NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI

DEPARTMENT OF CHEMISTRY

COURSE PLAN – PART I			
Name of the programme and specialization	**M.Sc. (Chemistry)**		
Course Title	**Electronic Structure Methods for Molecular and Solid State Systems**		
Course Code	**CH 631**	**No. of Credits**	**2 Theory + 1 Lab**
Course Code of Pre-requisite subject(s)	**Basic knowledge in quantum chemistry is desirable**		
Session	**January 2021**	**Section (if, applicable)**	
Name of Faculty	**Dr. Sunandan Sarkar**	**Department**	**Chemistry**
Official Email	**ssarkar@nitt.edu**	**Telephone No.**	**9153484492**
Name of Course Coordinator(s) (if, applicable**)**	**Dr. R. Karvembu**		
Official E-mail	**kar@nitt.edu**	**Telephone No.**	**9442268653**
Course Type (please tick appropriately**)**	✓ **Core course**	☐ **Elective course**	

Syllabus (approved in BoS)

Ab initio Methods: The Hatree SCF method – the Hatree-Fock equations – Koopmans' theorem – the Roothaan equations – concept of basis sets, electron correlation and configuration interaction, post Hatree-Fock theories.

Density Functional Theory: Principles of DFT – the Hohenberg-Kohn theorems – the Kohn-Sam equations – local density approximation (LDA), exchange-correlation functionals – gradient corrected functionals, hybrid functional and range separated hybrid functionals, DFT methods for van der Waals interactions, general performance overview of DFT.

Molecular Properties and Analysis: Predicting molecular geometry, optimization algorithms, potential energy surfaces (PES), frequencies analysis, zero-point energies and thermodynamic corrections, population analysis, natural bond order (NBO) analysis, molecular electrostatic potential, multipole moments, estimation of electron affinity (EA) and ionization potential (IP), computing molecular orbitals energies. Molecules in complex environments – Polarizable Continuum Models (PCM).

Surfaces and Low Dimensional Solids: Modelling strategies of periodic solids – lattice constants optimization, surface reconstruction, computing band structures and band gaps, density of states, quantum confinement effect, electronic structure of 1D and 0D systems, modification of electronic gap – designing of hybrid nanostructures. Quantum mechanical simulation of large systems – density functional tight binding (DFTB) approach.

Electronic Excited States: Time-dependent methods, vertical excitations, computing transition dipole moment, dark and bright states, analysis of natural transition orbitals (NTOs), attachment and detachment

densities, properties of charge transfer states. Excited-state optimization, computing emission energy, crossing between potential energy surfaces, conical intersections, electronic couplings between excited states. Applications in LED and Solar cells.

Practical Sessions (Programming, Modelling and Simulation):
1. Bash command and shell scripting and the basic structure of FORTRAN program.
2. Molecular modelling and visualization techniques. Searching for minimum energy structure – geometry optimization and computing the potential energy surface.
3. Frequency calculations – predicting IR spectra, computing normal modes, zero-point energy and thermochemical analysis.
4. Determination of the basis set required to predict the accurate structure, Conventional solution to the basis set superposition error (BSSE) – counterpoise correction.
5. Single point calculations – Mulliken population, NBO analysis, electrostatic potential, multipole moments, IP and EA, energies of HOMO and LUMO.
6. Basic of periodic system calculation – super cell approach, lattice parameter optimization, computing band structure, surface reconstruction, calculation of low dimensional solids.
7. Calculation of excited states properties – computing absorption spectra, visualization and plotting of attachment and detachment densities, characterization of charge transfer states.
8. Excited state geometry optimization – computing the emission energy. Solvent effects.

COURSE OBJECTIVES Introduction to electronic structure methods (quantum chemical approach) for molecular and solid state systems and their use in designing the efficient materials for potential applications.

MAPPING OF COs with POs

Course Outcomes	**Programme Outcomes (PO)** (Enter Numbers only)
Upon completing the course the student will be able to	
1. Explain the most important concepts of electronic structure theory	**PO1, PO3, PO4, PO7, PO8**
2. Understand the structure and reactivity of chemical and biological systems	**PO2, PO3, PO4, PO7, PO8**
3. Discuss the structural and physical properties of solids in different dimensions	**PO3, PO4, PO7, PO8**
4. Design and optimize the efficient materials for specific potential applications	**PO3, PO4, PO7, PO8, PO10**

COURSE PLAN – PART II

COURSE OVERVIEW

This course is offered as a elective course. This is a 2 credit theory and 1 credit lab course and three classes will be conducted per week.

COURSE TEACHING AND LEARNING ACTIVITIES (Add more rows)

S.No.	**Week/Contact Hours**	**Topic**	**Mode of Delivery**
1	III week of January	**Ab initio Methods:** Spin Operators, concept of Spin orbitals	Online

