ODYSSEY

User Guide
(Windows and Macintosh)

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* *Instructor's Edition only*

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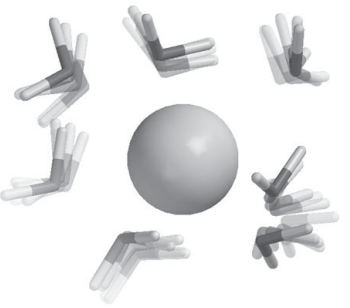
* *Windows only* ** *Macintosh only*

WORKING WITH *ODYSSEY*: THE ESSENTIALS



1.1 Welcome to ODYSSEY

ODYSSEY is a content-rich learning and simulation environment for molecular science. The software is designed to be used in two ways:

- ***Web-Style Browsing.*** Simply navigate through pages and follow links—No learning curve!

- ***Menu-Driven.*** Explore and visualize molecular systems with ***ODYSSEY's*** powerful, yet easy-to-use graphical interface.

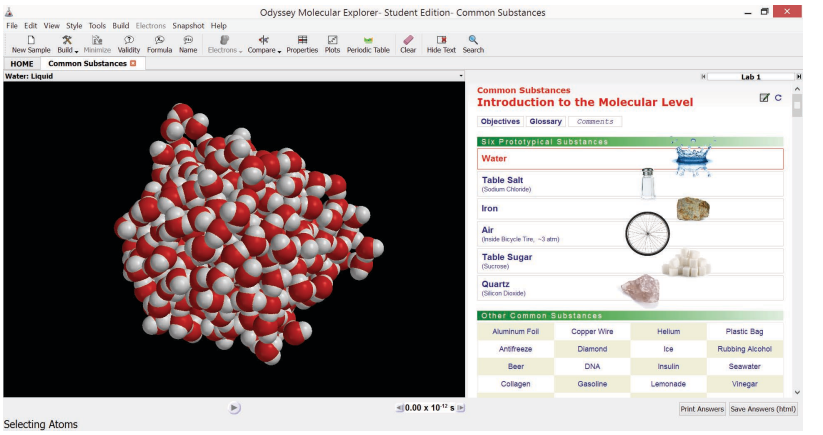
The next few pages explain everything you need to know to get started.

1.2 Manipulating Molecular Samples

- Start ***ODYSSEY*** via its icon on the Start screen or desktop (Windows) or via the Applications folder (Macintosh). ***ODYSSEY*** opens to its home page.

- To maximize screen size, select the "Maximize" icon in the upper right hand corner of the page (Windows) or upper left corner (Macintosh).

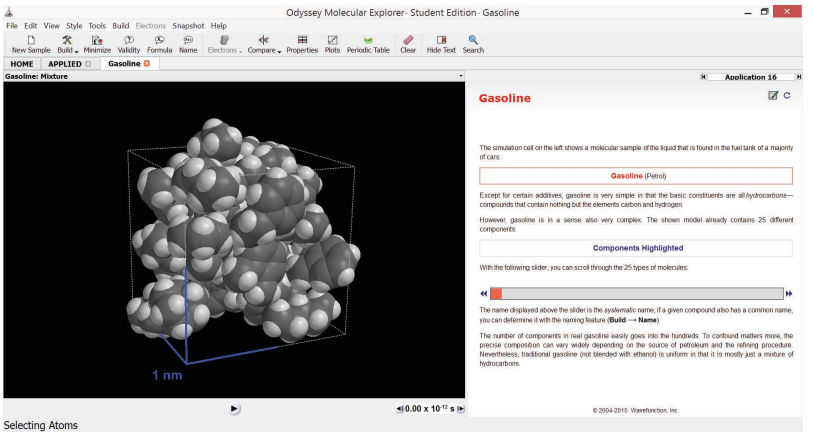
- Choose any of the topics on the home page.



- With a molecular sample displayed on the left side of the screen, verify the following functions:
  - Click and drag with the button (or left button) depressed to rotate the sample. Windows touchscreen: drag with finger.
  - Click and drag with the right button depressed to translate the model. Windows touchscreen: drag with two fingers or *long* press and drag with one finger; Macintosh trackpad (without a secondary click): Hold down the ⌘ key, depress the button, and drag.
  - Use the mouse scroll wheel to zoom in and out. Alternatively, hold SHIFT and then right-click and drag. Or use a *two-finger scroll* on the touchpad or trackpad (certain computers only). Windows touchscreen: use a pinch gesture.
- On many pages, you can start a physics-based *simulation* of the shown model by selecting the ▶ icon at the bottom. Select the icon again in order to stop the simulation.
- Exit by selecting the "Close" icon for the page (in the Windows version, the ✕ icon appears on the right hand side of the tab, in the Macintosh version, on the left). Closing the page takes you back to the home page.

1.3 Working with ODYSSEY Content

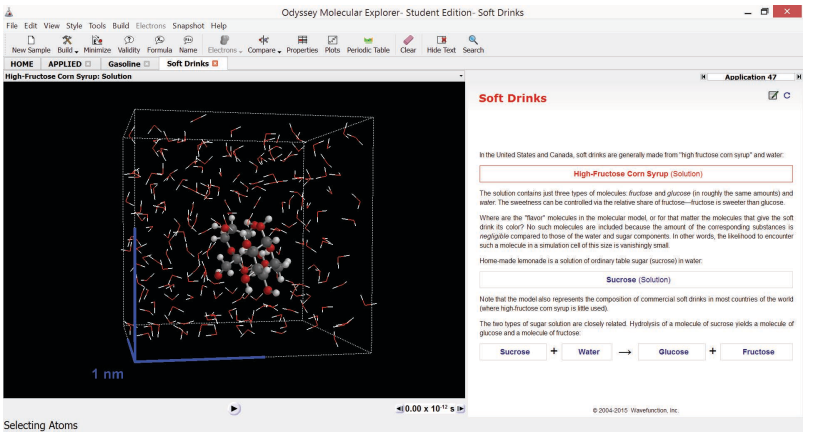
Select any of the topics available in the various sections of ***ODYSSEY*** (accessed via the buttons at the top of the home page).



- In many cases, the text includes “buttons” and other webpage-style controls. Selecting the buttons will trigger sample and visualization changes—try this out.

- Without closing the open page, go back to the **HOME** tab.

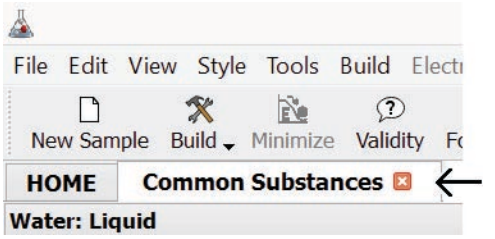
- Choose another topic.



- You now have two pages open at the same time. You can go back and forth between the two (and also go back to the **HOME** tab) by selecting the associated tabs.

- You can open as many pages as you wish. With a given topic open, you can also move to the previous or next topic by selecting the ◀| and |▶ icons that surround the “Number” field in the upper right corner of the text area.

- Closing any page is accomplished by selecting the "Close" icon for the page (in the Windows version, the ⊠ icon appears on the right-hand side of the tab, in the Macintosh version, on the left side).



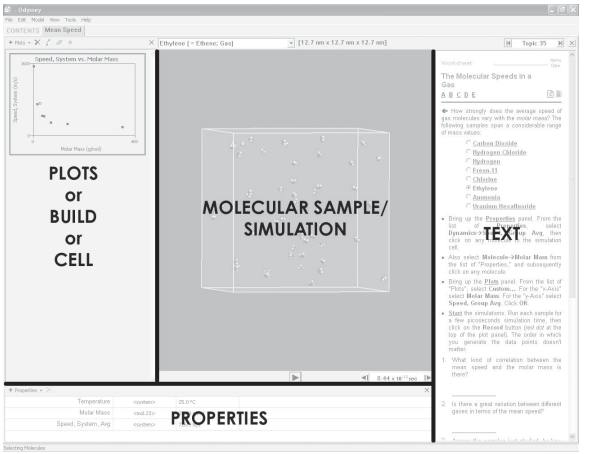
- By default, IUPAC Preferred Names are used for chemical compounds (= systematic names supplemented by a few common names that IUPAC continues to endorse). To display predominantly common names, open the **Tools** menu (Windows) or the **Odyssey** menu (Macintosh) and select **Preferences...**. Uncheck the "Use IUPAC Names" box, and then select **OK**.

- By navigating through hundreds of demonstrations, labs, and other types of pages, you can explore a world of fascinating chemistry. Use the simulation feature and find out for yourself what matter really is!

- Notes on how ***ODYSSEY*** operates and additional program features are documented in the remainder of this manual. For a concise overview of the main features of the program, please peruse the **New Users** link on the home page.

2.1 General Operation

2.1.1 Screen Layout



To change the size of the tiles for the *Sample*, *Text*, *Properties*, and *Plots/Build/Cell* areas:

- Position cursor on boundary between two tiles, click, and drag (or drag with finger).

2.1.2 ODYSSEY Icons

Simulations/Sequences:

- Start
- Stop
- Step Forward
- Step Reverse
- Change Frame

Properties:

- + Add Property — Add Property to List
- Remove Property from List
- Hide Properties Panel

Labs:

- Next Lab
- Previous Lab

Text:

- Page Refresh
- Notes
- Close Lab or Stockroom Page
- ANSWERS Show/Hide Answer Key*

Build:

- Build Mode
- Add
- Delete
- Make Bond
- Break Bond
- Simulation Cell
- Minimize
- Evaluate Structure
- Name Structure
- Molecular Formula

Plots:

- Add Plot
- Remove Plot
- Record Datapoint
- Edit Plot
- Clear Plot (Erase Datapoints)
- Hide Plots Panel

Other:

- Properties Table
- Plots Pane
- Electron Cloud
- Compare
- Hide Text Panel
- Periodic Table
- Clear Answers and Annotations

2.1.3 Toolbar

To display a toolbar with icons for commonly used operations:

- From the **View** menu, select **Toolbar**.

The size of the toolbar icons can be changed:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences**.

* *Instructor's Edition only*

- Choose among **Text Only**, **Extra Small Icons**, **Small Icons**, **Medium Icons**, **Large Icons**, or **Extra Large Icons**.

Note: In the Windows version, the toolbar can be (temporarily) moved to anywhere on the screen by dragging the "ridge" at its extreme left end.

2.1.4 Tabs

Whenever you open an item in **Home**, **New Users**, **Applied Chemistry**, or in the **Molecular Stockroom,** a new *tab* is created. You can go back and forth between tabs as desired. Generally, as many pages/samples as desired can be simultaneously open.

