DYNAMIC VISUALIZATION IN 3D OF CHEMICAL STRUCTURES

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Abstract

The advance of computer simulations to understand the behavior of material started in the '60, in recent years due to the computer power increase, simulations can predict the properties of materials with a great accuracy and speed.

Molecular Dynamics simulation is a technique for computing the equilibrium and transport properties of a traditional many-body system; the nuclear motion of the constituent particles obeys the law of

Classical mechanics. These simulations are very similar to real experiments.

During our courses at the Faculty of Chemistry of UNAM (National University of Mexico), the use of computer programs to model chemical events is increasing every year. Students simulate several experiments in order to understand the basic variables involved.

Keywords: Chemical reactions, Animation, Molecular Modeling, Reaction Mechanism, 3D visualization.

1 INTRODUCTION

To understand the behavior of chemical substances the use of Molecular Dynamics simulation is one of the key techniques for computing the equilibrium and transport properties of complex systems; the nuclear motion of the constituent particles obeys the law of classical mechanics. These simulations are very similar to real experiments.

When a real experiment is performed a sample of the material to be studied has to be prepared. This sample is connected to a measuring instrument (thermometer, manometer, calorimeter wtc.) and the property of interest is measured during a certain period of time. These measurements are subject to statistic noise; the longer the data are obtained the more accurate the measurements are. In Molecular Dynamics simulation, the same approach is followed, with the advantage that, (if the model is properly established) the data can be obtained with more accuracy, speed and more variables can be involved.

The use of Molecular Modeling programs allows the simulation of dynamic visualization of chemical entities in order to understand this behavior. Students improve their learning skills when they can simulate several variables and understand the basics of molecular behavior.

The use of 3D tools allows a better perception of the models and molecular structures.[1-14]

1.1 Programs

1.1.1 AtomSmith [15]

Is a very useful program for understandings the behavior of molecules. The use of the program help to think about and broaden, how the students can imagine molecules, and to explore the world of molecules by viewing, building and performing simulation of 3D molecular models. Exploring models in the program is as simple as loading a model and dragging the mouse to view the model in different environments.

There are versions for Windows and Mac "The Atomsmith Classroom" that has the full features of the program and reduce version for ipad. "Atom Smith, Molecule Lab".

It contains a collection of several hundred carefully selected molecules representing a broad range of fields including: Biology, Medicine, Physical Sciences, Organic Chemistry, Inorganic Chemistry, Physic Chemistry, Geology, Mineralogy.

In addition the system can search and load molecules from a collection of 25 million 3D models available in the PubChem database at the US National Institutes of Health, examples (Fig1-3)
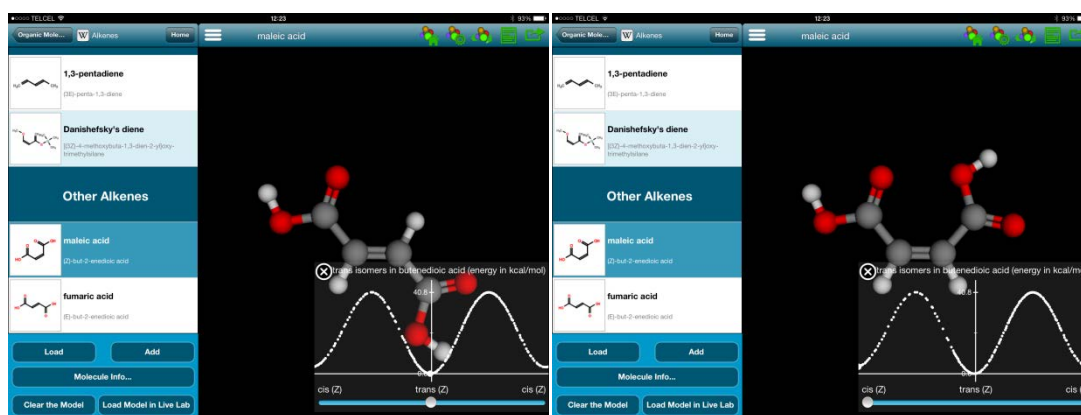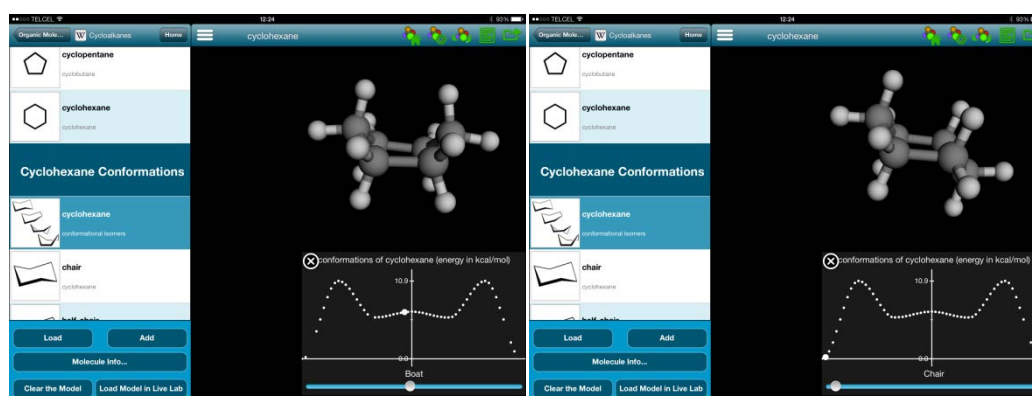
Fig 1 Cis trans isomerization

