

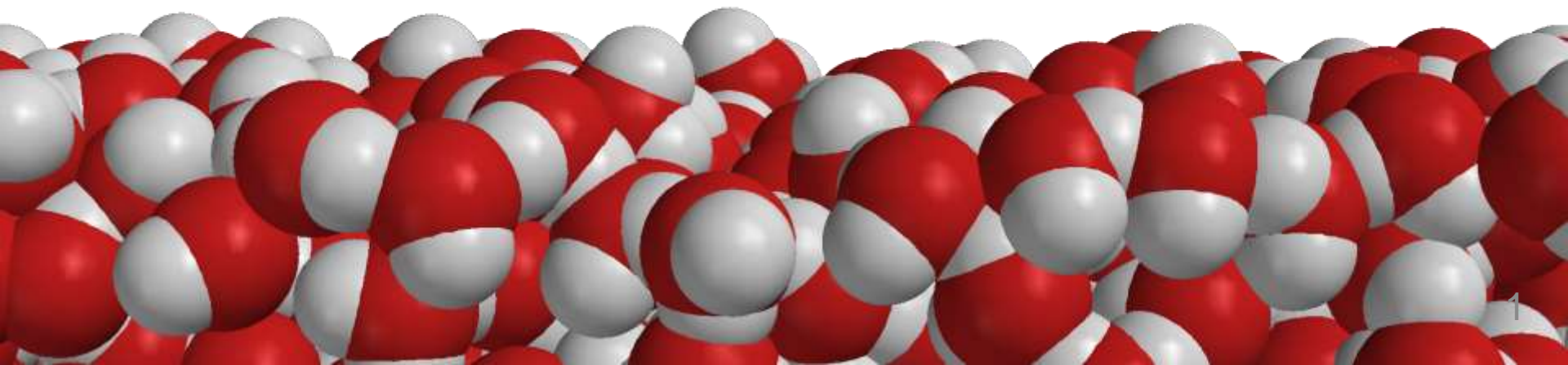
Working with **ODYSSEY**
Molecular Explorer

in the Chemistry Classroom

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Irvine, California 92612

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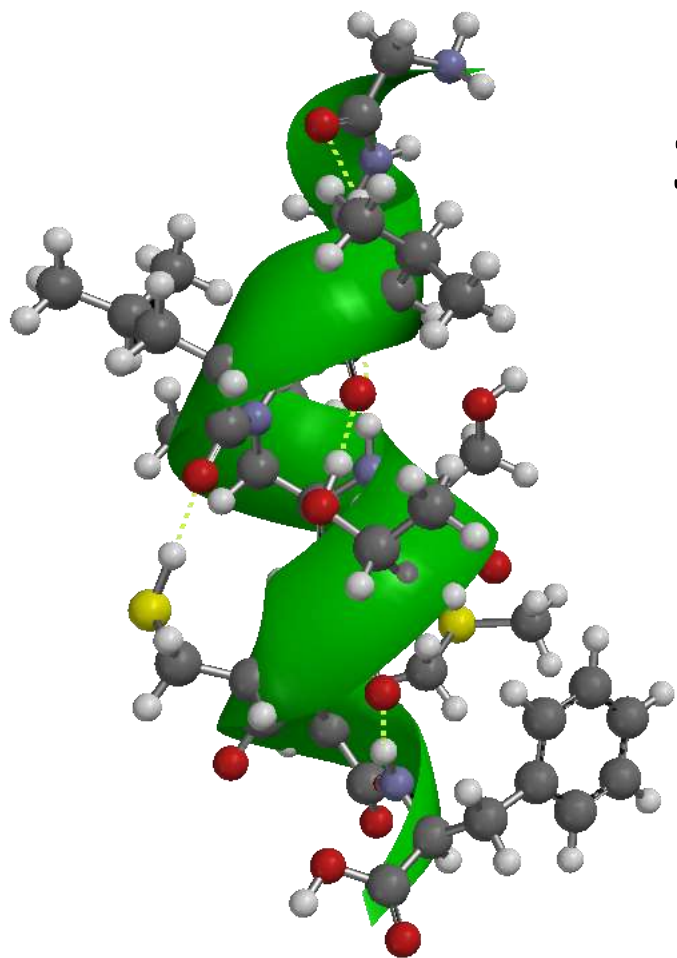
Molecular Modeling
Using Science to Teach Science

What Is **ODYSSEY** ?

