Comparative Study of Molecular Modelling Software for Science Education

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ABSTRACT

Teaching-learning processes of science through interactive software is the prerequisite of the present trend of education. Molecular modeling software is used to design and develop 2- dimensional, & complex 3-dimensional graphics and to visualize different Cartesian (x,y,z), dynamics, surface properties, and thermodynamics of inorganic, biological, and polymeric systems. This software provides a simulated and interactive molecular model of different molecules that enable stakeholders to design and develop the chosen topic as per their requirements. Molecular modeling software helps to enhance the perception, motivation, hands-on-practice and problem-solving trough critical thing and molecular behavior in actual they visualize. This paper gives a comparative study of various molecular modeling software viz., Chemdoodle, Hypercube, Avogadro, ChemAxon, Mole view and Chemsketch. The study also describes molecular model software and utilizes its activities. The findings of the study reveal that Avogadro is free and open-source software. It provides windows, Android and iOS-based maximum molecular modelling service to its stakeholders.

Keywords: *Chemdoodle, Hypercube, Avogadro, ChemAxon, Abalone II, Mole view, ChemSketch*

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1. Introduction

Computer technology, adopted in the chemistry since accessible in the public domain for predicting the structure and properties of molecules, is very helpful to different stakeholders viz., teachers, educators, students, technicians, doctors, scholars and scientists. Presently, the emerging technology in terms of molecular designer and analyzer enables the results up to a more precise and specific level. Molecular modelling software is the requirement of present teaching-learning processes for theoretical and practical subjects. Pedagogical usage of ICT is a deterministic factor in the classroom for Chemistry and Physics (Ouardouri, 2012; et al.). Ojha, (2016) studied the use of ICT in Chemistry Education and concluded that initiative to incorporate technology effectively into classroom instruction must begin with the curriculum objectives. It ensures a consistent goal. A mismatch between the values of the teacher and the technology initiative will cause an incorporation failure. Kumar, D. (2017) in his study reveals that students of Chemistry and life sciences discipline access and use moreinternet services for academic purposes. As exponentially increase the need to understand the design of the simple and complex molecular structure in 3D visualization, the demand for molecular modelling software increased respectively. Molecular modelling software may be defined as the software that includes all the theoretical and computational methods,and it is used to understand, design and development of the molecular structure in different dimensions interactively. The term "molecular modeling" usually conjures up two images: three-dimensional (3-D) depictions of small molecular structures and biological macromolecular structures, rendering in three-dimensional space the atoms of a molecule, whether it be something as simple as methane or as complex as ribulose (Smith 1998). In recent time, simulation is a very effective property of molecular modelling software which provide a clear 3D picture of molecular structure.

It enhances the scientific temperament among the various stakeholders. Geometries and interfaces present satisfactory agreement with molecular simulation and experimental data (Ghobadi and Elliott-2014). Simulation is being used to complete all the activities and experiments in an interactive method (Kumar, 2020). It provides an atomistic level of description for molecular structure. In the present scenario, various techno-pedagogical processes based on molecular modelling software are available online and office. Before its use, stakeholders need to find out the appropriateness of particular software. This paper discusses and compares the study of selected software is conduct.

2. Objectives of the Study

- To find out the free and open source molecular modelling software for Chemistry..
- To determine the supporting platform used by the molecular modelling software .
- To find out the basic tools available for the design and development of molecular structure.
- To determine the common facilities for building material for molecular structure.
- To determine the common facilities for binding molecular structure.
- To find out the overlying capabilities of selected molecular modelling software.

3. Limitations of the Study

The following study under titled 'Comparative Study of Molecular Modelling Software for Science Education' is limited to Chemistry.

4. Method

For this study, comparison of molecular modelling software for science education' different websites searched on internet. On the basis of, need and purpose of software in schooling education upto senior Secondary Stage, the following seven molecular modelling software were selected viz., Chemdoodle, Hypercube, Avogadro, ChemAxon, Mole view and ChemSketch. Further, comparison of the selected software conducted on the basis of :

a) license type
b) platform supported
c) tools available
d) building molecule
e) building material
f) overlying capability

5. Molecular modelling software and specific features

There are following seven molecular software discussed below as

5.1 Chemdoodle

This molecular modelling software specially designed for teachers and students for building structures from a starting atom to zig-zag line representation. It provides a stable structure to various molecules in shape and size that can be read and written in file formats. The molecular structure can be rooted as editable objects in Work, Microsoft Office and Open Office, in three dimensions, models generated in 3600 rotation. shapes of molecular structure can be rendered through individual choice.