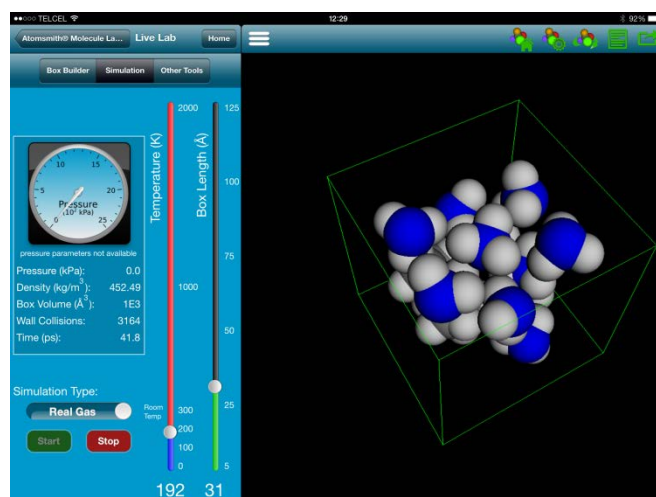

Fig 2 Ciclohexane chair and boat conformations.

Fig 3 Dynamic behavior of a mixture.

1.1.2   Odyssey [16]

Odyssey is learning and simulation environment for molecular science the program has several features to understand the behavior and properties of molecules. The dynamics can be controlled with many parameters, temperature, pressure, concentration, density. And properties as internal