2.1.5 Touchscreen/Trackpad/Mouse Functions

Windows: *Touchscreen**

General Functions	
Tap	Select
Long Press	Shortcut Menu
Drag	**Rotate** Entire Sample
Long Press + Drag or Two-Finger Drag	**Translate** Entire Sample
Pinch	**Zoom** Sample (or Resize Clipping Sphere)
Tap Molecule, then CTRL + Drag	Rotate One Molecule
Tap Molecule, then CTRL + **Long** Press + Drag	Translate One Molecule
Double-Tap Bond, then ALT + Drag Vertically	Rotate Around Bond[1]
Double-Tap Bond, then ALT + **Long** Press + Drag Vertically	Stretch Bond[1]
CTRL + Double-Tap	Invert Stereocenter
SHIFT + Drag Vertically	Z-Axis Rotate
Build Mode Only	
Tap	Perform Build Action
Double-Tap	*Insert* New
[1] Wrap-around red arrow indicates selection	

* *Keyboard is required for some functions*

Windows: *Touchpad or Mouse*
Macintosh: *Mouse or Trackpad with Secondary Click*

General Functions		
	Primary Button (usually left)	Secondary Button/ (usually right) or Secondary Click
Click	Select	Shortcut Menu
Depress + Drag	**Rotate** Entire Sample	**Translate** Entire Sample
Click on Molecule, then CTRL + Depress + Drag	**Rotate** One Molecule	**Translate** One Molecule
Double-Click on Bond, then ALT + Depress + Drag Vertically	Rotate Around Bond[1]	Stretch Bond[1]
Windows: CTRL + Double-Click *Macintosh*: ⌘ + Double-Click	Invert Stereocenter	–
Touchpad/Trackpad (Varies with Type): Pinch or Two-Finger Scroll or Scroll at Right Edge *Mouse with Scroll Wheel:* Roll Wheel *Always Works:* SHIFT + Secondary Button + Drag Vertially	**Zoom** Sample (or Resize Clipping Sphere)	
SHIFT + Drag Vertically	Z-Axis Rotate	**Zoom**
Both Buttons Depress + Drag	Define Area[2]	
Build Mode Only		
Click	Perform Build Action	–
Double-Click	*Insert* New	–

[1] Wrap-around red arrow indicates selection
[2] Style changes only

Macintosh: *Trackpad (Secondary Click Not Used)*

General Functions	
Click	Select
CTRL + Click	Shortcut Menu
Depress + Drag	**Rotate** Entire Sample
⌘ + Depress + Drag	**Translate** Entire Sample
Pinch or Two-Finger Scroll or SHIFT + ⌘ + Depress + Drag Vertically	**Zoom** Sample (or Resize Clipping Sphere)
Click on Molecule, then CTRL + Depress + Drag	Rotate One Molecule
Click on Molecule, then CTRL + ⌘ + Depress + Drag	Translate One Molecule
Double-Click on Bond, then OPTION/ ALT + Depress + Drag Vertically	Rotate Around Bond[1]
Double-Click on Bond, hold OPTION/ALT, then ⌘ + Depress + Drag Vertically	Stretch Bond[1]
⌘ + Double-Click	Invert Stereocenter
SHIFT + Depress + Drag Vertically	Z-Axis Rotate
Build Mode Only	
Click	Perform Build Action
Double-Click	*Insert* New
[1] Wrap-around red arrow indicates selection	

2.1.6 Page Refresh/Reload

Select the C icon next to the page title for a full refresh of a page. The action refreshes *all* samples of the current page. (Other tabs are unaffected by a refresh.)

A Reload option is also available in the shortcut menu (right-click; Touchscreen: long press; Macintosh trackpad: CTRL + Click) when the cursor is within the text area. However, the effect of this reload is limited: It only refreshes the HTML of the current page, i.e., it does not refresh the molecular samples.

2.1.7 Working Without the Text Panel

To hide the text panel of the current page (the toolbar must be shown):

- Select the icon.

The setting will be applied to all pages in the current session (but will not carry over to the next session).

2.1.8 Projector Friendly Colors

To switch to a background color scheme that is more suitable for classroom projection than the default black background color (the toolbar must be shown):

- From the **View** menu, select **Light Background**.

The setting is applied throughout the current session. Future sessions, however, will start with the normal (black background) color scheme.

2.1.9 Hiding the Status Bar

The status bar at the bottom of the window can be temporarily hidden:

- In the **View** menu, uncheck **Status Bar**.

2.1.10 Full Screen Mode

ODYSSEY can be put into presentation-style full screen mode:

- From the **View** menu, select **Full Screen**.

To exit full screen mode:

- In the **View** menu, deselect **Full Screen**.

2.1.11 Annotating

To annotate an ***ODYSSEY*** page:

- Select the icon at the top of the text panel. This opens a *Notes* page that accepts any "text" that is entered.

- Return to the originating page by selecting the **SAVE+CLOSE** link at the bottom of the *Notes* page.

The annotations for a given page are retained by the computer and will be shown whenever you return to the *Notes* page later.

2.1.12 Print Text Preview

Printable text items can be previewed:

- Choose **Print Text Preview** in the **File** menu.

2.1.13 Printing

Printing of Sample Snapshots:

- From the **File** menu, select **Print Sample Image...**.

Printing of Plots:

- Select the plot (it has a red border around it if selected).

- From the **File** menu, select **Print Active Plot...**.

Printing of Text Panel:

- From the **File** menu, select **Print Text...**.

Printing the Properties Table:

Use the computer's screen-capture facility (many machines have a special "Print Screen" key):

- Paste the screen shot into any picture editing program.

- Using the editing features of the picture editing program, crop the screenshot around the Table of Properties.

- Print the cropped picture directly from the picture editing program.

Printing of the Entire Screen:

- Use the screen-capture facility of your computer—many machines have a special "Print Screen" key.

- Paste the screen shot into any picture editing program.

- Print directly from the picture editing program.

2.1.14 Periodic Table

To display a periodic table of the elements:

- From the **Tools** menu, select **Periodic Table . . .**

The periodic table can be displayed with the following color overlays:

- *Default*: ***ODYSSEY*** atom colors

- Coloration by standard state (gas, liquid, or solid)

- Coloration by metallic character (metallic, semimetallic, or nonmetallic character)

- Coloration by valence electron configuration (s/p/d/f blocks; noble gases)

2.1.15 Short-Cut Menus

To access short-cut menus ("contextual" menus):

- Right-click (shortcut menus are available in the sample and text areas). On a Macintosh with a trackpad (or one-button mouse), use CTRL + Click. With a Windows touchscreen, use *long* press.

2.1.16 Copy and Paste

The clipboard is enabled (in the **Edit** menu, select one of three **Copy** options). This allows for easy export of pictures and data to Word documents, PowerPoint presentations, etc.:

- *Screenshots* can be retrieved from the sample area: Use **Copy Sample Image**

- *Plots* can be retrieved from the plots area: select the plot, then select **Copy Active Plot**

2.1.17 Answer Key*

For any individual page, the visibility of the answer key can be toggled on and off by selecting the ANSWERS icon at the top of the text panel.

To automatically show the answer key for *all* pages:

- From the **Tools** menu (Windows) or the **Odyssey** menu (Macintosh), select **Preferences...**

- Check **Show Answers by Default**.

2.2 Simulations and Samples

2.2.1 Starting and Stopping Simulations

Most molecular samples can be subjected to *molecular dynamics simulations* (= physical simulations in time):

- Use the ▶/⏸ button below the molecular sample in order to initiate and stop the simulations.

- Use the ⏭ button in order to advance in small time increments.

- Use the ⏮ button in order to go backwards in time in small increments.

* *Instructor's Edition only*

The choice of time step reflects the size of the system as well as expectations regarding the accuracy of such simulations. For large, user-built systems (>50 atoms) that have bonded hydrogen atoms, the timestep is initially set to 1 fs. For large user-built systems that contain no hydrogens, the time step is initially set to 2 fs and for user-built monatomic systems (such as noble gases), it is set to 5 fs. If simulations seem to progress with an occasional "slow-down" of all particle motion, this is due to automatic adjustments in the simulation procedure.

Note: The default time steps of user-built systems are chosen to allow for efficient simulations that advance quickly. For greater accuracy, and particularly to better resolve intramolecular vibrations, smaller time steps need to be chosen.

2.2.2 Sequences of "Frames"

Some samples (particularly those with "surfaces") can be viewed in a sequence that is *not* related to physical time:

- Use the  button below the sample to start and stop an animation of these sequences. Note that what is shown is *not* a physical simulation, but a simple animation of a number of prerecorded "frames".

- Use the  button to move one frame ahead in the sequence.

- Use the  button to move one frame back in the sequence.

- Use the  slider to manually control the sequence animation.

2.2.3 Switching Samples

Many pages have more than one sample associated with them. You can switch between them in two ways:

- The standard way to switch between samples is via radio buttons embedded in the text.

- Alternatively–and in particular if the text panel is hidden–

samples can be selected from the *pull-down menu* in the upper left corner of the sample area.

2.2.4 Moving a Selected Molecule within a Sample

A selected molecule (in samples where there is more than one molecule) can be moved relative to the other molecules:

- You can rotate the selected molecule by holding down the CTRL key while dragging the molecule (with the *left* button depressed when using a trackpad or mouse).

- You can translate the selected molecule by holding down the CTRL key while dragging the molecule after a long press (touchscreen) or with the *right* mouse button depressed (touchpad or mouse). Macintosh trackpad: Hold down the CTRL and ⌘ keys while dragging.

If you do not hold down the CTRL key while dragging, the rotation (left button) or translation (right button) will apply to the *entire* sample (= all molecules).

2.2.5 Changing Chirality

Tetrahedral stereocenters of chiral molecules can be inverted using ***ODYSSEY***. You can either invert all of the stereocenters simultaneously (thus generating the enantiomer) or invert individual stereocenters:

- To invert all of the stereocenters simultaneously, show the shortcut menu for any of the atoms and choose **Invert Molecule Chirality**.

- To invert just one stereocenter, show the shortcut menu for the stereocenter and choose **Invert Atom Chirality**. Alternatively, double-click/double-tap on the stereocenter while holding down the CTRL key (Windows) or the key (Macintosh).

Note: Only tetrahedral stereocenters can be inverted, not octahedral stereocenters.

2.2.6 *Saving Samples*

The currently displayed sample can always be saved as an `.xodydata` file into locations outside of the ***ODYSSEY*** folder (the ***ODYSSEY*** folder is Read Only in order to preserve the integrity of the software):

- From the **File** menu, select **Save Sample As...**.
- Navigate to the desired location, select a filename, and save the file.
- The saved sample is shown in a new tab.

The following restriction applies when saving samples:

- "Surface" information (Orbitals, Electron Density Distributions, Electrostatic Potentials, Polarity Maps) is not saved.

For export to Wavefunction's program ***SPARTAN***, samples can be saved in the `.spinput` format. Note that all "simulation cell-specific" information (such as the bounding box) is lost when saving in this format.

For exporting to other programs, the SMILES connectivity format can be used. You need to be in **Expert Mode** (See 2.7.7) to save in the SMILES format. Note that for charged species, the entire molecular charge will be assigned to a single atom.

