ADD-ON COURSE
OFFERED BY THE DEPARTMENT OF CHEMISTRY
BIJNI COLLEGE::BIJNI

Course Title	: Avogadro Software Learning in Chemistry
Course Code	: ASLC-101
Course Duration	**:** 30 Hours
Credit	: 2(1 Credit = 15 Hrs.)
Course Designed by	: Dipak Bhattacharyya, HoD & Assistant Professor
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Course Co-ordinator	**:** Mr. Nikhilesh Sutradhar, Assistant Professor
Approved by	**:** Governing Body, Bijni College, Bijni
Date of Approval	**:** 14-02-2025

Course Description:

The course deals with theoretical and practical studies on Avogadro a software. It teaches about application of the Avogadro software. It is a molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It is extensible via a plugin architecture,

Course Objectives:

- To equip undergraduate students with basic knowledge and skills related
- To chemical structure building and visualization using Avogadro software.
- To promote hands-on digital learning practices in chemistry.
- To enhance students' capability in applying software tools in chemical education and research.

Course Outcomes:

- Students were introduced to the Avogadro software interface and its tools for 3D molecular design.
- They learned to build molecular structures, perform geometry optimization, and visualize orbitals and vibrations.
- The course helped students build confidence in using chemical drawing software relevant for higher studies and research.
- Certificates were awarded to students after successful completion and evaluation.

Course Structure:

Day 1: Installing and Exploring Avogadro

- Download and install Avogadro from the official website.
- Understand the user interface: menu bar, toolbar, and 3D workspace.
- Learn how to rotate, zoom, and pan molecules.
- Resources: Watch beginner tutorials, read Avogadro documentation.

Day 2: Understanding File Formats and Basic Functions

- Open and save molecular structures in different formats (. cml, .xyz, .pdb).
- Use the undo/redo and reset view functions.
- Learn about coordinate systems in molecular visualization.
- Practice opening and modifying sample molecules from Pub Chem.

Day 3: Drawing Simple Molecules

- Use the drawing tool to create simple molecules like H_2O, CH4.
- Understand atomic valency and bond formation.
- Follow step-by-step tutorials and compare with real structures.

Day 4: Modifying Molecular Structures

- Add, remove, and modify atoms and bonds.
- Change hybridization states (e.g., sp^3, sp^2, sp).
- Adjust bond angles and torsions.
- Use the 'Auto Optimization' feature for corrections.

Day 5: Molecular Representations

- Explore ball-and-stick, space-filling, and wireframe models.
- Use element-based color schemes.
- Compare different representations for clarity.

Day 6: Customizing Visuals

- Change background color, labels, and display modes.
- Add element symbols and charge indicators.
- Experiment with visualization settings.

Day 7: Measuring Molecular Geometry

- Measure bond lengths, angles, and torsions.
- Use the 'Measure Tool' in Avogadro.
- Compare measured values with theoretical data.

Day 8: Geometry Optimization

- Perform molecular energy minimization using force fields.
- Understand why optimization is important.

- Compare structures before and after optimization.

Day 9: Calculating Basic Molecular Properties

- Find molecular mass, charge, and dipole moment.
- Use Avogadro's built-in property calculator.

Day 10: Understanding Electron Density and Surfaces

- Generate molecular surfaces and electron density maps.
- Load an example molecule and generate an electrostatic potential surface.

Day 11: Running Basic Quantum Chemistry Calculations

- Set up calculations (e.g., energy minimization, HOMO-LUMO orbitals).
- Choose force fields and methods (e.g., MMFF94, UFF).
- Run small calculations and analyze the output.

Day 12: Interpreting Results

- Understand energy values, dipole moments, and molecular orbitals.
- Compare optimized vs. non-optimized molecular structures.

Day 13: Vibrational Modes and IR Spectra

- Run vibrational frequency analysis.
- Interpret IR spectrum data.
- Compare vibrational modes of different molecules.

Day 14: Using Plugins and Extensions

- Explore available plugins for extended functionality,
- Install and test additional features in Avogadro.

Day 15: Building a Complex Molecule

- Construct a larger molecule like an amino acid or a simple drug molecule.
- Apply all learned skills in a practical project.

Day 16: Final Review and Next Steps

- Troubleshoot any issues encountered.
- Explore advanced learning resources.
- Review notes and practice on real-world molecules.

Suggested Readings:

1. "Avogadro 1.95.1 Released". GitHub. August 26, 2021. Retrieved September 24, 2021.
2. Hanwell, Marcus D; Curtis, Donald E; Lonie, David C; Vandermeersch, Tim; Zurek, Eva; Hutchison, Geoffrey R (2012). "Avogadro: An advanced semantic chemical editor, visualization, and analysis platform". J. Chemin form. **4** (1): 17. doi:10.1186/1758-2946-4-17. PMC 3542060. PMID 22889332.
3. Michael Salciccioli; Weiting Yu; Mark A. Barteau; Jingguang G. Chen; Dionisios G. Vlachos (2011). "Differentiation of O–H and C–H Bond Scission Mechanisms of Ethylene

Glycol on Pt and Ni/Pt Using Theory and Isotopic Labeling Experiments". J. Am. Chem. Soc. **133** (20): 7996–8004. doi:10.1021/ja201801t. PMID 21526776.

4. Open Babel documentation Author: Geoffrey R Hutchison; Noel M O'Boyle; Blue Obelisk (organization)
5. Avogadro website

Evaluation Process

1. A minimum of 75% class attendance is mandatory for course completion.5 marks will be assigned for attendance. 1 mark for 75%-80% attendance,2 marks for 81%-85% attendance, 3 marks for 86%-90% attendance,4 marks for 91%-95%attendance and 5 marks for 96%-100% attendance.
2. Evaluation will be based on- attendance, class tests/assignments, and practical.
3. Students must attend all the above-listed evaluation components.
4. To receive the course completion certificate, students must secure a minimum of 40% aggregate marks.
5. The percentage of Marks secured by students will be converted into a Grade as follows-

   40%-50%: Grade A

   30%-40%: Grade B

   20%-30%: Grade C