Some Features

- The models generated in 3D graphics can visualize and control over font, size and color in different angles with close observation.
- Own elements can be defined manually with different color set to apply to molecule rendering.
- Compass facilities available for the graphic to describe an orientation.
- For the visualization. Models can be rendered with transparent objects with or without back faces.
- Its generate several surface types and color functions for any number of atoms. Visualize the space of your structures in ways other editors cannot.
- Mesh algorithms, display types, normal's, colors and molecular model can customize
- Inbuilt facilities of Van der Waals, (VDW), solvent accessible surface and solvent excluded surfaces (SES) are available.
- A systematic view of atomic orbital models based on quantum numbers with the orbital widget.

5.2 HyperChem

HyperChem is an advanced molecular modeling platform that is used for 3D visualization, animation, quantum chemical calculations and molecular mechanics with dynamics quality, flexibility, and ease of

use. It includes the additional component of molecular structure, thermodynamics, spectra, and kinetics, etc. This software also supports other functions related to chemistry 3D design, such as protein simulations, molecular modeling, molecular visualization, calculations of chemical structures and other operations related to bioinformatics. Respective all, modelling and simulation of protein are specialized features of this software. This software can be used by teachers, researcher and students. Microsoft windows is the best supporting platform.

Some Features

- Convert 2D molecular sketch to a 3D structure and mechanics, molecular dynamics, and semi-empirical and molecular orbital methods, as well as density functional theory is also possible.
- Like other molecules, macromolecules and small molecules are also scriptable.
- The structure can be highlighting, displaying capabilities and draw complex molecules in 3D with the mouse. Further, a molecule can rotate, translate, and resize structures easily with supporting tools.
- Different types of atom, formal charge, atomic charge, atomic mass bond lengths, bond angles, torsion angles, and the bonding geometry of molecule ease to labelled.
- With a mouse click on model builder user can build peptides, nucleic acids from amino acid, nucleotide residue libraries , counter ions or create zwitterions, and inherit charges from templates for Amber, Charmm, and OPLS is supported.
- Library facility of readymade derivatives that can be integrated into the desired model.
- Display spectra including frequency, intensity and line-width envelopes.
- Display vectors attached to atoms indicating the relative force on the atom or its direction of motion in a normal mode.

5.3 Avogadro

Avogadro is a free and open-source advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics and materials science. It offers flexibility to edit different areas of chemistry through high-quality rendering and plugin architecture. This software storage capacity is very less on computers. Its support for Windows, Linux, and Mac. Avogadro has the plug-in architecture, interactive tools, commands and scripts. This software can be easily accessed and used by teachers and students.

Some Features

- It has the capability to enhance the semantic accessibility of chemical data.
- Avogadro library provides framework code and application programming interface (API) with three-dimensional visualization capabilities that can be used in research and education in the fields of physics, biology, chemistry and material science.
- Provide rich graphical interface using dynamically loaded plugins through the library.
- It also offers an easy-to-use builder, integrated support for downloading from common databases viz., PubChem and the Protein Data Bank.
- Molecular model can easily zoom in/out using the mouse button and moving into 3D.
- To optimizes molecular geometry, Auto Optimize tool given in the software which provides an interactive interface to shape a molecule geometry.
- It is also supported CML, XYZ, SDF, Mol2, and PDB files.

5.4 ChemAxon (MarvinView)

Cham axon is a standardized chemical structure representation tool kit. It helps to customize 3D molecular representation. It is free for academic purposes. This software can be download after register online with an email address. Users can easily edit and modify the molecular structure. Software It searches the molecules for structural problems and once an error is found, the software provides automatically a real-time solution.

Some Features

- Enable the fast and accurate drawing of chemical compounds, reactions viz., Markush structures and query molecules.
- The modeler has the facility to guide built-in structure and valence checkers.
- It provides live results for the property of the structure of the molecule.

- Thousands of molecules can be easily displayed through render in the matrix.
- Support different file formats includes .doc and .pdf.