2.2.7 *Saving Screenshots of Samples*

Screenshots of molecular samples can be saved:

- From the **File** menu, select **Save Sample Image As...**
- Choose a file name and one of the following file types:

  .jpg (compressed) - Windows and Macintosh

  .png (compressed, no loss) - Windows and Macintosh

  .bmp (uncompressed) - Windows only

- Save the graphics file to the desired location.

Tip: For best resolution, zoom in prior to saving the screenshot. In the Instructor's Edition, you can furthermore hide the text panel using the corresponding toolbar icon.

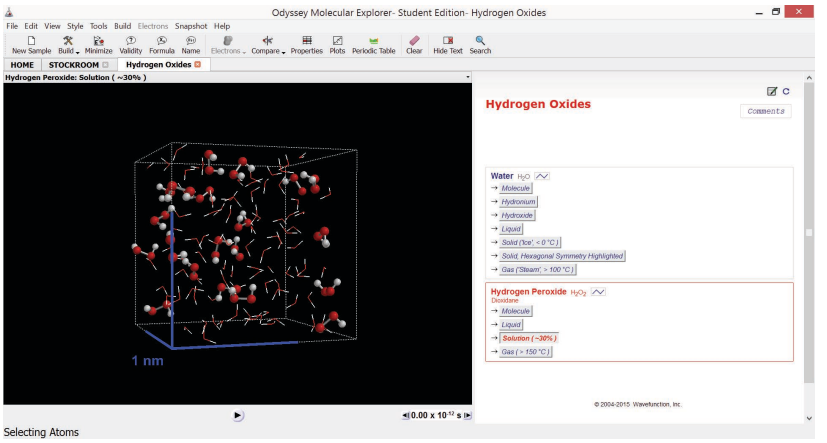
The *clipboard* (**Edit→Copy Sample Image**) can also be used to export pictures.

2.3 Visualization

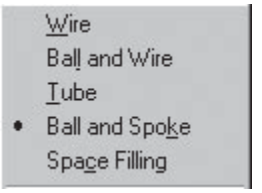
2.3.1 Styles

Molecular samples can be displayed in a variety of styles that are best illustrated using an example:

- On the **Molecular Stockroom** page, find "Hydrogen Peroxide" (use the Search capability or go directly to the **Hydrogen Oxides** page). Choose **Hydrogen Peroxide** as an **Aqueous Solution**.



- Try out the five styles, all available in the Style menu:



- The appearance of individual *atoms* can be customized:
  - From the **Edit** menu, choose **Select Atom** (which is, incidentally, the default).
  - Select any atom. The atom becomes highlighted. From the Style menu, choose the desired style (e.g., **Ball and Wire**).
  - Select the background to deselect the atoms.
- The appearance of *molecules* can also be customized:
  - From the **Edit** menu, choose **Select Molecule**.
  - Select one atom from one of the molecules (e.g., water). All atoms of the selected molecule become highlighted. From the **Style** menu, choose the desired style (e.g., **Space Filling**).
  - Select the background to deselect the atoms.
- Finally, the appearance of entire groups can be customized:
  - From the **Edit** menu, choose **Select Group**.
  - Select one atom from one of the groups (e.g., water). All atoms of the group become highlighted. From the **Style** menu, choose the desired style (e.g., **Tube**).
  - Select one atom from the other group (e.g., hydrogen peroxide). All atoms of *that* group become highlighted. From the **Style** menu, choose the desired style (e.g., **Ball and Spoke**).
  - Select the background to deselect the atoms.
- The **Hide** style turns off the visual display of parts of a system

(or even of *all* atoms of a system; useful if "Ribbon" or "Surface" displays are in place):

- From the **Edit** menu, choose **Select Group**.
- Select one atom from one of the groups (e.g., hydrogen peroxide). From the **Style** menu, select **Hide**. Only the other group remains visible.
- Select the background to deselect the hidden atoms.

- If the **Hide** style is invoked for all atoms of a system and the screen goes blank, the sample is not really gone. Just choose **Select All** from the **Edit** menu. Then, choose one of the regular styles from the **Style** menu and the sample will reappear.
- Atoms can also be selected depending on where they are drawn on the screen:
  - Depressing *both* buttons while dragging defines a rectangular screen area within which all atoms are selected.*

2.3.2 Hydrogen Bonds

To turn on hydrogen bond display (if such bonds are present in the sample):

- From the **Style** menu, select **Hydrogen Bonds**.

2.3.3 Lone Pairs

To display a *schematic* representation of lone pairs (where applicable):

- From the **Style** menu, select **Lone Pairs**.

Note: The schematic visualization of lone pairs is not always available. Lone pairs are never available for noble gas-like unbonded atoms or ions.

* *Not available for the Windows touchscreen and the Macintosh trackpad.*

2.3.4 *Dipole Arrows*

To turn on the display of molecular dipoles (*if* dipoles are present in the sample):

- From the **Style** menu, select **Dipole Arrows**.

Dipoles can be turned on *selectively*:

- Use **Select Molecule** or **Select Group** in the **Edit** menu (see the "Styles" section above for a demonstration of the "Select" feature) prior to turning on the dipole display.

2.3.5 *Collisions*

Display of collisions via "halos" can be turned on for gases, provided the physical density of the gas is not too large:

- From the **Style** menu, select **Collisions**, and then choose what type of collisions to display. The choices are **Molecule-Molecule**, **Molecule-Wall**, **All** or **None**.

2.3.6 *Reactive Events*

When reactions are allowed in the system, ***ODYSSEY*** can highlight the active reactions to make them easier to find.

- From the **Style** menu, select **Reactive Events** to toggle the highlighting of reactions.

2.3.7 *Trails*

Molecular trails or "trajectories" can be graphically traced:

- From the **Style** menu, select **Trails**.

Trails can be turned on *selectively*:

- Use **Select Molecule** or **Select Group** in the **Edit** menu (see the "Styles" section above for a demonstration of the "Select" feature) prior to turning on the trails display.

2.3.8 Velocities

Molecular velocities can be displayed graphically for systems with low enough densities:

- From the **Style** menu, select **Velocities**.

Velocities can be turned on *selectively*:

- Use **Select Molecule** or **Select Group** in the **Edit** menu (see the "Styles" section above for a demonstration of the "Select" feature) prior to turning on the velocities display.

Note: This attribute is not available for higher density samples.

2.3.9 Clipping Feature

The display of many molecular samples can be greatly simplified by only displaying atoms that are close to a user-set "center."

Using the clipping feature requires two steps:

- *Setting the Clipping Center:*

  Select an atom from the shortcut menu (right-click; touchscreen: long press; Macintosh trackpad: CTRL + Click), then select **Set Clipping Center**.

- *Choosing a Clipping Sphere Radius:*

  Select the clipping sphere by selecting the sphere (selection is indicated by a color change). Use the usual *zoom-in/zoom-out* functionality to adjust the size of the clipping sphere (use the scroll wheel or drag the mouse with the right-mouse-button + SHIFT key depressed or use a two-finger scroll if available for your touchpad or trackpad). Select the background when done.

Once a clipping center has been set, the use of clipping can be toggled from the menu bar:

- From the **Style** menu, select **Clipping**.

2.3.10 Charge Labels

To turn on the display of charge labels:

- From the **Style** menu, select **Charge Labels**, and then choose either **Net (Ionic)** or **Partial (Atomic)**.

2.3.11 Molecular Properties as a Color Value

Molecules can be colored according to their instantaneous kinetic energy, dipole moment or instantaneous binding energy (the bonding energy of a molecule and the energy of interaction of a given particle with all its neighbors).

- From the **Style** menu, select **Color by Property**.

- In the submenu, choose from **Translational Kinetic Energy**, **Binding Energy, Dipole Moment** or **None**.

The color scale ranges from *blue* through *white* to *red*:

- *Blue*: small kinetic energy / very negative binding energy / small dipole moment magnitude.

- *White:* intermediate values

- *Red*: large kinetic energy / less negative (or positive) binding energy / large dipole moment magnitude

As the simulation progresses, the numerical limits for defining the color scale are generally held constant. The range is never reduced; it is expanded if a smaller minimum or larger maximum is encountered. To display a particular range of values, open the **Style** menu, select **Color by Property** and then choose **Customize...**. If you select the **User-Defined** check box, you can then set the low and high values used for the coloration. Each of the three properties has its own range.

2.3.12 Ribbon Displays

Proteins and nucleic acids that contain explicit residue information (this includes samples that have been built with ***ODYSSEY***'s Peptide

or Nucleotide builder as well as PDB files from the Protein Data Bank) can be displayed as "Ribbon" models with a visual indicator for the backbone of the molecule:

- From the **Style** menu, select **Ribbons** (if the entry does not appear in the menu, then the underlying file does not contain the necessary residue information), then choose what type of ribbon to display. The choices are **Monochrome**, **By Secondary Structure**, **By Strand**, and **By Residue**.

Note: ***ODYSSEY*** uses hidden data to determine the ribbon information. For some files (such as those that have been heavily modified) this information is unavailable and ***ODYSSEY*** cannot display the ribbons needed to highlight the backbone.

2.3.13 Electron Density Displays

For systems with up to 30 atoms, ***ODYSSEY*** is capable of calculating a variety of electronic "surfaces":

- Electron Density Surfaces, both for a **High Density** isovalue and a **Low Density** isovalue

- **Polarity Maps** (Electrostatic Potential Maps)

To generate surfaces and change their appearance:

- From the **Electron Cloud** menu, select the name of the surface, e.g., **Polarity Map**.

- In the lower half of the menu, choose among **Solid**, **Transparent**, **Mesh**, or **Dots**.

2.3.14 Centering and Resizing

To center molecular samples:

- From the **Edit** menu, select **Center**.

To resize molecular samples:

- From the **Edit** menu, select **Resize**.

2.3.15 Comparing Two Samples

Two samples can be shown side-by-side for the purpose of comparing them:

- From the **View** menu (or using the **Compare** icon), select **Side-by-Side**. If you are on a page with multiple samples, you can pick one of them from the list. If there is no list (or if the list does not include what is desired), select **Search for more systems...** Use the search box to identify the desired sample, then select **OK**.

- To facilitate comparisons where samples are "shown on the same footing," the second sample is initially displayed with the zoom setting and style taken from the first sample. You may have to zoom in or out in order to get the desired view.

- One of the two samples always has the focus—it is indicated via a red frame. You change the focus by simply selecting the sample's background.

- A sample can also be compared "to itself". What this means is that a copy of the first sample is created. After creation of the copy, the two samples exist independently and can be manipulated separately.

- You can even compare two *user-built* samples: Create the first sample using the build functionality, then create a copy of this sample with **Compare** before(!) closing the build panel. Now modify the copy as desired (note that you cannot return to build mode after closing the build panel).

By default, only one sample at a time (the one with the red frame around it) can be subjected to simulations. However, the two samples can also be synchronized and run at the same time:

- From the **View** menu (or using the **Compare** icon), select **Synchronize**: The two Stop/Go simulation buttons below the two samples get replaced by one such button in the middle.

