

# Roving Around Molecules

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## Rover parts

The 3D geometry of atoms and molecules is difficult to grasp, but this knowledge is important. How can we give students a firsthand experience at the atomic level? Impressive demonstrations with expensive equipment have shown the value of computer-based molecular visualization to provide virtual experiences; there is strong

**Navigation.** In order to simulate the ability to move around molecules, we needed a way to show molecules from any perspective. This requires very fast software, because the illusion of smooth motion requires that the screen be redrawn at least 20 times per second, each time from a slightly different perspective.

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anecdotal evidence of the educational value of such immersive environments. We have now brought this experience to the desktop with the *Rover*, our newest addition to the Molecular Workbench, the Concord Consortium's award-winning molecular dynamics package. Interacting with the Rover can help students internalize accurate mental models of atomic-scale phenomena and develop an expert's ability to reason more effectively at different levels. No special glasses, prisms or other paraphernalia are required.

We have been using a Java molecular viewer called Jmol to display 3D objects. *Jmol* is ideal for Rover because it is fast, open source, and written in Java, our development language of choice. Jmol, however, did not originally support navigation—the ability of the user to move into and around molecules. Jmol simply views molecules from the outside. The molecule can be rotated and even displaced, like using a zoom lens, but always with the perception that the molecule is “out there.”

In order to overcome this limitation, we collaborated with the current chief

Jmol developer, Robert Hanson, Ph.D., to add navigation functionality to Jmol. Because it is open source software, we did not have to duplicate the considerable work and creativity that has already gone into Jmol. Instead, we were free to concentrate on adding the functionality we needed. Our additions are now available to Jmol users worldwide.

This new navigation capacity allows the user to appear to “fly” around molecules and explore structures from the inside. Even moving through macromolecules with thousands of atoms is handled smoothly and realistically.

**Animation Studio.** The Molecular Workbench is more than a simulation, it is also a complete system for authoring and delivering learning activities that use the simulations. As exciting as it is to move through a molecule, there are problems for end users if they get lost in the complexity and overlook significant features. Authors need ways to guide student experiences so that they navigate to the important parts of a molecule. To enable this, we created an Animation Studio, which allows authors to create virtual tours through molecules. A virtual tour consists of a series of scenes set by the author to introduce the fascinating molecular world and guide students through various structural patterns from different perspectives.

**Embedded annotation system.** Once students arrive at an interesting place in a molecule, they may need to be prompted with a question or given additional information. Inspired by Google Earth, we developed a system for inserting annotations into the molecular world. An annotation key, which is a customizable object embedded in the 3D space, can be attached to an atom, bond or chemical group, as illustrated in Figure 2. A link to other molecules or to a web page can be inserted into the annotation. The annotation capability is useful not only in making molecular explorations instructive, it also permits us to build a web space for any user to leave an

A side-by-side comparison of the default mode and the navigation mode

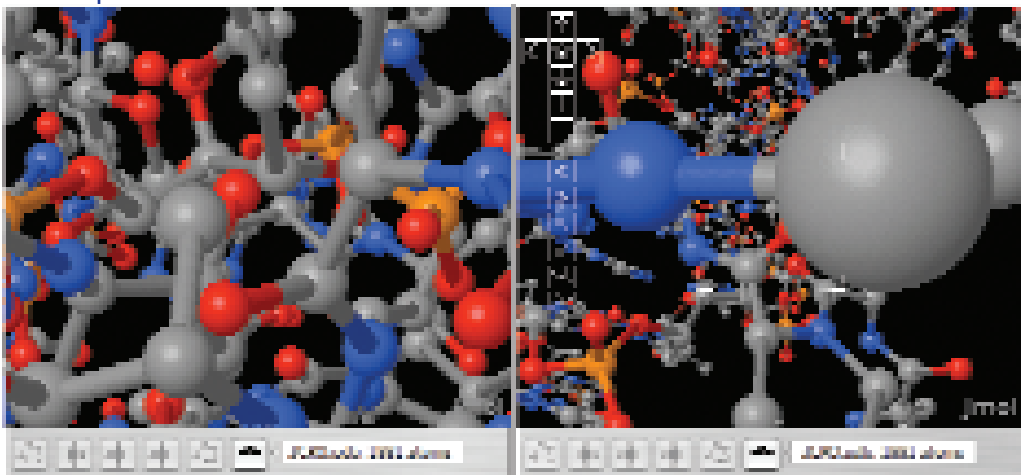
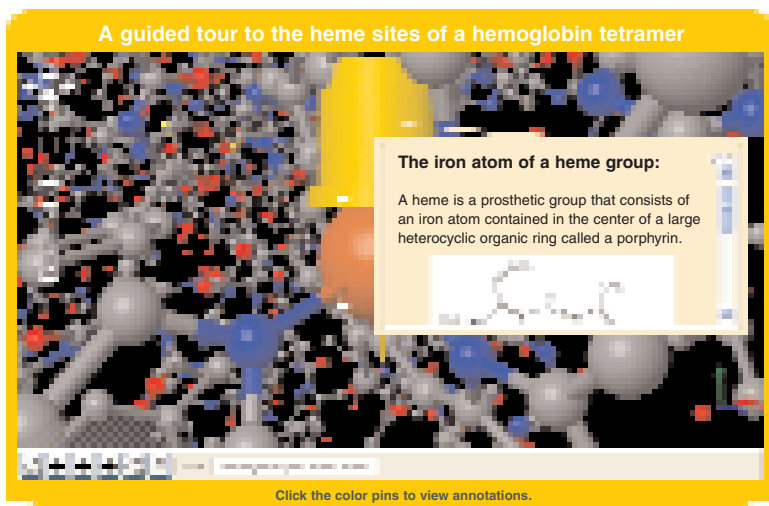


Figure 1 compares the original 3D capacity (left) with the navigation view (right) for the same molecule. The full 3D experience of molecules in motion is spectacular.