energy kinetic energy potential energy can be calculated. Odyssey is one of the most useful tools for teaching chemistry at different levels and different subjects. Analytical, Organic, Inorganic, Physic chemistry, Food Chemistry, Biochemistry and others.
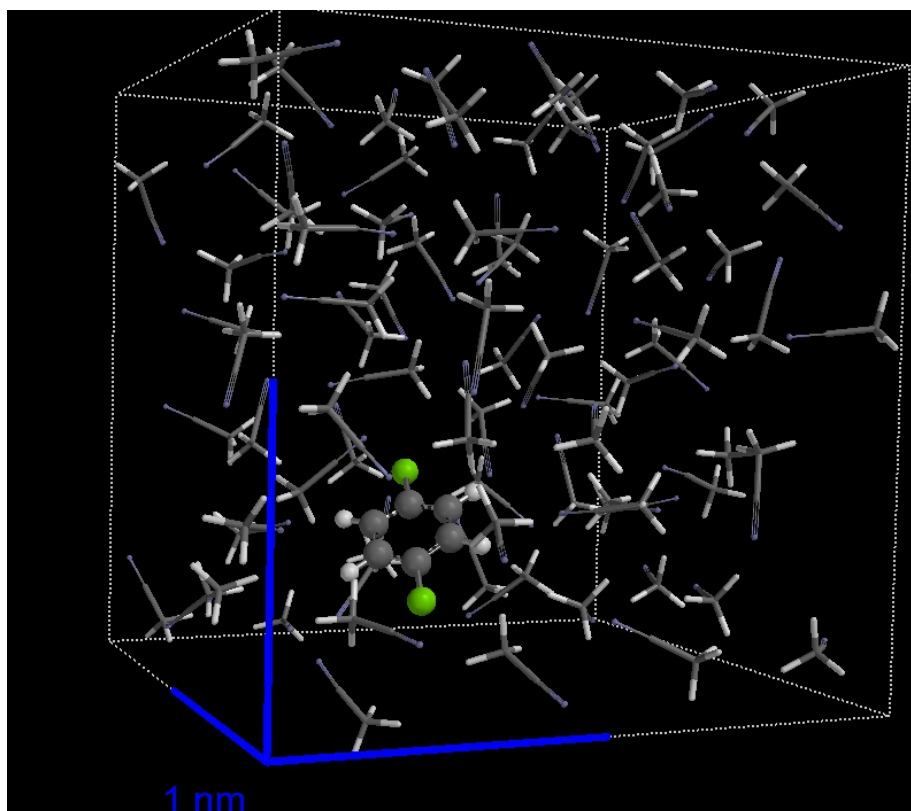
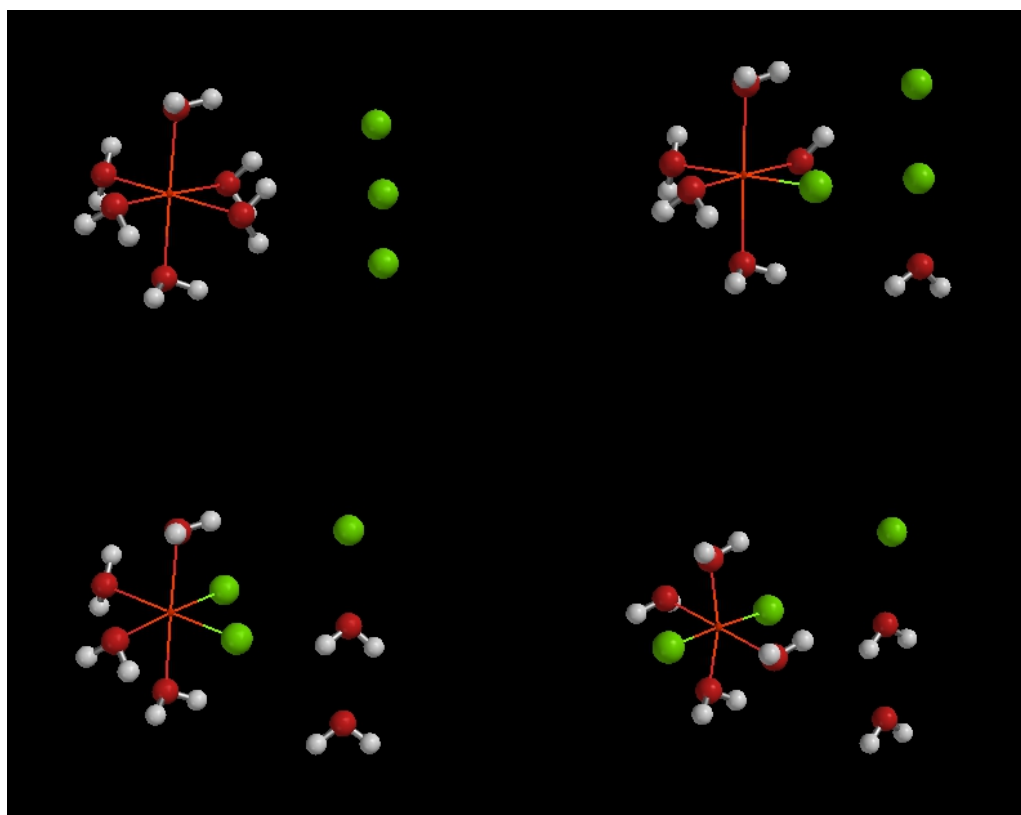Fig 4 1,4-dichlorobenzene in ethanenitrile solution
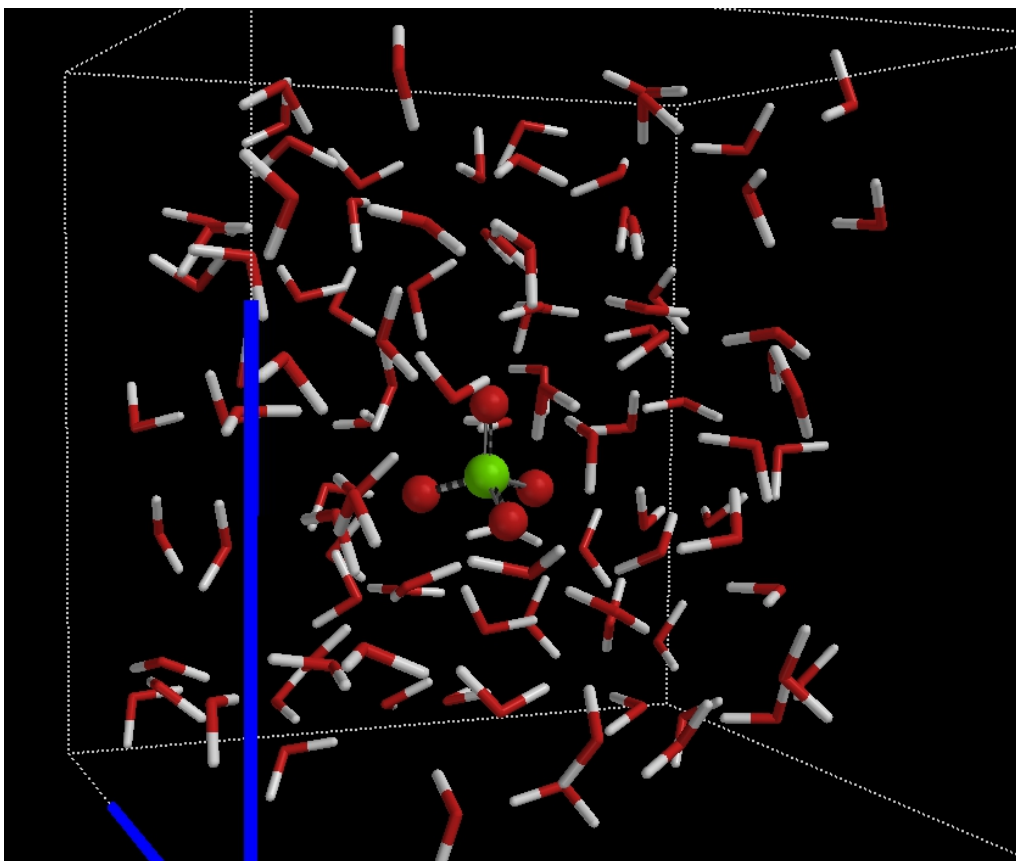

