1.	Title of the course	Classical Molecular Simulation Methods and Applications
2.	Course number	CY611L
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 molecular simulations and the state-of-the-art classical computer simulation methods used to study chemical, physical, and biochemical systems. To provide experiences on updated molecular simulation methodologies and strategies for enhancing efficiency.	
8.	**Course Content:** Phase-space, ensembles; Molecular modelling: hard potentials, soft potentials, multiatomic models; Forcefields: bonded and nonbonded interactions, polarizability; Monte Carlo techniques, Metropolis method, hybrid Monte Carlo, importance sampling, Markov chains; Molecular dynamics (MD) simulations, algorithms for time integration, methods for long-range electrostatic interactions; Thermostats; Barostats; Free energy calculations: umbrella sampling, histogram analysis, metadynamics and thermodynamic integration; Coarse-graining, multiscale methods, rare events algorithms, transition path sampling, hybrid MD; Development of forcefields; Applications in soft condensed matter, materials, and biophysical chemistry.	
9.	**Textbook(s):** 1. Allen M P and Tildesley D J, Computer Simulation of Liquids, 2nd Edition, Oxford University Press (2017). 2. Frenkel D and Smit B, Understanding Molecular Simulation: From Algorithms to Applications, 3rd Edition, Academic Press Inc (2023).	
10.	**Reference(s):** 1. Leach A R, Molecular Modelling: Principles and Applications, 2nd Edition, Pearson (2009). 2. Rapaport D C, The Art of Molecular Dynamics Simulation, 2nd Edition, Cambridge University Press (2004). 3. Graham C and Talay D, Stochastic Simulation and Monte Carlo Methods, Springer (2013).	