**Figure 2.** A pushpin key and its associated annotation. When the user navigates to the key and clicks on it, the annotation content comes up. The author of an activity controls the content of the annotation, which can contain text and graphics, plus links to other points in the molecule or web pages.

annotation to any molecule, which will then be seen by other users, similar to Google Earth or Wikipedia.

**Molecular Constructor.** This universal 3D constructor can be used to build any kind of molecule. Unlike other molecule builders, this tool works directly in 3D—there is no 2D-to-3D conversion. Most elements in the periodic table are supported with appropriate force field parameters determined according to their chemical properties. Building blocks such as amino acids, nucleotides and basic hydrocarbon molecules are provided for the user to rapidly sketch up complex molecular systems. A variety of tools are provided for the user to build 2-, 3-, and 4-body bonds, run energy minimization for selected atoms, cut/copy/paste molecules, and more. Figure 3 shows an example of what can be created with the Constructor.



**Molecular dynamics simulator.** All of Rover's capacity is embedded in the Molecular Workbench, a molecular dynamics package that models the

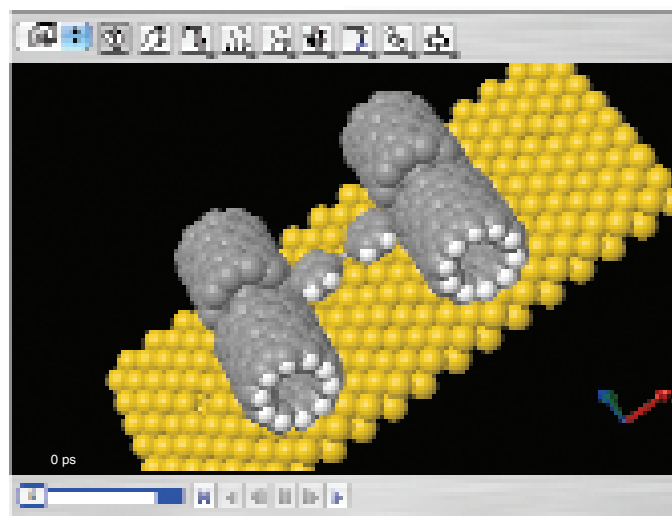
motion of molecules—their continual thermal vibrations and their responses to any applied forces. Consequently, students can see any Rover molecules in motion. Because the Constructor is part of Molecular Workbench, students can build molecules and then instantly run a simulation. This will reveal, for instance, whether a molecule is thermodynamically stable at different temperatures and how it might fold. This approach can potentially be useful in conveying the knowledge of chemistry in a trial-and-error way, similar to building a bridge and testing how much load would cause it to collapse. Figure 4 shows a snapshot of a molecular dynamics simulation on the subject of stereochemistry of the ethane molecule.

### Conclusion

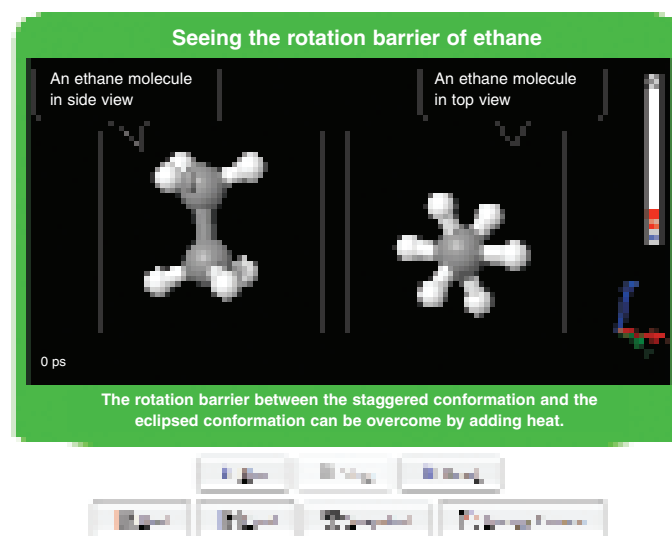
Getting a feel for the three-dimensionality of molecules is essential in the exploding fields of biotechnology, nanotechnology, modern medicine, genomics, bioinformatics, and electronics. These fields require a conceptual understanding of the physical properties of collections of atoms and molecules and the ways in which inter-

### LINKS Roving Around Molecules

-  **Molecular Rover**  
<http://rover.concord.org>
-  **Jmol**  
<http://www.jmol.org>



**Figure 3.** A molecular nano car with tires made of four short carbon nano tubes, all created using the Molecular Constructor. It sits on a gold crystal and can roll.



**Figure 4.** Part of a molecular dynamics simulation of ethane rotation. Two views of the same molecule are shown as it vibrates and rotates. At low temperatures, the molecule is trapped in the position shown, but as the temperature increases, the two ends can turn independently.

actions at the atomic scale relate to macroscopic properties. This understanding is difficult to acquire and is often shrouded in advanced mathematics and obscure terminology. The new Rover capacity in the Molecular Workbench provides an alternative, direct, and appealing route to this understanding. And “flying” through atoms and molecules is just plain fun!

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