Fig 5 Coordination Sphere Isomers
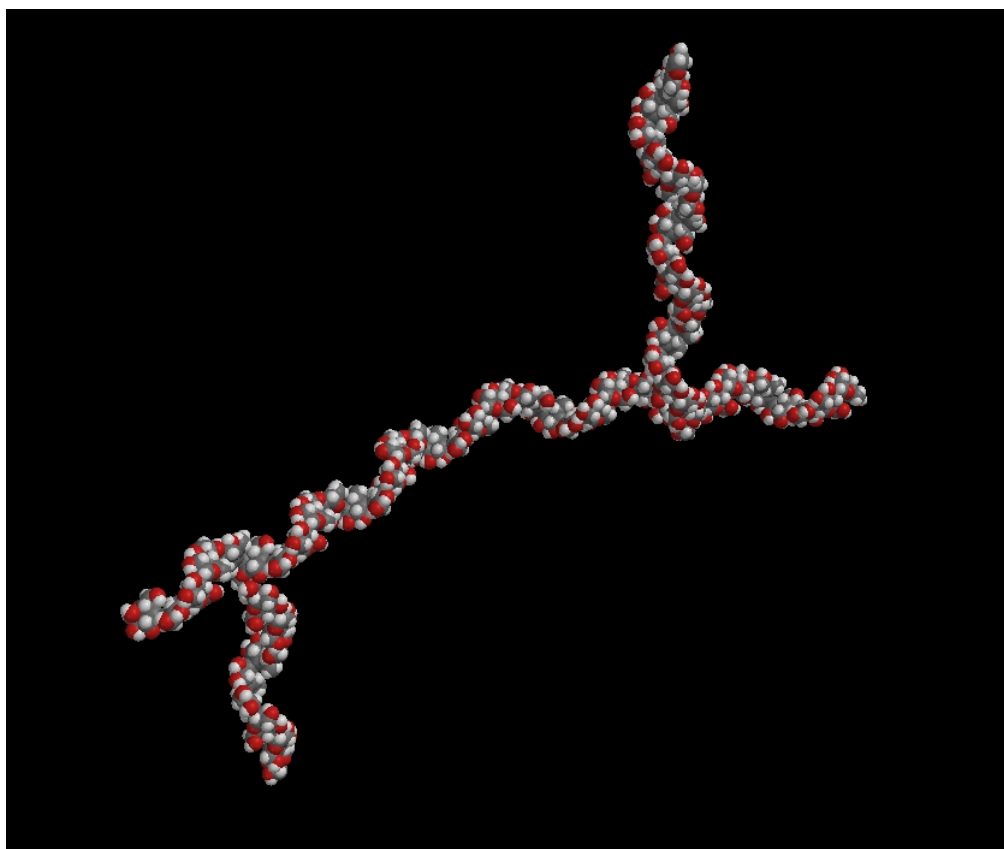