Synchronization only applies to the simulation capability—any visualization changes still only apply to the sample with the focus.

2.4 Properties

2.4.1 Measuring Physical Properties

To query the numerical values of physical properties:

- From the **View** menu, select **Properties**.
- From the **Add Property** menu (in the lower left corner), select the desired property, such as **Atom→Electronegativity**.
- If a selection is required, then this is indicated in the column to the right of the properties list; e.g., adding **Mole Fraction** to the list necessitates a **Select Group** action.

Additional properties are added to the panel via the "+ Add Property" button.

- If a property is added to the table, its numerical value will instantly be displayed (*if* it is a "system" property that does not require any selection *and* if the value is available without further need for simulation).
- Selections apply to the *active* property at any given time: You make a property "active" (property field background turns red to indicate selection) by selecting it in the list.
- If a property value is "Pending," then a simulation is required in order to calculate its value. The calculated number is filled in automatically as soon as it becomes available. When applicable, a proper selection (such as two atoms for a distance measurement) *must* have been made.

Some properties have both averaged and instantaneous values. To change between these, first select the property by selecting its name. If that property can be changed between averaged and instantaneous, a button (▾) will appear to the right of the property name. Selecting this button will let you choose between **Averaged** and **Not Averaged**.

Only properties that apply to the given molecular sample are

displayed, e.g., the entry **Mole Fraction** is absent for one-component systems or individual molecules.

To delete or hide property information:

- Any individual property can be removed from the list by selecting it (which makes it the *active* property) and by then selecting the ✕ icon to the right of "+ Add Property ▾."

- The entire "Properties" panel can be hidden by selecting the ⊠ icon ("local close button") in the upper right hand corner of the panel. The operation only *hides* the panel, i.e., it does *not* erase the property information.

2.4.2 Changing System Parameters

System parameters of bulk matter samples can often be changed. For these properties, a *slider* will appear when you select the property. The property can be changed by adjusting the slider, even while the simulation is in progress. (In the Windows version only, the value can also be changed with vertical *spinners*.) Some of the properties that can be changed are:

- *Temperature:*

  Add **Thermodynamics→Temperature** to the list of properties.

- *Volume:*

  Add **Thermodynamics→Volume** to the list of properties.

- *Number of Molecules/Atoms in One-Component Systems:*

  Add **System→Total Number of Molecules** (or **System→Total Number of Atoms** if monoatomic) to the list of properties.

- *System Composition in Multi-Component Systems:*

  Add **Composition→Number of Molecules** (or **Composition →Number of Atoms** if monoatomic) to the list of properties. Then select any group.

Note: In two-dimensional systems, **Area** replaces volume.

2.4.3 Changing Slider Limits

Built-in limits for temperature, volume, and composition sliders can be overwritten by explicitly requesting a property value outside of the default range:

- Select the numerical value field for the property and enter your desired value (excluding units).

Note: The limits of the corresponding slider are updated to include the newly requested value.

2.5 Plotting

2.5.1 Requesting Plots

ODYSSEY can generate numerous types of XY plots. In addition, ***ODYSSEY*** reports three kinds of histograms (for the molecular speeds, molecular kinetic energies, and dipole moments).

To request a plot:

- From the **View** menu, select **Plots**.

- Individual plots are added to the panel via the "  " button. You can add as many plots to the plots panel as you wish.

To clear a plot (= erase the data points):

- Select the  icon at the top of the plots panel.

To delete or hide plots:

- Any plot can be *removed* from the "Plots" panel by selecting it (= making it the *active* plot) and then selecting the  icon to the right of "  ."

- The entire "Plots" panel can be *hidden* by selecting the icon

("local close button") in the upper right hand corner of the panel. The operation only *hides* the panel, i.e., it does not erase the plot data.

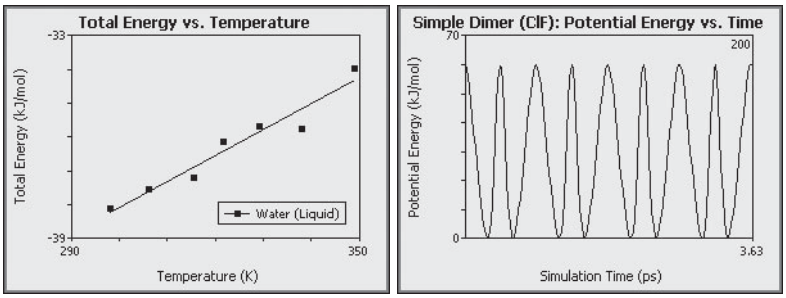
2.5.2 XY Plots

Most plots are obtained by actively recording measurements as a simulation is in progress or by following the time evolution of a selected property over the course of a similation. Examples include:

- *Total Energy* as a function of *Temperature*
- *Potential Energy* as a function of *Time*
- *Entropy* as a function of *Temperature*

More complicated plots that incorporate data from multiple samples can also be generated (see **Advanced** options below).

Examples of XY Plots



To generate an XY Plot (once the plot pane is up, see preceeding section):

- In the Plots panel, select the " Add Plot " button.
- From the list, select **XY Plot…**.
- Select the property for the *X Axis* and select the property for the *Y Axis*.
- You can choose **Use Average** and **What to plot** (the value, 1/value, log(value)) or use the defaults.
- Additional options can be invoked by selecting **Advanced**. Depending on the sample and X/Y properties chosen, the following may be available:

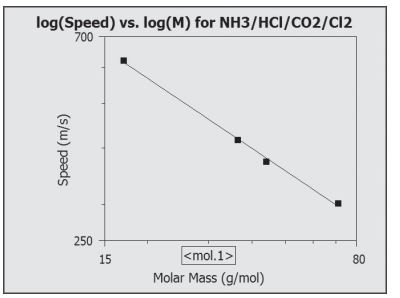
- **"Allow for multiple curves, with one curve for each sample"**

  This option will generate a plot with multiple curves. Each curve corresponds to a sample and recording data will add datapoints to the curve for the selected sample. The sample can be changed by either choosing among the samples in the text or by using the drop-down menu above the sample. *Only available for experiments with multiple samples*.

- **"Different samples are datapoints in a single curve"**

  This option generates a plot with each sample corresponding to a single datapoint. The record button is *not* active. If you choose this plot type, you may need to run each sample briefly to get that sample's datapoint to appear. The datapoint for the current sample is shown in yellow. As you run any of the samples, the datapoint that corresponds to that sample will move as the property values change. *This is only available for experiments with multiple samples.*

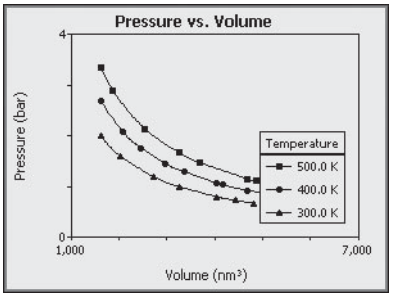
Example of a plot where different samples are datapoints in a single curve



- **"Allow for multiple curves that differ in the following parameter"**

  This option generates a plot that can have multiple curves. After choosing this option, you must select a property from the list. All of the datapoints that you record with the same value of this parameter will be in one curve. If you change the parameter property, the new datapoints you record will be in a separate curve on the same plot.

Example of an XY plot with a parameter



ODYSSEY automatically assigns different symbols for datapoints of different parameter values.

- **"One curve"**

  This option will generate a plot where each datapoint that is recorded is placed in a single curve. *This is only available for experiments that have a single sample.*

- Select **Next**.

- Choose among **Scatter Plot**, **Linear Fit**, **Point-to-Point**, and **Smoothed Fit**.

- If the axis property requires a selection, a rectangle will appear near the axis label. Select this rectangle (to make it active) and then select the desired entities in the model.

While the simulation is in progress, select the icon ("Record") in order to generate datapoints. Typically this is done while systematically varying one of the two properties (such as *Temperature* or *Volume*). The record button does not "light up" until sufficient data have been accumulated to allow for measurement. This may take several seconds or more for a given simulation.

ODYSSEY autoscales the X and Y axis ranges based on the minimum and maximum values that are encountered. If one of the limits exceeds the previous value, the range is updated.

Note: The resolution of plots with "Time" as the independent variable is not sufficient to capture extremely fast fluctuations, such as the potential energy (or intramolecular geometry) of *hydrogen*-containing flexible molecules.

2.5.3 Customizing XY Plots

To change the title, curve fit, or plotting function of a plot:

- Make the plot "active" by selecting it.
- Bring up the "Plot Edit" panel by selecting the  icon at the top of the plots panel.
- Several items can be customized:
    - Plot *Title*
    - *Labels* for the X and Y Axis
    - *Grid Lines* for the X and Y Axis
    - Explicit *Range* for the X and Y Axis
    - *Curve Fit* of **None**, **Point-to-Point**, **Smoothed Fit**, or **Linear Fit**.
    - Plotting function (e.g. X, 1/X, log(X))

2.5.4 Moving the Plot Legend

To move the legend of plots (e.g., in order to expose datapoints "hidden" behind the legend):

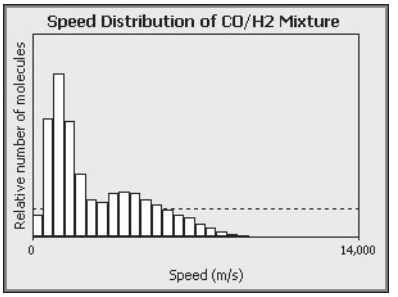
- Position the cursor on the legend, select, and drag.

2.5.5 Speed, Kinetic Energy, and Dipole Distributions

Three kinds of histograms can be generated:

- *Speed Distribution*: A histogram showing the probability of encountering speed values.
- *Translational Kinetic Energy Distribution*: A histogram showing the probability of encountering translational kinetic energy values.
- *Dipole Distribution:* A histogram showing the probability of encountering dipole moment values.

Example of
a Histogram
(Speed Distribution)



To generate a histogram:

- From the **View** menu, select **Plots**.
- From the list of "Plots" (upper left corner of the Plots panel), select either **Speed Distribution**, **Translat. Kinetic Energy Distribution**, or **Dipole Distribution**.

The appearance of a histogram can be customized:

- Make the histogram "active" by selecting it.
- Bring up the "Plot Edit" panel by selecting the icon at the top of the plots panel.
- Items available for customization include:
  - The histogram *Title.*
  - The histogram *Style*: **Bar** or **Line**.
  - The *Samples* setting: The default is **Single**. If set to **Multiple**, histograms for multiple samples (then automatically forced to be in the *Line* style) can be shown in the same plot.
  - *Labels* for the X and Y Axis.
  - The histogram range for the X Axis.
  - The number of tickmarks for the X Axis.
  - The number of histogram *Bins* within the range.

2.6 Building Your Own Samples

2.6.1 General Building

Opening the Model Kit:

- **File→New** creates a new molecular sample (without an accompanying text panel). The new model is in its own tab.

