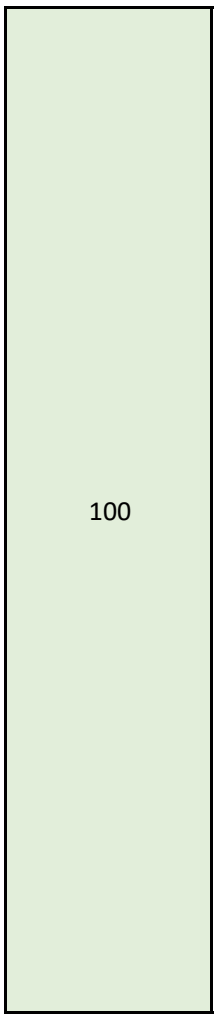
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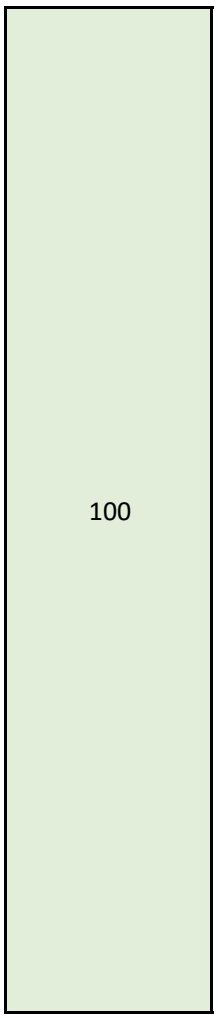
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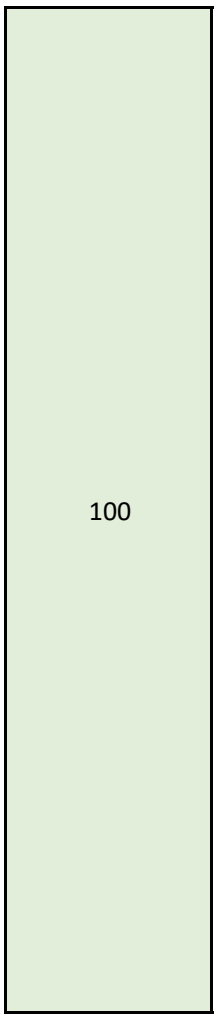
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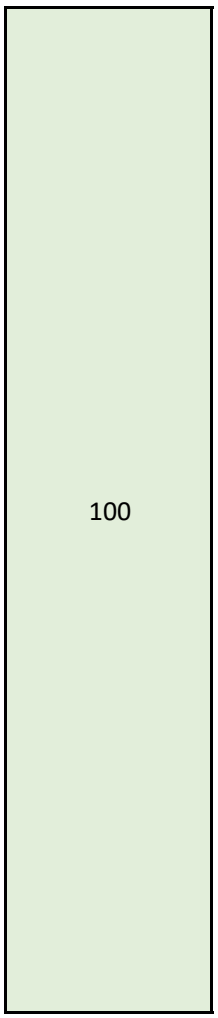
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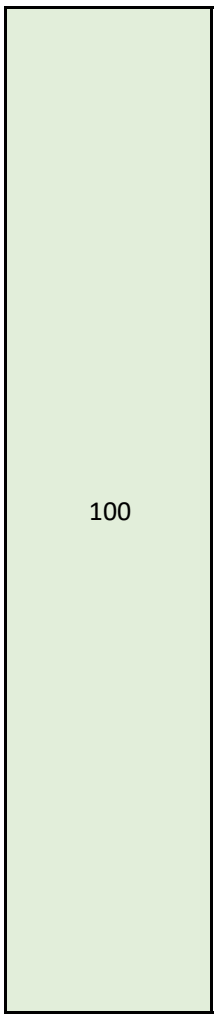
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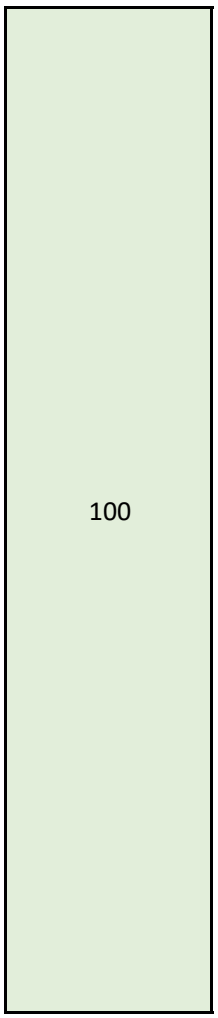
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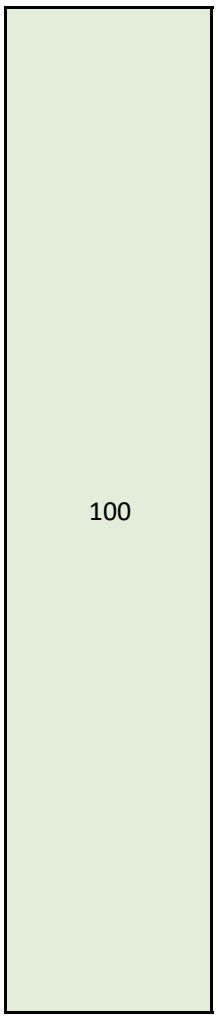
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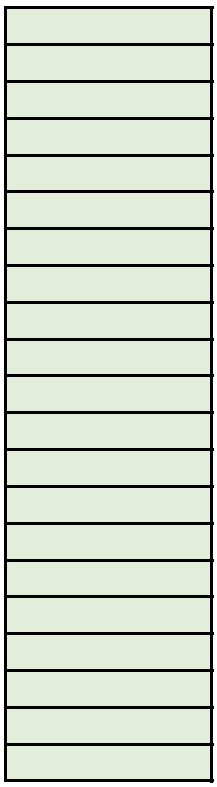

