INDIAN INSTITUTE OF TECHNOLOGY TIRUPATI
PROFORMA FOR NEW COURSE

1.	Title of the Course	Computational Methods in Materials Science
2.	Course Number	CY5023
3.	Status of the Course	Elective
4.	Structure of Credits	3-0-0-3
5.	Offered To	PG
6.	New Course/Modification to	New
7.	To be Offered by	Dr. Rajib Biswas and Dr. Arun K Manna
8.	To take effect from	January 2019
9.	Prerequisite	Nil
10.	Whether approved by the Department	Yes
11.	**Course Objective:** 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.	
12.	**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.	
13.	Text book(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).	
14.	Reference(s): 1. Attila Szabo, Neil S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory,* Dover Publications Inc., (1996). 2. M. P. Allen, D. J. Tildesley, *Computer Simulation of Liquids,* Oxford University Press, (2017).	