5.5 Mole view

Mole view is an open web-based molecular mechanism software. For its access and uses the requisite internet facility. Its facilitate to import file from another database like Crystallography Open Database, PubChem, RCSB Protein Data Bank and the Database. Through MolView, scientific databases include compound databases, protein databases and spectral databases, and records of these databases can be view as interactive visualizations using WebGL and HTML5 technologies.

Besides, it can be utilized for simulation, molecular modelling, protein assembly and chain representation. Teachers and students can easily practice this software for designing 3D molecular models and editors online.

Some Features

- At the same time, construct and visualize molecular structure 2D to the 3D on-screen.
- It helps to measure distances, angles and torsion angles in small molecules.
- Molecule spectra can be view through spectrum viewer through the tools menu.
- In the meantime of structure design, the error or mistakes can be correct through this software. In the case of the incorrect molecule, software shows In the wrong structure of a molecule addition atoms or new structures easily compare to check correctness.
- 2D and the 3D models of an atom or molecule directly download and use in design the presentation.

5.6 Abalone

Abalone is a molecular simulation software with two important things i.e., force filed for the simulation biomolecules and package of molecular simulation programme which include source code and demos. Abalone II contains proteins, hydrocarbons, heavy elements and molecules via a default FF.

Some Features

- Design Geometry optimization using Conjugate gradients, and Steepest descent
- Interface with quantum chemical programs with ORCA and NWChem.
- It contains chain builder, free mouse drawing, geometry editor, bonds detection by distance, overly and eliminating clashes
- It helps to design Force Fields of AMBER family, AMBER-ii, OPLS, DREIDING like FF for an arbitrary molecule, Semi-automated parameterization, and Implicit & explicit water models
- Its include GPU acceleration contains both MD and HMC
- Molecular dynamics work with Verlet, rRESPA, OPVL and OVVL fourth-order integrators and Replica exchange

5.7 Chemsketch.

Chemsketch is molecular modeling software that can be download either free or purchase for commercial purposes. Its free version contains limited features. It is a simple and educational purpose software. User can see the preview for better visualization and structure design.

Some Features

- Available facility to molecular rotation and multicolor visualization.
- Chemsketch work can be utilized in the PowerPoint presentation and word document.
- direction of arrows facilities available for equilibrium systems.
- Molecular design shows boiling point, molecular weight and density etc.
- Multiple templates with ions and functional groups available for the molecular design.
- User can modify the acid to the anion of the acid showing a negative charge.

6. Comparison of Molecular Modelling Software

In this study, compare various molecular modeling software based on different category's. In this section, we can classify the molecular modeling software into following categories, they are:

6.1 Based on license type

Avogadro and Mole View are only the software available free and open source. The other software Chemdoodle, Hypercube ChemAxon, Abalone and Chem Sketch available including advanced features for commercial purposes as highlighted in Table 1.

Table-1: Comparison based on license type

Molecular modeling Software		**Chemdoodle**	**Hypercube**	**Avogadro**	**Chem Axon**	**Abalone**	**Mole view**	**Chem Sketch**
Type								
License	**Free**	x	√*	√	√*	x	√	√
	Open	x	x	√	√	x	√	√
	Commercial	√	√	x	√*	√	x	√

Here, *limited version and commercial version advanced features

6.2 Based on platform supported

Chemdoodle, Hypercube ChemAxon, Abalone, Mole View and ChemSketch are only the software that is supporting Windows, Android and iOS platforms. Only Abalone is the software that supports the Windows operating system shown in Table 2.

Table-2: Comparison based on platform supported

Molecular modeling Software		Chemdoodle	Hypercube	Avogadro	Chem Axon	Abalone	Mole view	Chem Sketch
Type								
License	Windows	√	√	√	√	√	√	√
	Android	√	√	√	√	x	√	√
	iOS	√	√	√	√	x	√	√

6.3 Based on tools available

All seven software have the availability of basic tools facilities for the molecular structure shown in Table 3.

