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

Title: Modeling of Cluster Compounds

Objectives: The objectives of modeling of cluster compounds involve gaining insights into their structures, stability, bonding, reactivity, and spectroscopic properties. This knowledge aids in the interpretation of experimental data, the design of new cluster compounds, and the exploration of their potential applications in various fields, including catalysis, materials science, and nanotechnology.

Outcomes: At the end of this course, students will have broad knowledge of synthesis, applications, theoretical concepts, and computational studies of clusters of main block elements including boron hydride clusters, heteroboranes and macropolyhedral boranes.

Course Code: CSE-913

Credit Hours: 3-0

Course Contents:

1. Molecular Clusters
2. Theory and Concepts in Main-Group Cluster Chemistry
3. Homonuclear Boron Clusters
4. Steric effects in Metallocarbanes
5. Cluster of heavy group elements
6. Cages and clusters of heavy group elements
7. Chalcogenes clusters and cages
8. Clusters of transition metals and their applications
9. Fullerenes
10. Iron-Sulfur clusters in Biology

Course Contents with proposed contact Hours (Weekly plan):

Lecture wise Breakdown

W#1	Topics	Lect #
1	a. Overview of Cluster Chemistry b. Computational Methods	1-2
2	Theory and Concepts in Main-Group Cluster Chemistry	3-4
3	Homonuclear Boron Clusters a. Boron Hydride Chemistry b. 2e-3c bonding in Boranes c. Heteroboranes	5-6
4	a. Wades-Williams Formalism b. Macropolyhedral Boranes c. Stabilities of Macropolyhedral boranes relative to Single Clusters	7-8
5	a. The mno rule b. Major unexplored research areas in the chemistry of Boron Hydride Clusters c. Applications of Boron Hydride Clusters	9-10
6	Steric effects in Metallocarbanes	11-12

7	Stability of Metallocarbanes	13-14
8	Revision	15-16
9	**Mid Semester Exam**	17-18
10	Cluster of heavy group elements a. Borane analogues b. Clusters of aluminium, gallium and indium c. Cages and clusters of Group-14 elements	19-20
11	a. Clusters of silicon, germanium, tin and lead b. Computational studies of Group-14 clusters	21-22
12	Cages and clusters of heavy group elements a. P_n cages b. Cationic P_n^+ and As_n^+ clusters c. Bi clusters Computational studies of Group-15 clusters	23-24
13	Chalcogenes clusters and cages	25-26
14	Clusters of transition metals and their applications	27-28
15	Fullerenes	29-30
16	Iron-Sulfur clusters in Biology	31-32
17	Presentations + Revision + Problem Solving Assignment-1: Paper Submission	33-34
18	**End Term** ☺	35-36

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. Details are mention in the week wise breakdown.

Nature of Assessments

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