Fig 6 Perchlorate in water
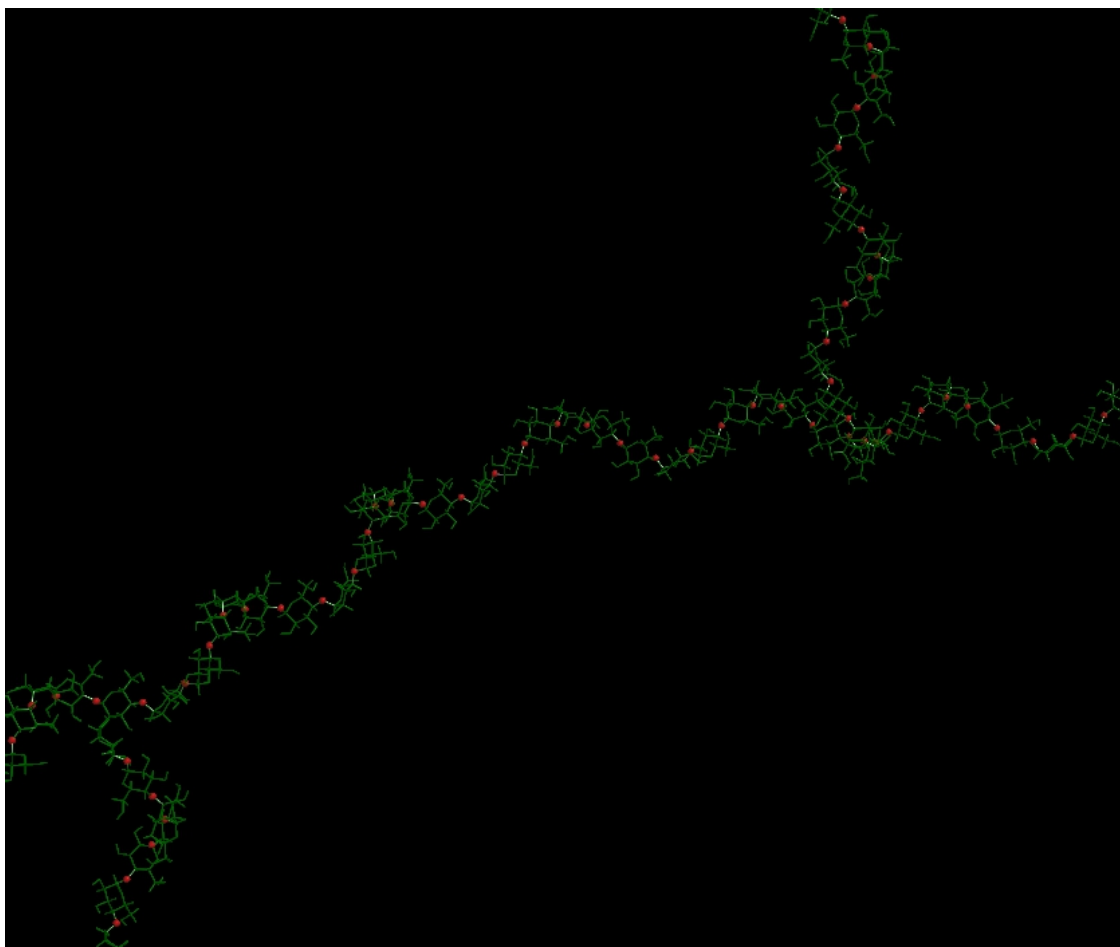