Molecular Explorer

How Is It Unique ?

3D Visualization & Simulation



- a) **At the Molecular Level...Always**
- b) **Very Science-Based...Always**
(Closely Related to “Real”
Molecular Modeling Programs)
- c) **Explorable...Always**

Content **AND** Practices **AND** Crosscutting Concepts

Traditional

~~**Content**
("Memorization")~~

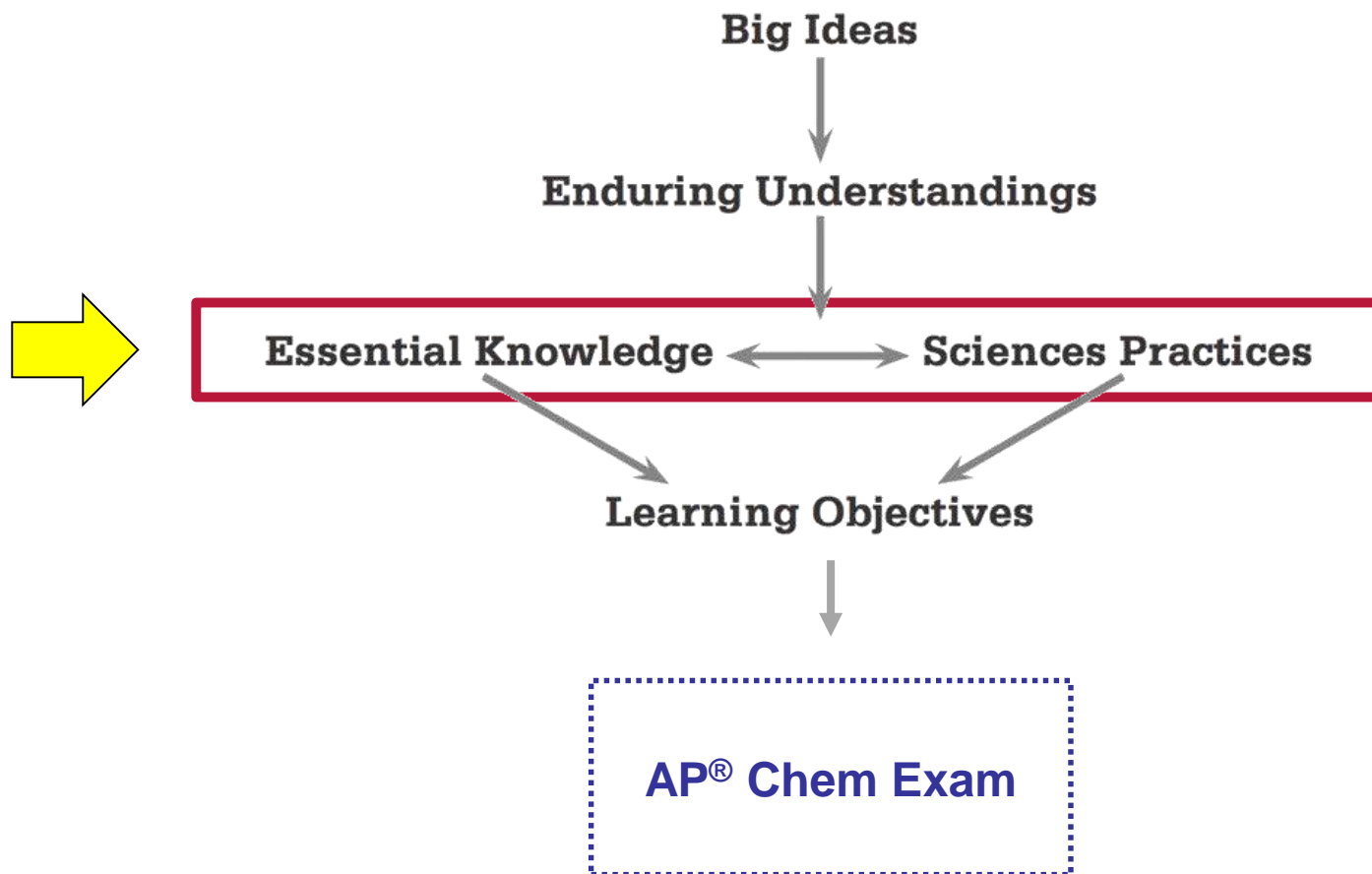
~~**Practices**
("Activities")~~



NGSS

Couple Content with Practices

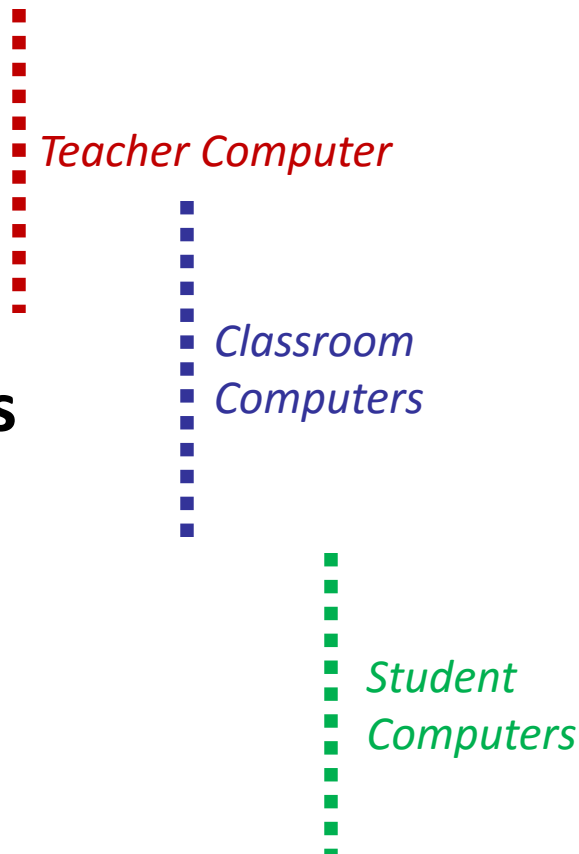
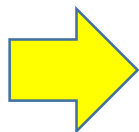
Knowledge + Skill = Exam Question