Course Outline

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

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.

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.

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 (1H 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 1H NMR absorption by various types of compounds.

5. Nuclear Magnetic Resonance Spectroscopy (13C NMR): The carbon-13 nucleus; carbon-13 chemical shifts; calculation of 13C chemical shifts; proton-coupled 13C spectra; spin-spin splitting of carbon-13 signals; proton-decoupled 13C spectra; Nuclear Overhauser Enhancement (NOE); cross-polarization: origin of the Nuclear Overhauser Effect; Analysis of some spectra.

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-

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; β1- and β2- 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.

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: SN1 Mechanism, SN2 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

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,

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.

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.

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

Introduction to Organic molecules, Functional groups and their structures
Lab on Molecular modeling and visualization with Gauss View 6.0
Lab on QM calculations with Gaussian.

Experiment 2 Getting started with calculations: Setting up and running calculation, energy calculation, interpreting energies and energy difference, dipole, higher dipole moments, molecular orbitals and modeling open shell systems.

Experiment 3 Structure and Analysis of organic Compounds: Survey of organic molecules, potential energy surface (PES) and single point energy calculation.

Experiment 4 Geometry Optimizations: geometry optimization of some organic molecules, Locating minima and maxima, convergence criteria, transition state calculations.

Experiment 5 Frequency Calculation: predict the infrared and Raman spectra of molecules (frequency and intensities calculation), characterizing stationary points, and compute zero point vibration and thermal energy correction.

Experiment 6 Basis set effects: Introduction different types of basis sets. Geometry optimization of some organic molecules with different basis sets and compares energies and find out the basis set effects of the molecules.

Experiment 7 Ion-ion interactions, Ion-dipole interactions, dipole-dipole interactions, ion-induced dipole interactions, hydrogen bonding, metal-ligand interactions, NMR calculation.

Experiment 8 Selecting an appropriate Theoretical method: Optimized geometry of some organic molecules with different methods, compare energy. Calculate HOMO-LUMO energies,

functional groups and their structures, Molecular modeling and visualization with Gauss View 6.0, QM calculations with Gaussian 16.

Experiment 2 Minimizing Molecular Structures: geometry optimization of some organic, convergence criteria, examining optimization results, locating transition structures, characterizing stationary points, interpreting normal mode information, strategies for handling difficult optimization cases.

Experiment 3 Modeling Large Systems (Gaussian ONIOM facility): Modeling QM: MM calculations of large molecule, ONIOM calculations of different transition metal complexes.

Experiment 4 Modeling Thermochemistry: Compound model chemistries for high accuracy energies, conformational searching and Boltzmann averaging, computing vibrational properties, compute zero point vibration and thermal energy correction.

Experiment 5 Methods and Basis set effects: Introduction different types of basis sets and methods, geometry optimization of some organic molecules with different basis sets, compares energies and find out the suitable method and basis sets.

Experiment 6 Predicting Chemical Properties: Modeling thermochemistry, predicting spectra of NMR, conformational searching, computing vibrational properties, IR and Raman Spectra.

Experiment 7 Modeling Chemistry in Solution: Continuum models of salvation, Properties in solution, predicting free energy in solution, predicting thermodynamic quantities.

Experiment 8 Predicting Free Energy Calculation: Free energy of solvation, solvation model based on SMD, including implicit and exclusive solvent model systems.

Programming in FORTRAN: Data Types, Constants, and Variables, Operation and Intrinsic Functions, Expressions and Assignment Statements, Numeric, Relational and Logical operations, Operator Precedence, single and mixed mode arithmetic, Fortran I/O and External Files.

Control Constructs: IF Constructs, Nested and Named IF Constructs, SELECT CASE Construct, Do Loops, Named and Nested Loops, Implied do loops.

Arrays and Programming Units: Declarations, Array Constructors, Array Sections, Array operations, Main Program, External Procedures, Internal Procedures, Subroutines, Functions.

Computing using FORTRAN: Construction and implementation of FORTRAN programs for solving problems in computational chemistry.
Books Recommended

1. Stephen J. Chapman, Introduction to FORTRAN 90/95.
2. Michael Metcalf, John Reid, Malcolm Cohen, Modern Fortran explained, Oxford University Press.
3. Gordon B. Davis & Thomas R. Hoffmann, FORTRAN 77: A Structured, Disciplined Style.