Fig 7 Amylopectin Molecule

Fig 8 Amylopectine repeating units.

1.1.3   VMD [17]

VMD is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more general molecules, as VMD can read standard Protein Data Bank (PDB) files and display the contained structure. VMD provides a wide variety of methods for rendering and coloring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VMD can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer.

The mouse can be used to manipulate the structure in the display window. There are three basic mouse modes: rotation, translation, and scaling. The mode can be changed from the Mouse menu in the main window, or by pressing r, t, or s on the keyboard while the mouse is in the graphics window. While experimenting, note how the cursor changes to indicate the mouse mode. In rotation mode, the left mouse button controls rotation about axes parallel to the screen, and the middle button controls rotation about the axis perpendicular to the screen. In translation mode, the left mouse button controls translation parallel to the screen, while the middle button controls translation in and out of the screen. Finally, in scaling mode, both the left and middle buttons control global scaling when the mouse is moved left or right, but the middle button causes larger changes.
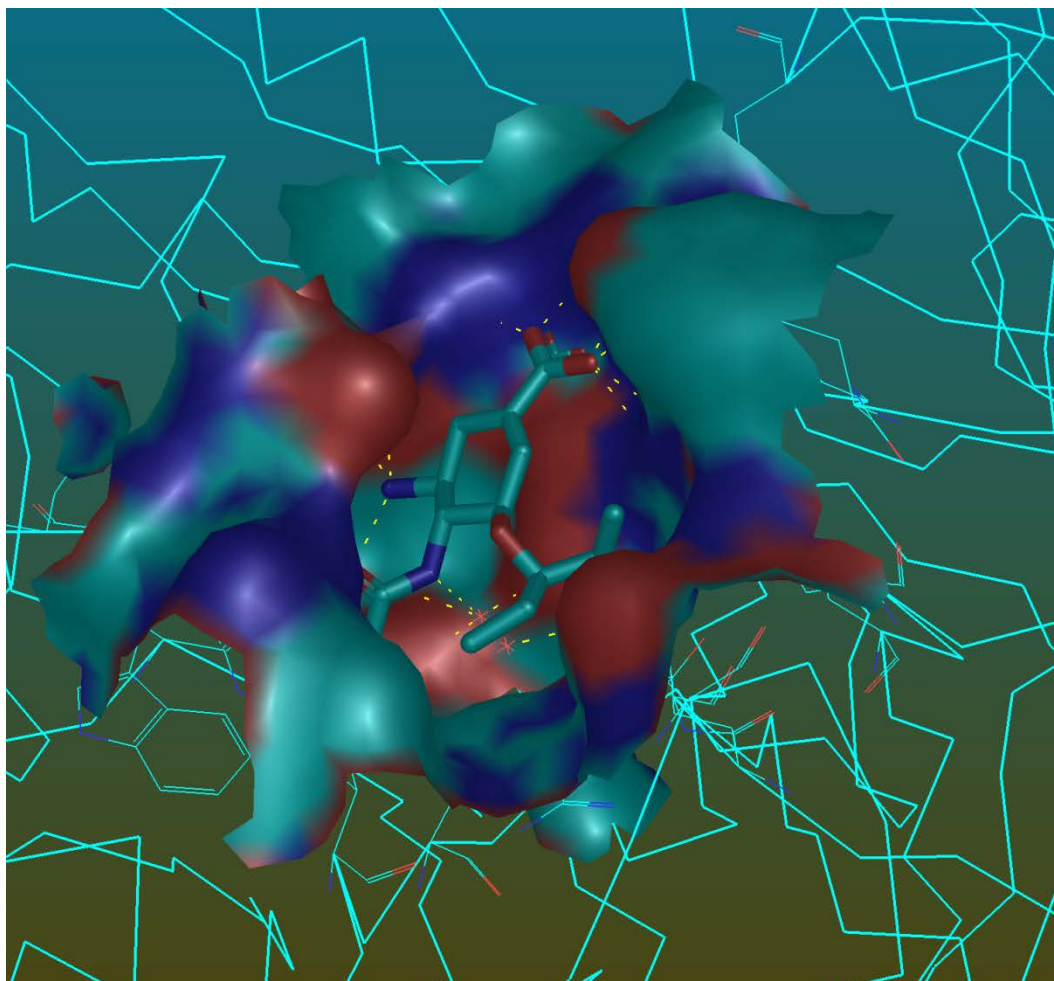
Fig 9 Active site