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How Can Be Used?

- **Direct Demonstrations**
(“The Molecular Perspective”)
- **Inquiry/Exploration**
(Ask Leading Questions!)
- **Computer Lab Experiments**
(Complement Wet Lab)
- **Take-Home Labs**
- **Enrichment**
- **Self-Study**



Scientific Content

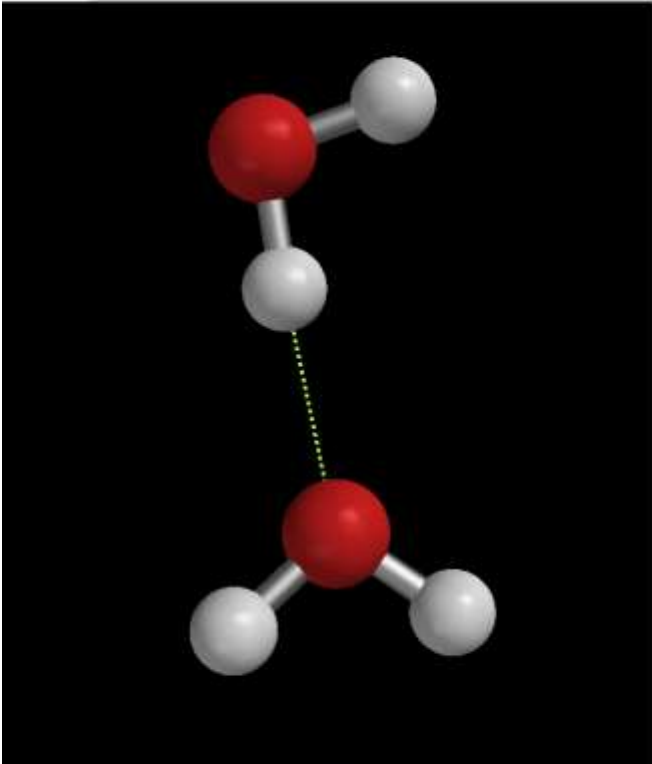
ODYSSEY Models + Teaching Units

Select a Content Level

File Edit View Style Tools Build Electrons Snapshot Help

New Sample Build Minimize Validity Formula Name Electrons Compare Properties Plots Periodic Table Clear Hide Text Search

HOME



ODYSSEY
Molecular Explorer

Welcome !

