Correlating symmetry and functionality of molecules

Course Title	Correlating symmetry and functionality of molecules	
Course Category	Pedagogy / Specialized Skills/ Research/ Generalized skills	
Relevant Discipline(s)	Chemistry/Chemical Engineering/Materials Science & Engineering	
Duration of course in equivalent integer no. of days (min 3 days, 1 day = 6 hrs of lectures/hands on sessions)	3 days (the actual classes will be scheduled over 6 days: 3 hours class on each day)	
Proposed dates	Class 1: 27 th November, 2020 6-9 PM Class 2: 28 th November, 2020 6-9 PM Class 3: 29 th November, 2020 6-9 PM Class 4: 4 th December, 2020 6-9 PM Class 5: 5 th December, 2020 6-9 PM Class 6: 6 th December, 2020 6-9 PM	

Brief Course Description and Course Contents

Module 1. Visualizing molecules through the lens of symmetry

In this module, we will try to explore the structure-function properties of molecules via the fundamental symmetric elements. Here, we will cover the following topics as per the following schedule:

Class 1 (3 hours Lecture)

- A. The connection between mathematics and chemistry
- B. Classification of molecules by point groups

Class 2 (3 hours Lecture)

- C. Description of Character Table and its use for differentiating molecules
- D. Generating Molecular Orbital (MO) diagrams with point group symmetry

Class 3 (3 hours practical session)

- E. Predicting the pattern of FTIR/Raman signals for metal carbonyl complexes
- F. Developing the MO diagram of transition metal complexes of variable geometry (Octahedral, Tetrahedral, Square planar) from the scratch

Module 2. Connecting the Chirality and Symmetry and their practical applications

In the second section of the class, we will discuss one of the critical parameter of molecules: the chirality as per the following schedule.

Class 4 (3 hours Lecture)

- A. The significance of Chirality
- B. Symmetric representation of chirality

- C. Monitoring chirality via optical rotation and circular dichroism (CD) spectroscopy *Class 5 (3 hours Lecture)*
- D. The molecular origin of CD spectroscopy
- E. The effect of magnetic field on CD spectroscopy
- F. Probing the secondary structures of proteins and DNA by CD spectroscopy

Class 6 (3 hours practical session)

G. Analyzing changes in the protein structures in solution via CD spectroscopy to comprehend biological implications of protein folding

The class notes and other reading materials will be provided during the class.

Instructor Details			
S.	Name of the	Departmen	Email
No.	Instructor	t	
1	Arnab Dutta	Chemistry	arnabdutta@chem.iitb.ac.i
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