VMD includes functions for analyzing molecular structures and trajectories. These functions access the internal VMD data structures to return or modify characteristics such as charge, mass, and position for individual atoms, residues, and molecules. More complex analysis capabilities, such as computing the RMS deviation or correlation functions of a dynamics trajectory, can then be implemented as Tcl scripts without the need to modify the VMD source code.
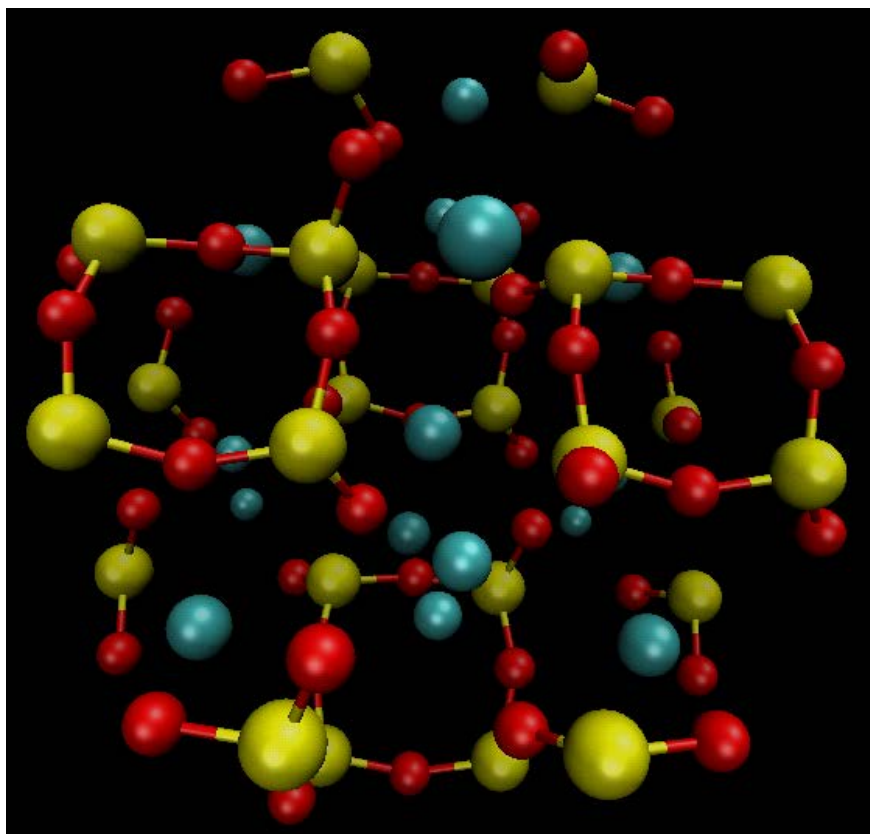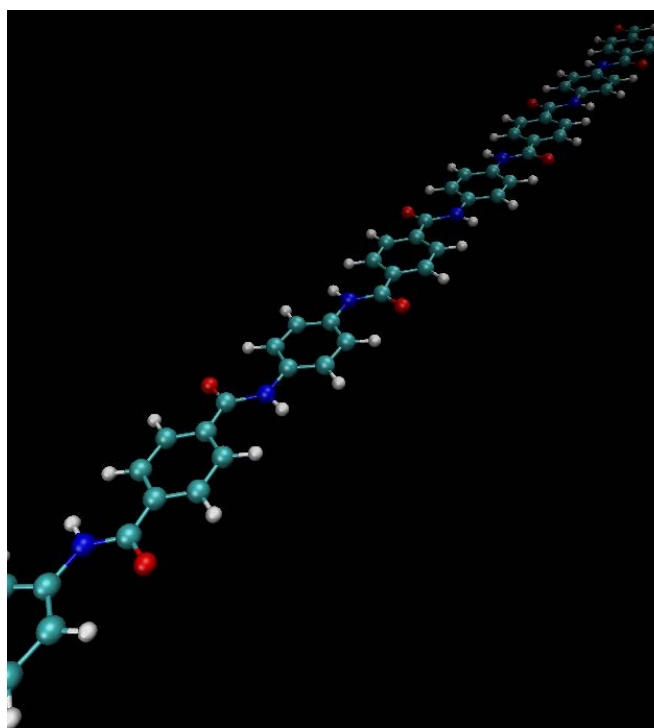
Fig 10_BaCuSi$_2$O$_6$

Fig 11 Kevlar

Simulation of polymers as the Kevlar can give insight about the intrinsic characteristics of the molecules, its aromatic rings with the amide bonds are responsible for the fire protection properties and it strength higher than steel, that is why it is used as bullet proofs textile.