Please choose a content level

- Introduction to Chemistry
- High School Chemistry
- AP® Chemistry*
- College Chemistry

Mahaffy-Tasker-Bucat-Kotz-Weaver-Treichel-McMurry
Chemistry: Human Activity, Chemical Reactivity

- Canadian Edition | Textbook
- International Edition | Tie-In

To change the content level later, go to
Tools → Preferences

To create your own content list, select
Content → My Favorites in Preferences.

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Selecting Atoms 0.00 x 10¹² s

High School: ~110 Units | AP[®] Chemistry: ~148 Units*

HOME

File Edit View Style Tools Build Electrons Snapshot Help

New Sample Build Minimize Validity Formula Name Electrons Compare Properties Plots Periodic Table Clear Hide Text Search

ODYSSEY Molecular Explorer

New Users Applied Chemistry Molecular Stockroom **Alignments** Customizing

[Edit List](#)
High School Chemistry
INSTRUCTOR'S EDITION
PASC
Chemistry through Inquiry

Matter and Measurements	29 Electron Sharing in Molecules	58 Pouring a Granular Material	84 Equilibrium and Temperature
1 Common Substances at the Molecular Level	30 Energetics of Covalent Bonding	59 Compressibility	85 Equilibrium and Pressure
2 Water—The Medium of Life	31 Polyatomic Ions	60 Molecular Motion in the States of Matter	Chemical Thermodynamics
3 States of Matter (2D)	32 Polar Bonds and Molecules	61 Overview of Intermolecular Forces	86 Thermal Conduction
4 States of Matter (3D)	33 Classifying by Bond Polarity	62 Dipole-Dipole Forces	87 Gas Expansions
5 Chemical Elements	34 Dipole Moments	63 The Molecular Polarity of Water	88 Entropy of the States of Matter
6 Types of Compounds	35 VSEPR Theory	64 The Attraction between Water Molecules	Main Group Elements
7 Types of Mixtures	36 Comparing Conceivable Shapes for a Molecule	65 Elements with Hydrogen Bonding	89 Alkali Metals
8 Chemical and Physical Properties	37 Multiple Bonds and Resonance	66 Comparing Ice with Liquid Water	90 Alkaline Earth Metals
9 Comparing Equal-Weight Samples	38 Probing Resonance: Ozone and Carbonate	67 Surface Tension	91 Boron Group
10 Identifying by Density	Gases	68 The Melting Transition	92 Carbon Group
11 Is Density a Constant?	39 Characteristics of Gases	69 Vapor Pressure	93 Nitrogen Group
12 Naming Molecular Compounds	40 The Density of Liquids and Gases	70 The Evaporation of Liquid Air	94 Oxygen Group
13 Percent Composition		71 Bonding in Crystalline Solids	95 Halogens
			96 Noble Gases

Selecting Atoms

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How Do I Customize the Table of Contents?

The screenshot shows the Odyssey Molecular Explorer interface. At the top, there is a navigation bar with icons for Compare, Properties, Plots, Periodic Table, Clear, Hide Text, and Search. Below this, the main header includes the Odyssey Molecular Explorer logo and a navigation menu with buttons for New Users, Applied Chemistry, Molecular Stockroom, Alignments, and Customizing. On the right side, there is an 'Edit List' button and text indicating 'High School Chemistry INSTRUCTOR'S EDITION' and the logo for 'I2A200 Chemistry through Inquiry'. The main content area is a grid of topics, each with a checkbox. The topics are organized into sections: 'Matter and Measurements', 'Main Group Elements', and others. A yellow arrow points to the 'Edit List' button, and two yellow arrows point to the checkboxes for 'Common Substances at the Molecular Level' and 'Water — The Medium of Life'.

Section	Topic	Checkmark
Matter and Measurements	Common Substances at the Molecular Level	<input checked="" type="checkbox"/>
	Water — The Medium of Life	<input checked="" type="checkbox"/>
	States of Matter (2D)	<input checked="" type="checkbox"/>
	States of Matter (3D)	<input checked="" type="checkbox"/>
	Chemical Elements	<input checked="" type="checkbox"/>
	Types of Compounds	<input checked="" type="checkbox"/>
	Types of Mixtures	<input checked="" type="checkbox"/>
	Elements, Compounds, and Mixtures	<input type="checkbox"/>
	Comparing Conceivable Shapes for a Molecule	<input checked="" type="checkbox"/>
	Visualizing Lone Pairs	<input type="checkbox"/>
Main Group Elements	Alkali Metals	<input checked="" type="checkbox"/>
	Alkaline Earth Metals	<input checked="" type="checkbox"/>
	Boron Group	<input checked="" type="checkbox"/>
	Carbon Group	<input checked="" type="checkbox"/>
	Nitrogen Group	<input checked="" type="checkbox"/>
	Gas Expansions (Extended)	<input type="checkbox"/>
	Entropy of the States of Matter	<input checked="" type="checkbox"/>
	Entropy and Temperature	<input type="checkbox"/>
	Entropy and Temperature (Extended)	<input type="checkbox"/>
	Compressibility	<input checked="" type="checkbox"/>