- **Build→Add** (and also **Build→Delete**) opens the builder to allow modifications of the shown molecular sample in the current experiment (the text panel is unchanged).

Adding to the sample:

- Select a building block from build panel.

- If starting with an empty sample, select the sample area to make the fragment appear. If a molecular structure already exists, select one of the *free valences* ("yellow spokes") of that structure to attach the fragment.

- Build your molecule by repeating the above steps.

- To start a new molecule *without* a connecting bond, *double-click* (or double-tap if using a touchscreen) on the background.

Deleting atoms:

- Selection of **Build→Delete** switches the program to "Delete Mode." Every selection will now delete the selected atom *until you leave* Delete Mode (usually by returning to **Build→Add**).

- Selection of **Build→Break Bond** switches the program to "Break Bond Mode." Every selection will now break the selected bond *until you leave* Break Bond Mode (usually by returning to **Build→Add**).

Changing the geometry:

- To change the *bond length*: Select a bond by double-tapping or

double-clicking on it. Hold the ALT key down and drag with the *right* button depressed. (*Note:* This does not work if the selected bond is part of a ring structure.) Touchscreen: Drag after a long press. Macintosh trackpad: Hold down first the OPTION/ALT key and then the ⌘ key while dragging.

- To "*rotate*" around bonds (that is, to change the dihedral angle): Select a bond by double-tapping or double-clicking on it. Hold the ALT key down and drag with the *left* button depressed. (This does not work if the selected bond is part of a ring structure.)

- To create *new* bonds: Select **Build→Make Bond** and select the *free valences* of any two atoms. (Note that the program will *continue* to create new bonds until you leave "Make Bond" Mode!)

Moving unconnected molecules relative to each other:

- Hold down the CTRL key while dragging the selected molecule with the left button depressed (→ rotate) or right button depressed (→ translate; Macintosh trackpad: Hold down the ⌘ key).

Minimizing the energy:

- From the **Build** menu, select **Minimize**. It is a good idea to do this at the end of the build session or even during the building procedure.

Correcting mistakes:

- From the **Edit** menu, choose **Undo** to undo an unwanted change. Undo can be applied multiple times to undo a series of unwanted changes.

- From the **Edit** menu, choose **Redo** to reapply the change reverted by Undo.

- To clear the entire sample, open the **Edit** menu and choose **Clear Sample**.

Finishing a build session:

- Select the **Close** ⊠ button in the upper right corner of the build panel.

- Selecting the **Start/Stop** button ( ) below the new sample also disables the builder and starts a room temperature simulation of the constructed system.

Other options and considerations:

- Hydrogens don't need to be added explicitly (all free valences will automatically convert to hydrogens at the conclusion of the build session).

- The toolbar (opened by selecting **Toolbar** in the **View** menu) gives access to convenient icons for essential building operations (**Add**, **Delete**, **Make Bond**, **Break Bond**, and **Minimize**).

- ***ODYSSEY*** requires explicit charges when building ions. Select **Set Charges...** in either the **Entry-Level** or **Advanced** builder, then use the up/down arrows to set the **molecular charge**. In build mode, charge is displayed for all charged species. *New molecules are always inserted with zero charge.*

2.6.2 Entry-Level Builder

Using the common organic building blocks present in the Entry-Level Builder, you can easily build complex organic molecules. To facilitate building common organic groups, sets of Groups and Rings are provided. To use these, select the **Groups** or **Rings** button, and then use the drop down menu to select the fragment of interest.

2.6.3 Advanced Builder

After opening the model kit:

- Switch to **Advanced** in the drop-down menu in the upper left corner.

- Select an **Element** from the drop-down periodic table (*argon* is the default).

- Select one of 12 different types of **Coordination** (the number and orientation of covalent bonds)

- To change the *bond order*: Select one of the four **Bond Order** icons, then double-tap or double-click on any existing bond. (The second bond type is for "partial double" or aromatic bonds.)

- To declare non-zero charges of built molecules, select **Set Charges**. In the subsequent dialog, use the up/down arrows to adjust the **molecular charge** for each molecule for which you need a non-zero charge.

Other options and considerations:

- The atom types can be changed at any time—simply select a new **Element** from the drop-down periodic table and double-tap or double-click on the atom(s) to be changed. (This does not change the number of valences.)

- Building of coordination compounds is facilitated with special building blocks from the **Ligands** drop-down menu at the bottom of the build panel.

2.6.4 Solid Builder

ODYSSEY's molecular builder includes a number of prototypical solid structure types. After opening the model kit, switch to **Solid** (drop-down menu in the upper left corner).

- In the drop-down menu in the Solid panel, pick one of five types: **Ionic Solids**, **Metallic Solids**, **Molecular Solids**, **Covalent Network Solids**, or **Bravais Lattices**.

- Select one of the structures in the corresponding submenu. Tap or click in the sample area to make the solid structure appear.

- You can change the number of replications of the basic cell with the Replication fields. (A reasonable default is provided that is big enough to be interesting but small enough to simulate effectively.)

- For many of the solid types, you can also change the atom types and the charges. For example, there are several different solids that have the same structure as Sodium Chloride. ("Sodium Chloride Type" is available in the Ionic Solids section.) Both

NaCl and CaO have this structure, but to build CaO, you would need to change Na to Ca and change Cl to O, then make sure that the charges are +2 and -2, respectively. For known structures the correct cell size is used, otherwise a rough estimate is used.

Note: 1) If the "start" button below the sample is faded out, the structure cannot be subjected to simulation. 2) The dimensions of the solid unit cell can be changed with the **Solids** tab of the **Simulation Cell** Builder.

2.6.5 Peptide Builder

After opening the model kit, switch to **Peptide** in the drop-down menu in the upper left corner.

- There are three different options for building peptides: **Single Amino Acid**, α **Helix**, and β **Sheet**. You can choose between these using the radio buttons at the bottom of the peptide builder.

- For the **Single Amino Acid** selection, the chosen amino acid is displayed and can be inserted by clicking/tapping (or double-clicking/double-tapping for non-empty samples) on the background.

- For α **Helix** and β **Sheet**, selecting the amino acids adds them to the sequence panel. The amino acid sequence can be inserted by clicking/tapping (or double-clicking/double-tapping for non-empty samples) on the background. The sequence panel can be cleared by selecting the **Clear** button.

2.6.6 Nucleotide Builder

After opening the model kit, switch to **Nucleotide** in the drop-down menu in the upper left corner.

- There are five different options for building nucleotides: **Single Nucleotide (DNA)**, **Single Nucleotide (RNA)**, **DNA (Double Strand)**, **DNA-RNA**, and **RNA (Single Strand)**. You can choose between these using the radio buttons at the bottom of the nucleotide builder.

- For the **Single Nucleotide** selections, the chosen nucleotide is displayed and can be inserted into an empty sample by selecting the background. (You can only insert with the Nucleotide Builder into empty samples. To clear the sample, open the **Edit** menu and select **Clear Sample**.)

- For the three strand selections, selecting the nucleotide adds them to the sequence panel. The sequence panel can be cleared with the **Clear** button. The nucleotide sequence can be inserted into an empty sample by selecting the background.

2.6.7 Bulk Sample Builder

To build bulk samples that are confined to containers with rigid walls (appropriate for gases):

- Use the molecule builder to build one molecule of each component of a mixture. (It does not matter how the molecules are spatially arranged.)

- From the **Build** menu, select **Simulation Cell**. By default, the molecule is in **Vacuum** at room temperature. (The **Temperature** can be explicitly declared in a textbox.)

- Switch to the **Gas** tab for building samples of gas. Declare the desired **Temperature** and **Pressure** in textboxes at the top of the cell build panel.

- Declare the desired number of molecules using the textbox that is labeled with the empirical formula of the molecule. For multicomponent mixtures, more than one textbox is present.

- The ratio of the simulation cell side lengths (aspect ratio) can be set at the bottom of the cell build panel (**Cell Ratio**). The default is for a cubic cell.

- Select **Apply** to initiate the creation of the simulation cell. A progress bar will be displayed that indicates the progress of the build operation.

To build bulk samples that use periodic boundary conditions (appropriate for liquids and solutions):

- Start similarly to building gases, but switch to the **Liquid** tab after bringing up the **Simulation Cell** build panel. Declare the desired **Temperature** and **Density** at the top of the panel. Declare the desired number of molecules using the textbox(es) that is (are) labeled with the empirical formula(s) of the molecule(s).

- The ratio of the simulation cell side lengths can be set at the bottom of the cell build panel (**Cell Ratio**). The default is for a cubic cell.

- By default, periodic boundary conditions will be used for all three dimensions. Use the drop-down **Periodic Boundary Conditions** menu at the bottom of the panel to limit the periodicity to less than three dimensions; rigid walls will be used instead. (If you request rigid walls for all three dimensions, the resulting sample will have three rigid walls, like a gas sample.)

- Select **Apply** to initiate the creation of the simulation cell. A progress bar will be displayed that indicates the progress of the build operation.

- If the simulation cell building step does not finish after a few minutes, then **Abort** and repeat with a set of "less challenging" system conditions.

To change the temperature and/or density of *existing* solid samples (retrieved from the stockroom or built with the **Solid** builder):

- Switch to the **Solid** tab after bringing up the **Cell** build panel.

2.6.8 Adding Labels

Labels (as many as desired) can be attached to all samples:

- Select **Build→New Label**, then *double-click* (or double-tap) on the background. Add any text.

- To edit an existing label, select the label from its shortcut menu (right-click; touchscreen: long press; Macintosh trackpad: CTRL + Click) and select **Edit Label**.

- To move an existing label, select the label and use the same method that you use otherwise for translating individual

molecules (see Section 2.1.5).

- To delete a label, select the label from its shortcut menu (right-click; touchscreen: long press; Macintosh trackpad: CTRL + Click) and select **Delete Label**.

2.6.9 Changing Chirality While Building

Tetrahedral stereocenters of chiral molecules can be inverted by *double-clicking* (or, where applicable, *double-tapping*) on the stereocenter while holding down the CTRL key (Windows) or the ⌘ key (Macintosh).

You can also invert stereocenters via the shortcut menu (right-click; touchscreen: long press; Macintosh trackpad: CTRL + Click) choose **Invert Molecule Chirality** (will invert all stereocenters simultaneously) or **Invert Atom Chirality** (will invert just the selected stereocenter).

2.6.10 Energy Minimization

To minimize the energy of a sample:

- From the **Build** menu, select **Minimize**.

Systems with a boundary (typically gases, liquids, or solids) are minimized at *constant volume*.

For some samples, the energy minimizer and the dynamics option are deliberately disabled. If you really must minimize the energy of such a system, you can still do so after *saving* the sample as a new file.

2.6.11 Name Structure

To find the name of a molecule or system:

- From the **Build** menu, select **Name**.