Table-3: Comparison based on tools available

Tools	Chemdoodle	Hypercube	Avogadro	Chem Axon	Abalone	Mole view	Chem Sketch
Navigate	√	√	√	√	√	√	√
Bond-Centric Manipulate	√	√	√	√	√	√	√
Manipulate	√	√	√	√	√	√	√
Selection	√	√	√	√	√	√	√
Auto-Rotate	√	√	√	√	√	√	√
Auto-Optimize	√	√	√	√	√	√	√
Measure	√	√	√	√	√	√	√
Align	√	√	√	√	√	√	√

6.4 Based on building molecules

Among all software, only Chemdoodle and Avogadro fulfill the condition of the molecular building shown in Table 4.

Table 4. Comparison based on building molecules

Tools	Chemdoodle	Hypercube	Avogadro	Chem Axon	Abalone	Mole view	Chem Sketch
Importing Molecule	√	√	√	√	√	√	√
Importing from PDB	√	√	√	x	x	√	x
Building a Peptide	√	√	√	√	√	√	√
Building DNA/ RNA	√	√	√	√	x	x	√
Building Nanotubes	√	x	√	x	√	x	x
Insert Fragments	√	√	√	√	√	x	x
Building with SMILES	√	x	√	√	x	x	√

6.5 Based on building Material

Avogadro and ChemAxon are only two software have all the building material as compared in Table 5.

Table-5: Comparison based on binding molecules

Tools	Chemdoodle	Hypercube	Avogadro	Chem Axon	Abalone	Mole view	Chem Sketch
Building a Supercell	√	x	√	√	√	x	x
Making a Crystal slab	X	x	√	√	x	x	x
Building a polymer	√	√	√	√	√	√	√
Perceiving symmetry	√	√	√	√	√	√	√
Reducing Crystal	√	x	√	√	x	x	x
Scaling Crystal Cell	x	x	√	√	x	x	x
Molecule-surface Interactions	√	√	√	√	x	x	x

6.6 Based on overlaying capabilities

Chemdoodle, Hypercube and Avagadro software have all the overlying capabilities includes additional features viz., Graphics, simulation and Interactive. The ChemAxon, Abalone, Mole View and Chem Sketch have only 2D and 3D overlying capabilities as highlighted in the table 6.

Table-6: Comparison based on overlaying capabilities

Molecular modeling Software Type		Chemdoodle	Hypercube	Avogadro	Chem Axon	Abalone	Mole View	Chem Sketch
Overl-aying capability	2D	√	√	√	√	√	√	√
	3D	√	√	√	√	√	√	√
	Animation	√	√	√	x	x	x	x

	Other	Graphics	Simulation Interactive	Simulation Interactive	x	x	x	x

Please note that the characteristics and features may be varied according to the individual software.

7. Molecular Modelling Software

As the software discussed, there are the following websites/links are given to the further area of study/research.

Table-7: Website/Links for Molecular Modelling Software

Software	Website/link
Chemdoodle	https://www.chemdoodle.com/3d
Hypercube	http://www.hyper.com/
Avogadro	https://avogadro.cc/. https://sourceforge.net/projects/avogadro/postdownload
ChemAxon	https://chemaxon.com/
Abalone	http://www.biomolecular-modeling.com/Abalone/
Mole view	http://molview.org/
ChemSketch	https://www.acdlabs.com/resources/freeware/chemsketch/download.php

8. Findings

- Avogadro and Mole View are only the software available free and open source.
- Chemdoodle, Hypercube ChemAxon, Abalone, Mole View and ChemSketch are only the software that is supporting Windows, Android and iOS platforms.
- All the seven software, Chemdoodle, Hypercube, Avogadro, ChemAxon, Mole view and Chemsketch have the availability of basic tools facilities for molecular structure.
- Chemdoodle and Avogadro fulfill the condition of the molecular building.
- Avogadro and ChemAxon are only two software have all the building material used in molecular modelling.
- Chemdoodle, Hypercube and Avagadro software have all the overlying capabilities includes additional features viz., Graphics, simulation and Interactive.

9. Conclusion

Molecular modelling software amplifies actual reality of molecule to provide the real time information. Different molecular modular have different characteristics and features to design and develop the visualization of molecule in 3D, graphic, animation and simulation respectively. Comparison of modelling software reveals that user can select the appropriate software for desired requirement. Additional, Avogadro is very supportive modelling software that provide advance feature and ease to download, access and use by different stakeholders. This software work in offline mode that is the present need of remote areas where internet service interrupted. These software engage the different stakeholder to learn the diverse molecular structure in different perspective that generate new and varied knowledge.

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