School of Interdisciplinary Engineering and Sciences (SINES)
National University of Sciences & Technology (NUST)

Title: Computational Chemistry

Objectives: The goal is to acquire knowledge in Computational Chemistry and some basic skills to solve problems of chemical interest. Except for learning some basic theoretical models, the emphasis is to learn about its maximum possible applications. This course is designed so that the students will learn a variety of commonly used computational chemistry techniques, such as geometry optimization, location of transition states, conformational analysis, and prediction of possible reaction mechanisms.

Outcomes: At the end of the course students will be able to

a) Decide how the problem in hand would be modeled
b) Which software to choose
c) Which computational methods are suitable for simulations
d) Analyze the simulation data

Course Code: CSE-878

Credit Hours: 3-0

Course Contents:

1. Introduction
2. Methods used in Computational Chemistry
3. Combined QM/MM Methods
4. Model selection and performance
5. Applications of Computational Chemistry

Course Contents with proposed contact Hours (Weekly plan):

Lecture wise Breakdown (1 Hour Lectures + 2 Hours Lab)/ Week

W#1	Topics	Lect #
1	Introduction to Computational Chemistry	01
2	Potential Energy Surface	02
3	Geometry Optimization	03
4	Computational Chemistry Methods using HPC a. Classical Methods i. Molecular Mechanics	04
5	Computational Chemistry Methods using HPC a. Classical Methods i. Molecular Mechanics	05
6	Assignment Computational Chemistry Methods using HPC a. Classical Methods i. Molecular Mechanics	06
7	Computational Chemistry Methods using HPC a. Classical Methods i. Molecular Mechanics	07
8	Computational Chemistry Methods using HPC b. Quantum Mechanics	08

9	MID SEMESTER EXAM	
10	Computational Chemistry Methods using HPC b. Quantum Mechanics	09
11	Computational Chemistry Methods using HPC c. Combined QM/MM Methods	10
12	Computational Chemistry Methods using HPC d. Combined QM/MM Methods	11
13	Optimization Techniques	12
14	Optimization Techniques	13
15	Model Selection and Performance	14
16	Application of Computational Chemistry in various fields	15
17	Presentations + Revision + Problem Solving	16
18	**End Term** ☺	

Details of lab work/workshop practice, if applicable:

Lab sessions will mainly focus on the hands-on training in connection with the lectures taught in class.

Recommended reading, including textbooks, reference books with dates

1. "Introduction to Computational Chemistry", Frank Jensen, 3rd Edition, Wiley, **2016**
2. "Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics" Errol G. Lewars, 3rd Edition, Springer, **2016**
3. "Essentials of Computational Chemistry", 2nd Edition, Christopher J. Cramer, John Wiley and Sons, Ltd, **2002**.
4. "Molecular Modeling: Principles and Applications", 2nd Edition, Andrew Leach, Pearson, **2001**
5. "Encyclopedia of Computational Chemistry", 5th volume, John Wiley and Sons, Inc. **1998**.
6. "Practical Strategies for Electronic Structure Calculation", Warren J. Hehre, Wavefunction, **1995**.
7. "Ab initio molecular orbital theory" Warren J. Hehre, Random, P. V. R. Schleyer and J. A. Pople, John Wiley and Sons, **1985**.

Nature of Assessments

Homework/ Assignments:	5%
Quizzes:	5%
MSE:	30%
Final Exam:	40%
Project:	20%