If it can, ***ODYSSEY*** will report the name of the molecule(s). Molecules with more than 200 atoms cannot be named. For many common molecules, ***ODYSSEY*** will display both the systematic name and the common name.

2.6.12 Evaluate Structure

ODYSSEY contains a facility to evaluate the chemical reasonableness of user-built or pre-built structures. To use this feature:

- From the **Build** menu, select **Validity**.

ODYSSEY will produce a list of questionable bonding centers, or will report that the model seems reasonable.

Note: Structures with more than 2,000 atoms cannot be evaluated.

2.7 Preferences

2.7.1 Setting the Text Size

The text size can be altered independent of the screen resolution:

- From the **View** menu, select **Zoom Text→Zoom In (**or **→Zoom Out)**.

The program will remember your choice in future sessions.

2.7.2 Physical Units

ODYSSEY uses the following default settings for property units in the *Properties* panel and in *Plots*:

Length:	nm/pm
Temperature:	°C
Pressure:	atm
Energy:	kJ/mol

To change the default settings:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.

- Adjust the radio buttons within Units to reflect your desired settings.

ODYSSEY will apply new settings to current and future sessions.

2.7.3 Boundary Display Style

ODYSSEY generally employs "Periodic Boundary Conditions" when simulating condensed phase samples (liquids and solids).

By default, the visualization is such that the molecules "leave" and "re-enter" the simulation cell as "complete entities". In a second visualization style, the molecules are shown "clipped" when positioned on one of the boundaries, i.e., part of a given molecule is shown on one side of the simulation cell and part on the other side. (This doesn't necessarily mean that the molecules get physically clipped–molecules usually interact as "complete entities".) To make this alternative style the default setting:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.

- Select **Alternate Visualization of Periodic Boundaries**.

- Select **OK**.

Note that the underlying simulations are completely unaffected by the visualization setting. Also, note that some systems (such as liquid sulfur) have a *fixed* setting for the boundary visualization, i.e., they are unaffected by the default setting in **Preferences**.

2.7.4 Hydrogen Bonds Style

By default, hydrogen bonds are drawn as thick broken (dashed) lines so as to be easily recognizable in complex systems. For a more subtle display of hydrogen bonds:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.

- Uncheck **Emphasize Hydrogen Bonds**.

- Select **OK**.

2.7.5 Color Preferences

The default colors of the background and atom types can be set by the user:

- From the **Edit** menu, select **Color**. Select either the *background* or an *atom* of the desired chemical element.

- Adjust the mix of the three primary colors as desired (or select **Default** for a reset).

- Close the dialog by selecting .

Note that the color settings are global, i.e., they affect the display of *all* samples once the change has been made.

2.7.6 Reduced Graphics for Slower Machines

The graphical resolution sample can be set to *lower quality* whenever a given model is dynamically updated (either through user-induced rotation or via a physical simulation). This can help speed up the program when used with low performance graphics cards.

To change the graphics performance setting:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.

- Check (select) **Reduced Graphics for Slower Machines**.

- Select **OK**.

2.7.7 "Expert" Setting

The "Expert" Setting is for ***ODYSSEY*** users that are familiar with the details of molecular dynamics simulations. If selected, the following queries are enabled by default:

Properties Panel:

- Potential Energy
- Intermolecular Energy
- Total Energy
- Pressure
- *PV*/*nRT* (Compression Factor)
- Dihedral Angle

Plots:

- Radial Pair Distribution Function

"Expert" users are also able to save samples in the SMILES connectivity format for export to other programs.

To enable the "Expert" setting:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.
- Check (select) **Expert**.
- Select **OK**.

When in **Expert** mode, the **Tools** menu includes an **Expert Keywords...** option. It gives access to an input field where keywords for simulations can be set explicitly, such as:

- TIME_STEP=0.5 - use a fixed time step of 0.5 femtosec
- NVT - use an ensemble where the number of particles, the volume, and the temperature are held constant
- NVE - use an ensemble where the number of particles, the volume, and the energy are held constant
- BOX - enclose the system in a container
- PBC - use periodic boundary conditions
- CUT_OFF=7.0 - evaluate electrostatic interactions up to a distance of 7.0 Angstrom

- SHAKE_BOND - constrain the bond lengths to their equilibrium values

- TEMP_MIN=100.0 - set the minimum allowed temperature to 100 K

- TEMP_MAX=1000.0 - set the minimum allowed temperature to 1000 K

- VOLUME_MIN=10.0 - set the maximum allowed volume to 10% of the initial volume

- VOLUME_MAX=500.0 - set the maximum allowed volume to 500% of the initial volume

Note: These and other keywords are only intended for true expert users, i.e., users who are intimately familiar with the technology of molecular-level simulations. Typical users of ***ODYSSEY*** will never need to declare or alter keywords.

2.7.8 IUPAC and Common Names

Molecules can be shown using their common names or their IUPAC (mostly systematic) names. To change between the two, open the **Preferences** panel: From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), choose **Preferences...**. Then check or uncheck the "Use IUPAC Names" option. Select **OK** to save your choice.

2.7.9 Dipole Orientation

Samples with dipoles can either be displayed with the arrow pointing from positive to negative or from negative to positive (the latter is the IUPAC default). To change between these two settings, open the **Preferences** panel (from the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), choose **Preferences...**). Then check or uncheck the "Dipoles Negative to Positive (IUPAC)" option. Select **OK** to save your choice.

2.7.10 Sound Effects

The user can control whether a sound effect is generated whenever one of the **Style→Collisions** options is selected *and* two molecules collide.

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**.

- Check (or uncheck) **Play Sounds**.

2.8 Using ODYSSEY with Other Programs, Files, and Documents

2.8.1 Reading PDB, XYZ, SMILES, ChemDraw, and ISIS/Draw Files

ODYSSEY imports standard PDB files: (`.pdb`), XYZ files (`.xyz`), SMILES string files (`.smi`), ChemDraw files (`.cdx`), and ISIS/Draw files (`.skc`)

- Use the **Open...** dialog in the **File** menu.

2.8.2 Compatibility with Wavefunction's SPARTAN

ODYSSEY → SPARTAN:

- Samples must be saved in the `.spinput` format before they can be opened with ***SPARTAN***. All atomic coordinates are fully recognized. However, "simulation cell-specific" information (such as the bounding box) is lost.

SPARTAN → ODYSSEY:

- Files of type `.spartan` can be opened with ***ODYSSEY***. Structural data and visualization features are fully recognized. Minor differences in the display may exist.

- "Surface" data (Electron Densities, Potentials, Orbitals) can only be preserved in the Instructor's Edition and then only by saving an entire lab in the `.odylab` format.

- If quantum mechanical calculations have been run on the file, ***ODYSSEY*** will use the *calculated* atomic charges (scaled so that each molecule has a whole number charge).

- For `.spartan` files that contain just one system, molecular dynamics will be available. For `.spartan` files with more than one system, molecular dynamics will not be available. Instead, a "Frameslider" will be present (see section 2.2.2 for information about Framesliders).

2.8.3 Using ODYSSEY with PowerPoint

ODYSSEY can be hyperlinked in PowerPoint presentations. You have the choice among the following possibilities:

- Hyperlinking individual samples (no accompanying text included)

- Hyperlinking molecular labs*

- Hyperlinking ***ODYSSEY****'s* home page.

The subsequent items provide corresponding instructions.

Note: When you run PowerPoint and use ***ODYSSEY*** hyperlinks, it is useful to open ***ODYSSEY*** beforehand (this makes the opening of simulations faster). It is not necessary to close ***ODYSSEY*** when moving from hyperlink to hyperlink since *one* copy of the program will be used for all of the linked simulations.

2.8.4 Hyperlinking Individual Samples

- Save the sample that you want to hyperlink as an `.xodydata` file in a folder of your choice. Note that "surface" data such as electron densities, potentials, and orbitals) will be lost (→ link through the initial page to access such samples).

* *Instructor's Edition Only*

- Creating the hyperlinks in PowerPoint:

    - Windows: Use the "Hyperlink" attribute and navigate to the location of your saved `.xodydata` file.

    - Macintosh: Use the "Action Settings" attribute (i.e., do *not* use the "Hyperlink" attribute). In the drop-down menu for "Hyperlink to", select "Other File..." and navigate to the location of your saved `.xodydata` file.

*2.8.5 Hyperlinking Molecular Labs**

ODYSSEY molecular labs (teaching units) can be hyperlinked into PowerPoint presentations:

- Switch for the molecular lab that you want to hyperlink from **Normal** to **Text Edit** (at the bottom of the text section).

- Select **Save Lab** (in the lower right corner), and in the subsequent dialog select either **Save as Teacher Lab** (includes comments and answers to questions if any are present) or **Save as Student Lab** (excludes comments and answers). Pick a location of your choice for the `.odylab` file that is about to be saved.

- In PowerPoint create a hyperlink to the saved `.odylab` file – ***ODYSSEY*** will open automatically when selecting the hyperlink in the PowerPoint presentation.

2.8.6 Hyperlinking the Home Page

If you link to ***ODYSSEY***'s initial page, you can access any lab and/or sample, via that hyperlink:

- In your PowerPoint slide, select the object that you wish to hyperlink.

- Right-click and select **Hyperlink**.

- Browse for the name of the ***ODYSSEY*** executable:

* *Instructor's Edition Only*

- Windows: The executable in the ***ODYSSEY*** folder is either "OdysseyStudent.exe" (Student Edition) or "OdysseyInstructor.exe" (Instructor's Edition). In most cases, you will find the ***ODYSSEY*** folder in the "Program Files→Wavefunction" folder.
- Macintosh: The executable is either "Odyssey X.X Student.app" (Student Edition) or "Odyssey X.X Instructor.app" (Instructor's Edition). In most cases, you will find the file in the "Applications" folder.

Selecting the object in the PowerPoint slide (when in presentation mode) will take you to the initial page of ***ODYSSEY***. You can go wherever you wish from there.

2.8.7 Saving ODYSSEY Pictures

Screenshots of samples can be saved in a variety of formats that allow for inclusion in other documents (Microsoft Word files, Web Pages, etc.):

- From the **File** menu, select **Save Sample Image As...**.
- Choose a file name and one of the following file types:

  .jpg (compressed) - Windows and Macintosh

  .png (compressed, no loss) - Windows and Macintosh

  .bmp (uncompressed) - Windows only
- Save the graphics file to the desired location.

Tip: For best resolution, zoom in prior to saving the screenshot. In the Instructor's Edition, you can furthermore hide the text panel using the corresponding toolbar icon.

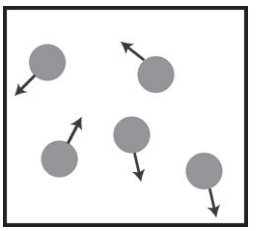
The *clipboard* (**Edit→Copy Sample Image**) can also be used to export pictures.

