

## CH-907 Advanced Physical Chemistry

Credit Hours: 3-0

**Prerequisite: Nil**

### **Course 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.

### **Course Outcomes**

Students will learn the core concepts of computational chemistry and learning basic principles and methods used for Computational chemistry and Computer-based molecular design. Students will also learn to use a series of open source tools and libraries and apply them for Molecular Modeling and Simulations. This course covers the basic theories need for computation followed by molecular mechanical and quantum mechanical model theories.

### **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

### **Recommended Books**

1. "*Molecular Modeling: Principles and Applications*", 2nd Edition, Andrew Leach, Pearson
2. "*Encyclopedia of Computational Chemistry*", 5th volume, John Wiley and Sons, Inc.

3. "*Practical Strategies for Electronic Structure Calculation*", Warren J. Hehre, Wavefunction,

1995.

4. "*Ab initio molecular orbital theory*" Warren J. Hehre, Random, P. V. R. Schleyer and J. A. Pople, John Wiley and Sons, 1985.

5. "*Essentials of Computational Chemistry*", 2nd Edition, Christopher J. Cramer, John Wiley and Sons, Ltd, 2002.