1.	Title of the course	Introduction to Molecular Dynamics Simulations
2.	Course number	CH512L
3.	Structure of credits	2-1-0-3
4.	Offered to	PG
5.	New course/modification to	Modification To CH5032/21
6.	To be offered by	Department of Chemical Engineering
7.	To take effect from	July 2022
8.	Prerequisite	CoT
9.	**Course Objective(s):** To introduce the concepts of atomistic simulation techniques and apply them to process systems.	
10.	**Course Content:** Introduction to thermodynamics and statistical mechanics; Introduction to molecular dynamics; Numerical differentiation; Numerical integration and optimization: velocity Verlet, leapfrog, steepest descent, conjugate gradient; Probability density function; Ensembles: canonical, microcanonical, grand canonical; Interaction modelling: bonded and non-bonded, Coulombic, particle mesh Ewald method; Topology and simulation parameters; Periodic boundary conditions; Radial distribution function; Auto-correlation functions; Applications: fluid phase equilibria, transport of ions/molecules at pore scale, polymeric materials, crystalline materials.	
11.	**Textbook(s):** 1. Alavi S, *Molecular Simulations: Fundamentals and Practice*, 1st Edition, John Wiley & Sons (2020). 2. Frenkel D and Smit B, *Understanding Molecular Simulation: from Algorithms to Applications*, 2nd Edition, Academic Press (2001).	
12.	**Reference(s):** 1. Haile J M, *Molecular Dynamics Simulation: Elementary Methods*, 1st Edition, Wiley (1997). 2. Tuckerman M, *Statistical Mechanics: Theory and Molecular Simulation*, 1st Edition, Oxford University Press (2010).	