SCIENTIFIC BACKGROUND

3.1 Molecules in Motion: The Basic Idea Behind Dynamic Simulations

ODYSSEY's simulations are very different from the simulations you may have encountered in other science media products. The motion of molecules does not arise because a human designer used a software tool to create an animation. Instead, ***ODYSSEY*** uses the basic laws of nature in order to represent molecular matter. The motion of molecules is an *outcome* of applying these laws, very much like the forces of gravity determine how the planets in the solar system move. In short, there is no "movie" file anywhere in ***ODYSSEY***.

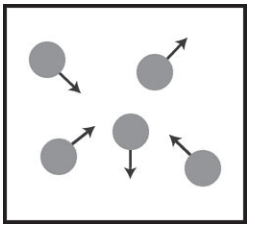
Suppose you want to simulate liquid water. When you load an ***ODYSSEY*** page with liquid water as the sample, you retrieve from a file the positions and velocities of water molecules in a simulation cell *at an arbitrary moment in time*. The following picture symbolizes the "start configuration"—for simplicity we represent water molecules as single spheres:



In order to perform a simulation, ***ODYSSEY*** must do several things:

1. Calculate the *forces* acting between the molecules—this is done using a set of rules that were developed by chemists and other scientists in years of laborious research. While partly empirical, the rules are based on a strict physical analysis of the forces that act between atoms.

   The arrows in the following picture represent the computer's knowledge of the forces acting on the molecules:

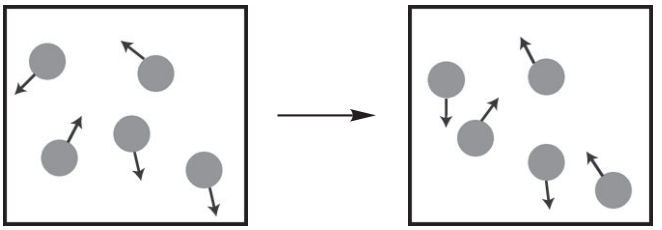


2. Next, ***ODYSSEY*** applies a formula that has been known since 1686! Newton's Second Law states that the force acting on an object and the object's *acceleration* are proportional:

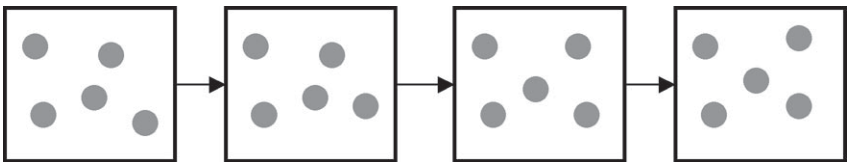
$$F = m \bullet a$$

Since we already know the force acting on a given water molecule (see above) and since the mass of a water molecule is well-known, we can now calculate the molecule's acceleration. Knowing the molecule's acceleration, however, amounts to being able to predict where it will move to and what its new velocity will be! More formally, this is called solving the "equations of motion," and it is really no different than predicting the trajectory and velocity of a satellite that is fired off into space (all we need to know are the "initial conditions").

If we apply this procedure to all water molecules in the simulation cell (in fact, it is applied to all molecules at once), we get the next snapshot of our system, or the next "time step":



Molecular dynamics. In order to sustain a full-fledged simulation, all that is required is to repeat the same steps, again...and again… and again:



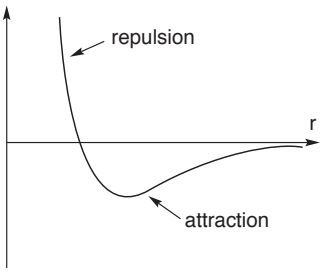
When you watch a simulation of liquid water in ***ODYSSEY***, the computer is calculating "time steps". (The program actually makes several steps between screen updates.) The steps are separated by approximately 10^{-15} sec of physical time—a very short time indeed! Typically, the computer calculates several thousand time steps during a simulation (up to hundreds of thousands of steps for some systems).

In the "start configuration" as well as at any time thereafter, each molecule has not only a position, but also a certain *velocity*. In fact, where the molecule will move to in the next step is affected by both the force acting on the molecule *and* its velocity. The molecule's velocity is updated step after step, just like its position.

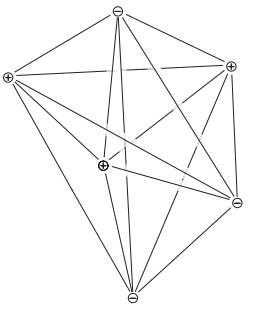
3.2 Calculation of Molecular Interactions

For each sample, ***ODYSSEY*** calculates the energy of interaction between the atoms that are present, regardless of whether the sample is an isolated molecule or a bulk phase with many molecules. The "potential function" is very complicated–there are many hundreds of parameters for the elements and valence states encountered in chemical compounds. At least conceptually, however, the potential function can be thought of containing the following main terms:

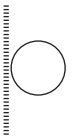
- Intermolecular *attractive* energy: an energy term that represents van der Waals forces (dispersion forces) between non-bonded atoms.
- Intermolecular *repulsive* energy: a steeply repulsive energy term for steric interactions at short distance that makes a close "overlap" of non-bonded atoms very unlikely.



- *Coulomb* energy (both inter- and intramolecular): energy term due to the assignment of "effective charges" to all the atoms of a molecule; at the intermolecular level, this energy represents charge-charge, charge-dipole, and dipole-dipole interactions.

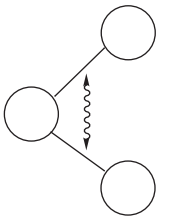


- *Repulsive interactions* between the molecules of the system and the confining walls (if there are any).

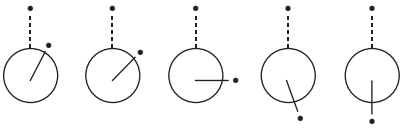


- Intramolecular energy of *bond-stretching*: the spring-like energy that it takes to distort a bond from its equilibrium bond distance. *Note:* This energy term (and sometimes also the following one) does not vary over time if ***ODYSSEY*** keeps the molecular geometry rigid.

- Intramolecular energy of *angle-bending*: the energy that it takes to distort any three bonded atoms from their preferred bond angle.



- Intramolecular energy of *rotation around dihedral angles*: a periodic function that describes the relative energies of the various "staggered" and "eclipsed" conformations of any four consecutively bonded atoms.



There are other terms, but essentially, it is the sum of these energies that yields the total energy of a given system. Calculation of the *derivatives* of the total energy with respect to the coordinates of all atoms yields the intermolecular forces that are at the heart of the algorithm that takes the system from one time step to the next (→Chapter 3.1). As the energy depends on the coordinates of *all* atoms in the system, the calculation must be repeated even when only a single atom moves.

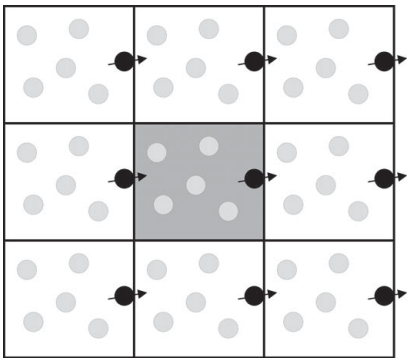
3.3 Why Do Molecules of Liquids Sometimes Disappear?

When you carry out a simulation of a gas in ***ODYSSEY***, you see molecules moving inside a container. That impression is perfectly appropriate: The molecules are confined by rigid "walls" from which they bounce off again and again as the simulation evolves.

However, when you carry out a simulation of a liquid the situation is somewhat different. You may notice that some molecules or atoms seem to *leave* the simulation cell, i.e., when close to one of the boundaries they often seem to be "gone" a few moments later. If you look carefully you will also notice the opposite, namely "new" molecules or atoms that seem to *enter* the simulation cell. Superficially, this coming and going is often perceived as a slight "flicker" at the simulation cell boundaries.

Why does this happen? The answer is that there really aren't any "boundaries" when ***ODYSSEY*** simulates a liquid or solid—despite the obvious presence of a simulation cell! The trick is called *periodic boundary conditions*, and it is the approach which allows us to simulate true bulk matter (i.e., not a few molecules of liquid water, but the substance you get from the tap) even when we only have a very small simulation cell to work with.

Essentially, the simulation cell "wraps around" in each of the three dimensions. A good way to visualize this is to imagine that the simulation cell is surrounded by a set of identical *replicas*:



If a molecule in the center cell moves, then all its "copies" in the replica cells move at the same time—a perfectly coordinated motion.

Focus on the highlighted molecule. If the molecule "leaves" the central simulation cell towards the right, the molecule's replica enters at the same time from the left. In effect, we have allowed the molecule to cross the system boundary while not losing anything—the system density remains perfectly constant.

The huge advantage of this approach is that there are no walls in the system that can interfere with the calculated bulk properties. Just think of a glass of water: The vast majority of the $\sim 10^{23}$ molecules in the glass are *not* close to any of the container walls. Periodic boundary conditions allow us to accomplish the same in a simulation. In effect, the cell boundaries become a device for organizing the simulation rather than a representation of an actual container.

3.4 Rigid Molecules and the Speed of Simulations

If you monitor the *intra*molecular bond distances during an ***ODYSSEY*** simulation, you may notice that often they do not change. Why? Keeping the molecules partially rigid is a common device for "speeding up" the simulations; it allows for using a larger physical time step than would otherwise be possible.

The rigidity is an excellent approximation of the real physical situation for very stiff hydrogen-containing bonds. More generally, it is of relatively little consequence for many calculated properties.

3.5 Do the Calculated Properties Reproduce Experimental Data?

In many cases, there is qualitative agreement between calculated and experimentally measured properties. Particularly "trends" (such as variation with atomic mass, variation with dipole moment, or variation with temperature) are often predicted correctly. Predictions that are quantitatively correct are rare as the program employs models that are computationally inexpensive and therefore imperfect.

While not very common, outright failures also occur. However, it should be kept in mind that the presence of failures and limitations is a defining characteristic of all models—not only scientific models, but also models anywhere else. The pedagogical value of models

derives from their ability to be experimented with, not from being perfect replacements of the "real thing."

3.6 Does ODYSSEY Assume Ideal Gas Behavior?

ODYSSEY never assumes ideal gas behavior. Gas molecules are always modeled as particles of finite volume that exhibit non-negligible interactions (if sufficiently close).

Nevertheless, ideal gas behavior will be observed in many situations, namely whenever the physical conditions happen to closely correspond to the assumptions that are implicit in the Ideal Gas Law.

3.7 Gravity in ODYSSEY

You may have noticed that if you turn a partially filled simulation cell "upside down", the liquid doesn't flow to the bottom. The reason for this at first glance strange behavior is not the omission of the Earth's gravitational field (it is easy to include), but the fact that gravitational forces are so weak that they do not make a difference on the time scale of molecular simulations. *Much* longer simulations (and macroscopic sample sizes) would be needed to observe gravity-driven flow.

Incidentally, even macroscopic samples can behave the way molecular samples behave in ***ODYSSEY***. All that is needed is an environment where the effects of gravity are not noticeable–as is the case for any orbiting spacecraft. One could well say that ***ODYSSEY*** conveys an idea of what handling substances on the International Space Station would feel like!

