1.	Title of the course	Computational Methods in Materials Science
2.	Course number	CY516L
3.	Structure of credits	3-0-0-3
4.	Offered to	PG
5.	New course/modification to	Modification To CY5023/6
6.	To be offered by	Department of Chemistry
7.	To take effect from	July 2022
8.	Prerequisite	Nil
9.	**Course Objective(s):** In addition to the underlying theory, this course will also provide hands-on experiences on some of the state-of-the-art computer simulation methods used to study chemical, physical, biochemical systems. Particular emphasize will be given to solve problems in materials science	
10.	**Course Content:** Classical Molecular Simulation: Ensemble, Molecular Dynamics, Monte Carlo techniques, Metropolis method, Hybrid Monte Carlo, Wang-Landau sampling, Applications: Lennard-Jones system and Ising model Free Energy Calculations: Umbrella sampling, WHAM analysis, Transition Matrix Monte Carlo, Metadynamics Quantum Simulations for Multi-electronic Systems (Atoms, Molecules, and Solids): Wave function theory (WFT), Density functional theory (DFT), Exchange correlation functionals, Basis Sets, Basics of solids state physics, Pseudopotentials, Applications in atoms, molecules, nanostructures and solids.	
11.	**Textbook(s):** 1. Daan Frenkel, Berend Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press (Computational Science), (2001). 2. Robert G. Parr, Weitao Yang, Density-Functional Theory of Atoms and Molecules, Oxford University Press, (1989).	
12.	**Reference(s):** 1. Attila Szabo, and Neil S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications Inc., (1996). 2. Allen M P, and Tildesley D J, *Computer Simulation of Liquids*, Oxford University Press (2007).	