[A-3]COURSE SYLLABUS

1. Course Description (Approximately 100 words)

This course deals with computations that deal with the applications of statistical mechanics of chemical problems. The molecular dynamics method, constrained dynamics and simulations on liquid Ar and water are considered in detail. The Monte Carlo method for thermodynamic properties and its applications for the evaluation of integrals is considered next. Biomolecular simulations include applications to polypeptide conformations and structures of RNA and DNA.

2. Course Goals and Objectives (Approximately 100 words)

Invent new algorithms to globally optimize at the worldwide level the use of raw materials, energy, and environmental impact of chemical processes.

Develop new and powerful computational methods, applicable from the atomic and molecular level to the chemical process and enterprise level, that will enable multiscale optimization.

3. Textbook (Title, Author, Publisher, Year of Publication, etc.)

Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Sep 21, 2016 by Errol G. Lewars

4. Reference

Introduction to Computational Chemistry Feb 6, 2017 by Frank Jensen

5. Course Requirements and Grades

CAT 30%
EXAM 70%

6. Course Calendar

Week	Main Content
1	Potential Models
2	Concept of Periodic Boundary Conditions (PBC)
3	Generalized coordinates
4	Solution of equations of motions using Finite Difference Methods
5	Basics of Statistical Mechanics - concept of ensemble; time average vs. ens
6	Concept of Temperature in simulations
7	Development of a molecular dynamics (MD) code for Lennard-Jones fluids
8	MID-TERM EXAM
9	Monte Carlo (MC) method,Development of a MC code, Analysis of simulatec
10	Polypeptide conformations - I (Aqueous and non aqueous media)
11	Polypeptide conformations – II
12	Polypeptide conformations – III
13	Structure of DNA and RNA-I, Structure of DNA and RNA-II
14	FINAL EXAMINATION