VMD provides an interface to initialize a new simulation, and can serve also to monitor and control certain simulation parameters. After a simulation is started and a connection between VMD and the application is made, molecular structures are communicated to VMD as they are calculated.
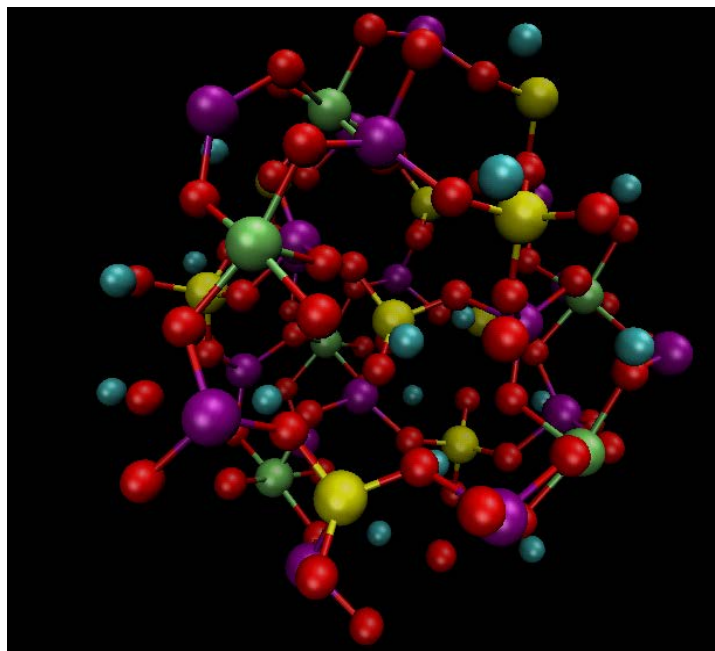

Fig 12 $Ca_3Ti_2Si_2(Al,Ti,Si)_3O_{14}$

Once a connection to a running simulation has been established, VMD provides options to modify simulation parameters, such as the temperature, and remote connection parameters, such as the frequency with which coordinate sets are communicated from the simulation program to VMD. [17]
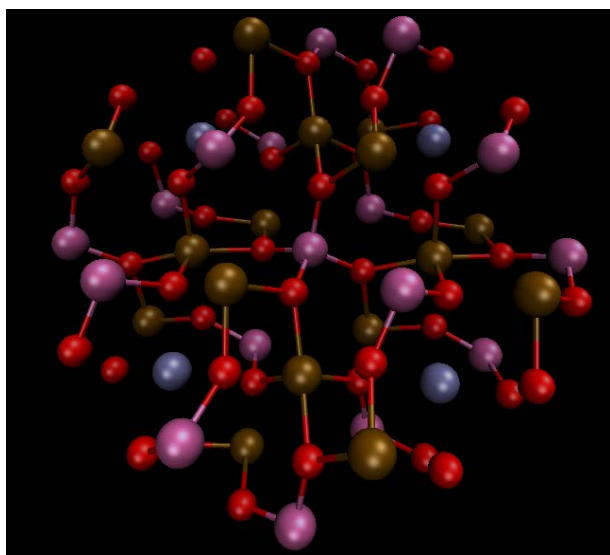

Fig 13 $Mg_{1.75}Fe_3Y_{.7}Ge_2O_{12}$

2 CONCLUSIONS

The use of Molecular Modeling programs allows the simulation of dynamic visualization of chemical entities in order to understand this behavior. Students improve their learning skills when they can simulate several variables and understand the basics of molecular behavior.

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Fig 1,2,3 were done using Atom Smith.

Fig 4,5,6,7,8 were done using Odyssey

Fig 9,10,11,12,13 were done using VMD.

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