20CY114 COMPUTATIONAL CHEMISTRY LAB

Hours Per Week :

L	T	P	C
-	-	4	2

Course Description and Objectives:

This course bring the hands on experience on various computational tools which are essential for this modern era to execute the research task in chemistry. Also, this lab will teach the role of computer in the research field of chemistry.

Course Outcomes:

The goal of this lab course is to provide the hands on experience in the molecular modeling. Upon completion of the course the student will be able to:

COs	Course Outcomes
1	Understand the basics of computer in chemistry
2	Utilize the tools available for chemical problems
3	Apply the chemical knowledge to draw various chemical structures using the software.
4	Analyze 2D & 3D chemical structures
5	Explore various chemical and protein databases

1. Explore the MS office (Word Doc).

2. Explore the MS office (Power point).

3. Explore the MS office (Excel).

4. Installation of Chem-sketch or Chem-draw.

5. Draw the chemical structures using Chemsketch (Open chain compounds).

6. Draw the chemical structures using Chemsketch (Cyclic compounds).

7. Analyse various chemical databases.

8. Understand and analyze protein data bank (PDB).

9. GAMESS (http://www-jmg.ch.cam.ac.uk/cil/gamess/dft.html).

10. Draw the chemical structures using VESTA.

11. QunatumEspresso (https://www.quantum-espresso.org/)

Reference Books:

1. http://www-jmg.ch.cam.ac.uk/cil/gamess/dft.html

2. https://www.quantum-espresso.org/

3. A Handbook of Computational Chemistry – A Practical Guide to Chemical Structure and Energy Calculations by Tim Clark.

4. Density Functional Theory: A Practical Introduction. Authors: David S. Sholl and Janice A. Steckel, 2009 (WILEY).

5. The ABC of DFT. Author: Kieron Burke