Set/Unset Checkmarks

How Do I Create My Own Table of Contents?

Mac

Win

Preferences...

Preferences

Content: My Favorites

Length: nm or pm Å

Temperature: °C K °F

Pressure: atm kPa mm Hg bar

Energy: kJ/mol kcal/mol

Property Table Font Size:

Label Font Size: Fixed

Toolbar: Show Text

Use IUPAC Names

Dipoles Negative to Positive (IUPAC)

Emphasize Hydrogen Bonds

Emphasize Collisions

Play Sounds

Show 1 nm ruler on Cells

Alternate Visualization of Periodic Boundaries

Show Answer Key by Default

Reduced Graphics for Slower Machines

Enable Authoring of New Labs

Expert Developer

View: Perspective Orthogonal

Restore Defaults Full Reset Export Favorites OK Cancel

Custom Table!

1 Common Substances at the Molecular Level

2 Water - The Molecule of Life

3 Elements, Compounds, and Mixtures

Set Checkmarks

Unset Edit button

1. Select the Full AUI toolbar in the upper right corner.

2. Set checkmarks for all user toolbars.

3. De-select the 'Edit' button in every toolbar.

Learning About the Program / Refreshing Your Memory

The screenshot displays the software's main window with a menu bar (File, Edit, View, Style, Tools, Build, Electrons, Snapshot, Help) and a toolbar. Below the toolbar, there are two main sections:

- New User Tutorials:** A grid of 14 numbered lessons. A yellow arrow points to this section from a box labeled "ODYSSEY in 14 Lessons".
- Examples for Building New Models:** A grid of 20 numbered molecular models. A yellow arrow points to this section from a box labeled "Building Examples".

Text in the interface includes: "Increase the text size: Ctrl + Shift + PLUS-key", "Decrease the text size: Ctrl + MINUS-key", and "ODYSSEY Molecular Explorer".

**ODYSSEY in
14 Lessons**

Building Examples

Science Matters!

File Edit View Style Tools Build Electrons Snapshot Help

New Sample Build Minimize Validity Formula Name Electrons Compare Properties Plots Periodic Table Clear Hide Text Search

HOME APPLIED

Applied Chemistry

Industrial Chemistry

1	Top 10 Inorganic Chemicals	4	Syngas
2	Top 10 Organic Chemicals	5	Oxyfuel Welding
3	Common Solvents	6	High Explosives

Polymers

7	Recyclable Plastics	12	Silicone
8	Poly lactide	13	Polycarbonate
9	Rubber	14	Kevlar
10	Nylon	15	Plexiglass

Energy and Transportation

16	Natural Gas	18	Octane Rating
17	Gasoline	19	Fuel Additives

Agriculture

Pharmaceutical Chemistry

33	Top 10 Prescription Drugs	39	Small Molecule Prescription Drugs
34	Pain Medications	40	Inhalation Anesthetics
35	Penicillin	41	Intravenous Anesthetics
36	Peptide Antibiotic	42	Inhaler Propellants
37	Chemotherapy	43	Essential Amino Acids
44	Mayonnaise	47	Artificial Sweeteners
45	Wine	48	Soft Drinks
46	Chocolate	49	Wine
50	Chocolate	50	Chocolate

Biology

51	Enzymes I	58	Oxygen Transport I
52	Enzymes II	59	Oxygen Transport II
53	Enzyme Inhibitor	60	Metabolic Energy

Sanitation

70	Soap	72	Disinfectants
71	Shower Cleaner	73	Dry Cleaning

Analytical Chemistry

74	Solvents	77	EDTA
75	Partition Coefficient	78	UV Spectroscopy
76	pH Indicator	79	Superheavy Carbonyl

Materials Chemistry

80	Brass	83	Two-Dimensional Carbon
81	Liquid Crystals	84	Two-Dimensional Silicon
82	Carbon Nanotubes		

Supramolecular Chemistry

85	Interlocked Molecules	88	Grant Spoked Wheel
86	Catenaenes	89	Endohedral Fullerenes
90	Carbon Nanotubes	91	Carbon Nanotubes