2	III week of January	Hartree product wavefunctions Many electronic wavefunctions	Online
3	IV week of January	Ground state and excited state energies of 2e systems, Concept of Singlet and Triplet states	Online
4	I week of February	The Hatree SCF method – the Hatree-Fock equations - Koopmans' theorem – the Roothaan equations	Online
5	II week of February	concept of basis sets, electron correlation and configuration interaction, post Hatree-Fock theories.	Online
6	III week of February	**Density Functional Theory:** Principles of DFT – the Hohenberg-Kohn theorems – the Kohn-Sam equations	Online
7	IV week of February	local density approximation (LDA), exchange-correlation functionals – gradient corrected functionals,	Online
8	I week of March	hybrid functional and range separated hybrid functionals, DFT methods for van der Waals interactions, general performance overview of DFT.	Online
9	II week of March	**Molecular Properties and Analysis:** Predicting molecular geometry, optimization algorithms, potential energy surfaces (PES), frequencies analysis, zero-point energies and thermodynamic corrections,	Online
10	III week of March	population analysis, natural bond order (NBO) analysis, molecular electrostatic potential, multipole moments, estimation of electron affinity (EA) and ionization potential (IP), computing molecular orbitals energies. Molecules in complex environments – Polarizable Continuum Models (PCM).	Online
11	IV week of March	**Surfaces and Low Dimensional Solids:** Modelling strategies of periodic solids – lattice constants optimization, surface reconstruction, computing band structures and band gaps, density of states, quantum confinement effect, electronic structure of 1D and 0D systems,	Online
12	I week of April	modification of electronic gap – designing of hybrid nanostructures. Quantum mechanical simulation of large systems – density functional tight binding (DFTB) approach.	Online
13	II week of April	**Electronic Excited States:** Time-dependent methods, vertical excitations, computing transition dipole moment, dark and bright states, analysis of natural transition orbitals (NTOs), attachment and detachment densities, properties of charge transfer states.	Online
14	III week of April	Excited-state optimization, computing emission energy, crossing between potential energy surfaces, conical intersections, electronic couplings between excited states. Applications in LED and Solar cells.	Online

15	I week of March	**Practical Sessions** (Programming, Modelling and Simulation): Bash command and shell scripting and the basic structure of FORTRAN program.	Online
16	II week of March	Molecular modelling and visualization techniques. Searching for minimum energy structure – geometry optimization and computing the potential energy surface. Determination of the basis set required to predict the accurate structure, Conventional solution to the basis set superposition error (BSSE) – counterpoise correction.	Online
17	III week of March	Frequency calculations – predicting IR spectra, computing normal modes, zero-point energy and thermochemical analysis.	Online
18	IV week of March	Single point calculations – Mulliken population, NBO analysis, electrostatic potential, multipole moments, IP and EA, energies of HOMO and LUMO.	Online
19	I week of April	Basic of periodic system calculation – super cell approach, lattice parameter optimization, computing band structure, surface reconstruction, calculation of low dimensional solids.	Online
20	II week of April	Calculation of excited states properties – computing absorption spectra, visualization and plotting of attachment and detachment densities, characterization of charge transfer states.	Online

COURSE ASSESSMENT METHODS (shall range from 4 to 6**)**

S.No.	Mode of Assessment	Week/Date	Duration	% Weightage
Theory				
1	Test 1	I week of Mar	60 minutes	25
2	Assignment 1	II week of Feb	2 days	10
3	Test 2	II week of April	60 minutes	25
CPA	Compensation Assessment*	III week of April	60 minutes	25
3	Final Assessment *	II week of May	2 hours	30
Practicals				
4	LAB assessment (viva-voce)	IV week April	3 hours (10 minutes)	10

***mandatory; refer to guidelines on page 4**

COURSE EXIT SURVEY (mention the ways in which the feedback about the course shall be assessed)

1. Feedback from students during class committee meetings.
2. Anonymous feedback through questionnaire at the end of the semester.

COURSE POLICY (including compensation assessment to be specified)

MODE OF CORRESPONDENCE (email/ phone etc)
ssarkar@nitt.edu; Tel. No.:9153484492
COMPENSATION ASSESSMENT POLICY
1. This assessment is for those students who missed Test I/II due to genuine reasons.
2. Compensation assessment will be conducted during the III week of April.

ATTENDANCE POLICY (A uniform attendance policy as specified below shall be followed)

- At least 75% attendance in each course is mandatory.
- A maximum of 10% shall be allowed under On Duty (OD) category.
- Students with less than 65% of attendance shall be prevented from writing the final assessment and shall be awarded 'V' grade.

ACADEMIC DISHONESTY & PLAGIARISM

- Possessing a mobile phone, carrying bits of paper, talking to other students, copying from others during an assessment will be treated as punishable dishonesty.
- Zero mark to be awarded for the offenders. For copying from another student, both students get the same penalty of zero mark.
- The departmental disciplinary committee including the course faculty member, PAC chairperson and the HoD, as members shall verify the facts of the malpractice and award the punishment if the student is found guilty. The report shall be submitted to the Academic office.
- The above policy against academic dishonesty shall be applicable for all the programmes.

ADDITIONAL INFORMATION, IF ANY

FOR APPROVAL

Dr. Sunandan Sarkar
S. Sarkar
Course Faculty _____ **CC- Chairperson** _____ **HOD** _____ 05/02/2021

Guidelines

a) The number of assessments for any theory course shall range from 4 to 6.

b) Every theory course shall have a final assessment on the entire syllabus with at least 30% weightage.

c) One compensation assessment for absentees in assessments (other than final assessment) is mandatory. Only genuine cases of absence shall be considered.

d) The passing minimum shall be as per the regulations.

B.Tech. Admitted in				P.G.
2018	2017	2016	2015	
35% or (Class average/2) whichever is greater.		(Peak/3) or (Class Average/2) whichever is lower		40%

e) Attendance policy and the policy on academic dishonesty & plagiarism by students are uniform for all the courses.

f) Absolute grading policy shall be incorporated if the number of students per course is less than 10.

g) Necessary care shall be taken to ensure that the course plan is reasonable and is objective.