A familiar phenomenon that crucially depends on the presence of gravitational forces is the formation of neat interfaces. In ***ODYSSEY***, you will in fact find models of immiscible liquids that show fairly straight interfaces, but this is only because they have been *set up* to show the "expected" pattern.

3.8 Condensing Gases

Given sufficient simulation time and a sufficiently low temperature, samples of gas will eventually show condensation. However, the condensation will happen via the formation of irregular molecular clusters rather than through the formation of a "neat" horizontal interface. The reason for this is the insignificance of gravitational forces on the time scale of molecular simulations.

3.9 Why Won't Liquids Freeze?

ODYSSEY focuses on real simulations of physical phenomena, rather than on cartoon-style animations. While the freezing transition can be simulated, it is very hard to do and requires sample sizes and time scales that lie beyond the scope of ***ODYSSEY***.

3.10 Why Doesn't the Density Change When Melting?

ODYSSEY performs its simulations with unit cells of constant volume. The user has to manually adjust the volume in order to represent changes in density:

- From the **View** menu, select **Properties...**.
- From the **Add Property** menu, select first **System → Density** and then **Thermodynamics → Volume**.
- Adjust the volume with the provided slider so as to reach the desired density.

Alternatively, the Build → Simulation Cell → Liquid tab can be used for density adjustments.

3.11 Why Won't Molecules Dissociate?

Although ***ODYSSEY*** is capable of simulating the breaking and forming of covalent bonds, such systems require special algorithms and a very detailed description of the reaction. This information is not

automatically available. Unless the system has been set up beforehand to include reactions, chemical change with breaking of covalent bonds therefore cannot happen.

3.12 Why Won't Ions Dissolve Across an Interface?

While ***ODYSSEY*** is capable of representing a large variety of physical and chemical processes, the program cannot directly carry out real-time simulations when the time scale of the process in question does not fit within the typical picosecond (10^{-12} sec) time range that is accessible to the program.

The process of dissolving an ionic solid falls into this category. In principle, ions may well break away from the solid, but the process is an extremely "rare event" and in practice will not be observed.

3.13 Identification of Hydrogen Bonds

ODYSSEY identifies a hydrogen bond when an atom with an attached hydrogen is close to another atom and *all* of the following criteria are satisfied:

- The partnering atoms must involve a *known* hydrogen bond donor and a *known* hydrogen bond acceptor. Oxygen, nitrogen, and fluorine are the most important formers of hydrogen bonds, but not necessarily in all valence states. In liquid water, for example, sp^3 oxygen acts as both a donor and an acceptor of hydrogen bonds. The sp^2 oxygen of carbonyl groups, on the other hand, can only act as an acceptor and must pair up with some other donor if it is to form a hydrogen bond.

- The distance between the hydrogen atom and the acceptor atom must fall within a range of 122-260 pm.

- Overtly bent hydrogen bonds are excluded by requiring that the angle $\angle$ (hydrogen atom-donor atom-acceptor atom) is smaller than a set value. For example, for oxygen and nitrogen this angle is 30°.

3.14 Calculation of Enthalpies, Entropies, and Free Energies

For select compounds under a certain set of conditions (temperature, pressure, and phase), ***ODYSSEY*** calculates common thermodynamic functions:

Entropy:

ODYSSEY displays standard entropies. The algorithm used depends on the complexity of the given system and involves combinations of analytical statistical thermodynamic theory and empirical formulas (with the latter representing best fits of experimental data).

Enthalpy and Free Energy:

For some substances ***ODYSSEY*** calculates enthalpies (equivalent to heats of formation) and free energies from empirical formulas that represent best fits of experimental data. Following the usual approach of thermochemistry, both (!) the standard enthalpy and the standard free energy are taken as zero when dealing with an element in its standard state at 25°C (even though the entropy is of course not zero).

In order to allow for an intuitive interpretation of temperature changes, the program also adopts a unique reference state, i.e., the displayed values are always relative to the elements in their standard states at 25°C. Note that this is different from what is implicit in the NIST-JANAF thermochemical tables and similar data collections. If such tables give heats of formation (or free energies) as a function of temperature, the assumed reference state is temperature dependent because the enthalpy of formation (or free energy) of the stable phase of an element is by definition zero for all temperatures. ***ODYSSEY*** refrains from working with varying reference states.

TEACHING USAGE

4.1 Simulating the Liquid-Vapor Transition

The liquid-vapor transition can easily be simulated for many systems:

- Retrieve a sample of liquid from the Molecular Stockroom, or build one yourself using the Model Kit (you will need to know the density of the desired liquid).
- From the **View** menu, select **Properties...**.
- From the **Add Property** menu, select first **Thermodynamics → Temperature** and then **Thermodynamics → Volume**.
- Start the simulation.
- Overwrite the Volume Field by a number that is at least 100 times bigger than the number shown.
- Resize the view of the simulation cell: **Edit → Resize**.
- To speed up the process of evaporation, select "Temperature" and increase its value with the slider provided.

4.2 Incorporating Simulations into Presentations and Classwork

To incorporate ***ODYSSEY*** simulations into lectures, laboratory experiments, and homework assignments:

- Make the corresponding molecular sample (normally an `.xodydata` file) available on a computer that has ***ODYSSEY*** installed.
- Run the corresponding simulation live and use the visualization and system manipulation features of the ***ODYSSEY*** interface.

See Section 2.8.3 for help on linking ***ODYSSEY*** simulations directly in PowerPoint.

Note: Since ***ODYSSEY*** is organized around the paradigm of live, interactive simulations, corresponding "movies" cannot be saved.

4.3 Can ODYSSEY Be Used with Interactive Whiteboards?

ODYSSEY is well suited for classrooms that are equipped with Smartboards or other interactive whiteboards.

4.4 Annotating Pages

All ***ODYSSEY*** pages can be individually annotated:

- Click (or tap) on the "document" icon (looks like a piece of notebook paper) at the top of the text panel. This opens a Notes page that accepts any text that is entered.

- Return to the originating page by selecting the **SAVE+CLOSE** link at the bottom of the Notes page.

The annotations for a given Experiment or Stockroom entry are retained by the computer and will be shown whenever you return to the corresponding Notes page later.

COMPUTER QUESTIONS AND TROUBLESHOOTING

5.1 Graphics Performance

If the graphics performance is unsatisfactory when using the "Space-Filling" style:

- In the **Tools** menu (Windows) or **Odyssey** menu (Macintosh), select **Preferences**.
- Check **Reduced Graphics for Slower Machines**. Confirm **OK**.

5.2 Running on Battery

If the graphics performance is unsatisfactory when running on battery:

- In the **Tools** menu (Windows) or **Odyssey** menu (Macintosh), select **Preferences**.
- Check **Reduced Graphics for Slower Machines**. Confirm **OK**.

On some computers, you may notice a certain "jumpiness" of the simulations while running on battery. This is due to repeated and automatic cycling of the processor between different clock speeds. Changing the power management setting of your machine to "Presentation" is likely to remedy this problem.

5.3 Graphics Hardware Acceleration*

Try to lower the "Graphics Hardware Acceleration" if ***ODYSSEY*** crashes immediately after installation:

- Go to **Start Menu→Settings→Control Panel→Display→ Settings→Advanced→Troubleshoot**.

* *Windows only*

- Set the "Hardware Acceleration Slider" to the highest setting that still allows the program to run properly.

5.4 Windows Operating System Requirements

ODYSSEY requires Windows 10, Windows 8, or Windows 7.

5.5 Macintosh Operating System Requirements

ODYSSEY requires macOS 10.14 Mojave, macOS 10.13 High Sierra, macOS 10.12 Sierra, OS X 10.11 El Capitan, or OS X 10.10 Yosemite.

5.6 Differences Between Pre-Built and User-Built Samples

When building molecules and bulk phase samples from scratch, ***ODYSSEY*** draws on a set of all-purpose rules and parameters (since the structure space of chemistry is huge and the computer obviously doesn't exactly know what you are after). Pre-built samples in ***ODYSSEY***, on the other hand, are often defined with custom settings that help with improving the general quality of the model.

As a consequence, user-built samples will occasionally not "behave as well" as the pre-built samples. However, it is rare for a user-built sample to behave completely differently.

5.7 Problems with Collision or Velocity Highlighting

The "Collisions" and "Velocities" attributes (in the **Style** menu) are only available for samples whose density is not too high (this protects the computer from problems such as being overwhelmed by collision counting in higher density samples). A rule of thumb is that letting the pressure drop to less than ~10 atm (use **Build → Simulation Cell → Gas**) will make the attributes available.

5.8 Vapor Molecules Don't Seem to Move Fast Enough

When comparing gases with liquids or solids, the molecular motion in the former often appears to be "slow" rather than fast. Why is that?

In order to facilitate observations of a wide variety of systems, ***ODYSSEY*** *autoscales* the size of the simulation cell to the screen size regardless of the physical state of the substance. As gas phase simulation cells are typically much bigger than condensed phase simulation cells (compare the "1 nanometer lines" in the corners of the simulation cells), the net motion in the gas phase *is* in fact much faster than the net motion in the liquid phase.

5.9 Creating File Associations in Windows

Before you can hyperlink an ***ODYSSEY*** file into a PowerPoint presentation, you may have to register the `.xodydata` file extension with the Windows operating system (in this way PowerPoint will know that it needs to start ***ODYSSEY*** when encountering hyperlinks to `.xodydata` files):

1. Try to directly open the `.xodydata` file by double clicking (or double tapping) on its icon. If ***ODYSSEY*** starts up and the model displays, you don't need to do anything else.

2. If ***ODYSSEY*** doesn't start up, *right-click* (or long press) on the `.xodydata` file and select **Open with…**, and then select **Choose default program**. In the resulting dialog, navigate to the ***ODYSSEY*** folder and select "OdysseyStudent.exe" (Student Edition) or OdysseyInstructor.exe (Instructor's Edition). In most cases, you will find the ***ODYSSEY*** folder in the 'Program Files→Wavefunction' folder of 'Local Disk (C:)'.

Any file of the type `.xodydata` can now be hyperlinked into PowerPoint slides via the 'Hyperlink' attribute. All features of the ***ODYSSEY*** interface (simulation control icons, etc.) are fully available.

5.10 Opening Saved Models with "Drag and Drop"

All ***ODYSSEY*** files (`.xodydata`, `.odyssey`, or `.odylab`) and also all `.spartan` files can be opened by dragging the file onto the desktop shortcut created by the installer.

5.11 Importing From Other Modeling Programs

ODYSSEY reads `.pdb` files (generated by most other modeling programs and also the file format of many databases) as well as `.spartan` files (generated by Wavefunction's program ***SPARTAN***). In addition, it reads ChemDraw, ISIS/Draw, XYZ and SMILES files. Use **File → Open** in order to import an external file or use "Drag and Drop".

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