Areas of Interest

~100 Elements | ~700 Inorganic and Organic Compounds


Odyssey Molecular Explorer - Instructor's Edition - STOCKROOM

File Edit View Style Tools Build Electrons Snapshot Instructor Help

New Sample Build Minimize Validity Formula Name Electrons Compare Properties Plots Periodic Table Clear Hide Text Search

HOME STOCKROOM

Molecular Stockroom



Elements

B Br C Cl F Fe H He N O P S Si

Hydrogen

Helium

Lithium Beryllium Boron Carbon Nitrogen Oxygen Fluorine Neon

Sodium Magnesium Aluminum Silicon Phosphorus

Potassium Calcium Scandium Titanium Vanadium Chromium Manganese Iron Nickel Copper Zinc Gallium Germanium Arsenic

Rubidium Strontium Yttrium Zirconium Niobium Molybdenum Technetium Radium Silver Cadmium Indium Tin Antimony

Cesium Barium Lanthanum Hafnium Tantalum Tungsten Rhenium Iridium Gold Mercury Thallium Lead Bismuth

Francium Radium Actinium Rutherfordium Dubnium Seaborgium Bohrium Hassium Meitnerium Darmstadtium Roentgenium Copernicium Flerovium

Lanthanides: Cerium Praseodymium Neodymium Promethium Samarium Europium Gadolinium Terbium Dysprosium Holmium Erbium Thulium Ytterbium Lutetium

Actinides: Thorium Protactinium Uranium Neptunium Plutonium Americium Curium Berkelium Californium Einsteinium Fermium Mendelevium Nobelium Lawrencium

Inorganic

CO₂ HCl HNO₃ H₂O H₂SO₄ NaCl NaOH NH₃ SiO₂

Aluminum Compounds Calcium Compounds Hydrogen Halides Nitrogen Compounds Sodium Compounds Chromium Compounds Mercury Compounds

Ammonium Compounds Carbon Compounds Hydrogen Oxides Phosphorus Compounds Strontium Compounds Cobalt Compounds Nickel Compounds

Arsenic Compounds Cesium Compounds Interhalogens Potassium Compounds Sulfur Compounds Copper Compounds Platinum Compounds

Tin Compounds Zinc Compounds

f-Block:

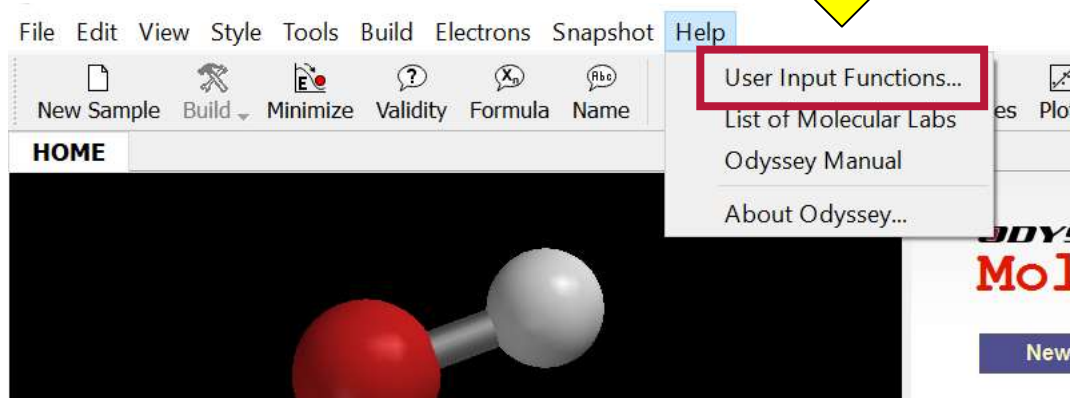
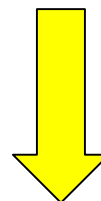
Shortcuts
(Particular Compounds)

Collections
(Multiple Compounds)


User Input Functions

Touchscreen, Trackpad, Mouse

In-Program Reference:
Help Menu
(Tailored for Windows/Macintosh)



