1.	Title of the course	Modern Electronic Structure Methods and Applications
2.	Course number	CY612L
3.	Structure of credits (L-T-P-C)	3-0-0-3
4.	New course/modification to	Modified with CY516L/COMPUTATIONAL METHODS IN MATERIALS SCIENCE
5.	To be offered by	Chemistry
6.	Prerequisite	CoT
7.	**Course Objective(s):** To introduce state-of-the-art electronic structure methods and their implementations to study complex structure-property relationships in atoms, molecules and solids through hands-on exercises.	
8.	**Course Content:** Electronic structure methods for many-electron systems; Wavefunction based ab initio methods: Hartree-Fock theory and post Hartree-Fock ones, Koopmans' theorem, static and dynamic correlation; First-principles density functional theory (DFT) and time-dependent DFT (TDDFT): Kohn-Sham and generalized Kohn-Sham formalisms, Janak's theorem, exchange-correlation hole, exchange-correlation functionals and TDDFT kernels, basis sets; Pseudopotentials: norm-conserving and ultrasoft ones; Applications: electronic structure of atoms, molecules, nanostructures and solids.	
9.	**Textbook(s):** 1. Szabo A and Ostlund N S, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications Inc. (1996). 2. Martin R M, Electronic Structure: Basic Theory and Practical Methods, 2nd Edition, Cambridge University Press (2020).	
10.	**Reference(s):** 1. Ullrich C A, Time-Dependent Density Functional Theory: Concepts and Applications, Oxford University Press (2019). 2. Parr R G and Yang W, Density-Functional Theory of Atoms and Molecules, Oxford University Press (1989).	