- **Rotate**
 - Drag (Touchscreen)
 - **Left** Button + Drag (Trackpad / Mouse)

- **Translate**
 - **Long** Press + Drag (Touchscreen)
 - **Right** Button + Drag (Win Touchpad / Mouse)
 -  + **Button** + Drag (Mac Trackpad)

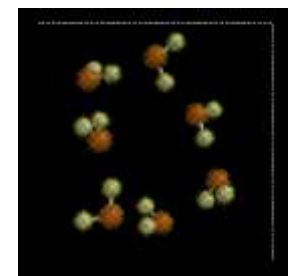
- **Zoom**
 - **Pinch** (Touchscreen / Trackpad)
 - **Scroll Wheel** (Mouse)

Further options are available, especially for older computers
→ Consult ***User Input Functions...*** in the **Help** menu

CTRL key not held down



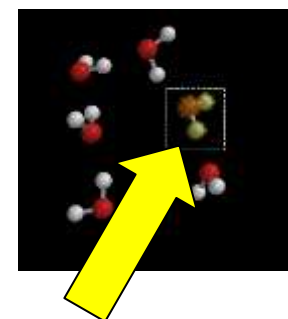
Rotate / Translate
Entire Model
(= All Molecules)

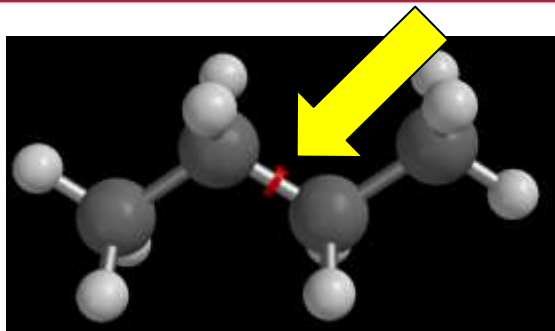


CTRL key held down



Rotate / Translate
Selected
Molecule Only





- **Double**-tap / **double**-click on bond to select it (Red wrap-around arrow confirms selection)

- ALT key not held down →

Rotate Model

Translate Model

- **ALT key held down** →

Rotate Around Bond

Change Bond **Length**



Drag (Touchscreen)

Left Button + Drag



Long Press + Drag (Touchscreen)

Right Button + Drag

 + **Button** + Drag (Mac Trackpad)

Visualization

Model Styles and Other Display Options

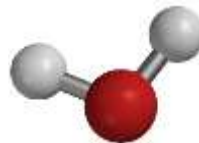
Start with **Space Filling** — it shows what things “really look like”

- Molecular shape
- Packing in solids and liquids
- Emptiness of gases



To see details, switch to **Ball and Spoke** (or **Ball and Wire**)

- Covalent bonds
- Distance / Angle measurements !



Tube — very useful in conjunction with hydrogen bonds



Wire — useful for the solvent of solutions

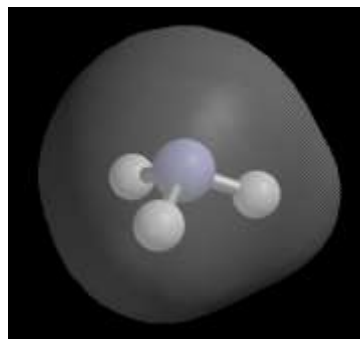
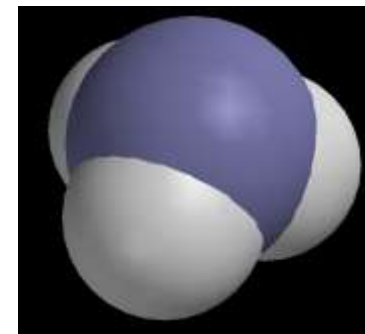


→ **Ball and Spoke** is the default style for the build panels

→ Use **Space Filling** for gases...or you will hardly see anything !

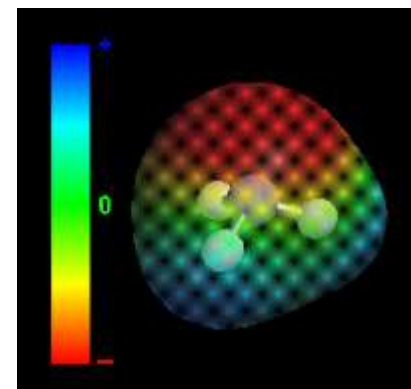
Molecular Shape / Polarity

- Space Filling** style — Approximate Shape



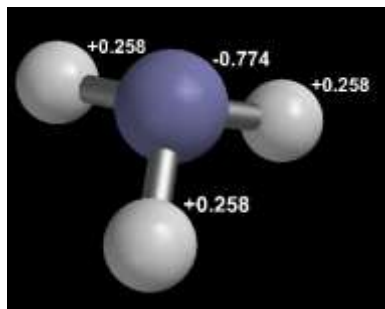
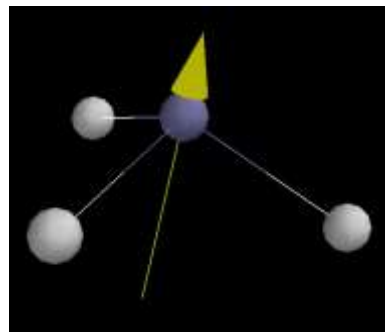
- Outer Surface** — True Shape
(Electron Cloud, ~98% of the total density)

- Polarity Map** — True Shape + Polarity



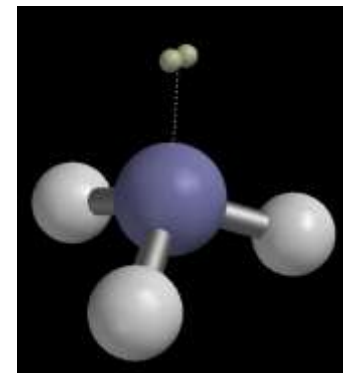
Molecular Shape / Polarity

- Dipole Arrow(s)** —
Combine with **Ball and Wire**
(or **Wire**) style



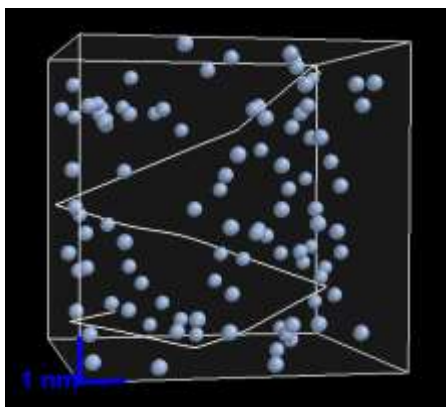
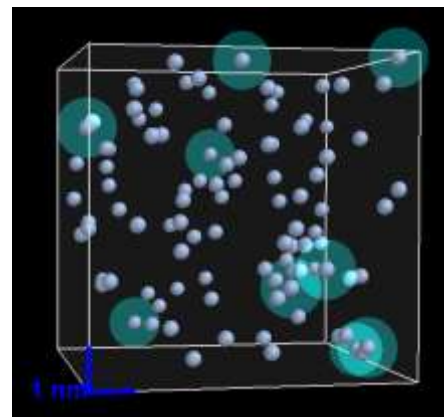
- Charge Labels** — Atomic Partial Charges

- Lone Pairs** — Cartoon Representation



Gas Laws / Kinetic Theory

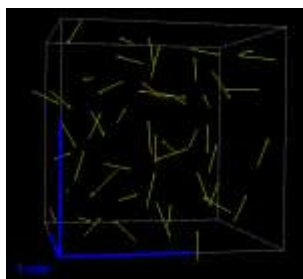
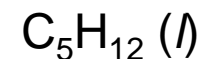
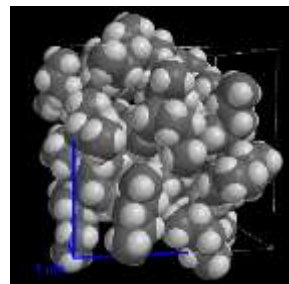
- ❑ **Collisions** —
select **Molecule-Wall**
→ Concept of “Pressure”



- ❑ **Trails** — *Right-click* on an atom
and select **Set Trail**

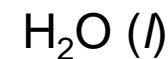
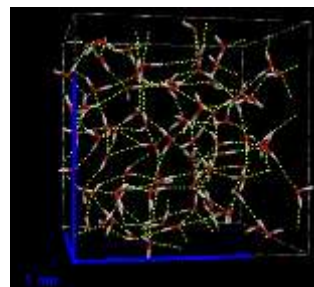
Intermolecular Forces

- Space Filling** style
→ *Dispersion forces*



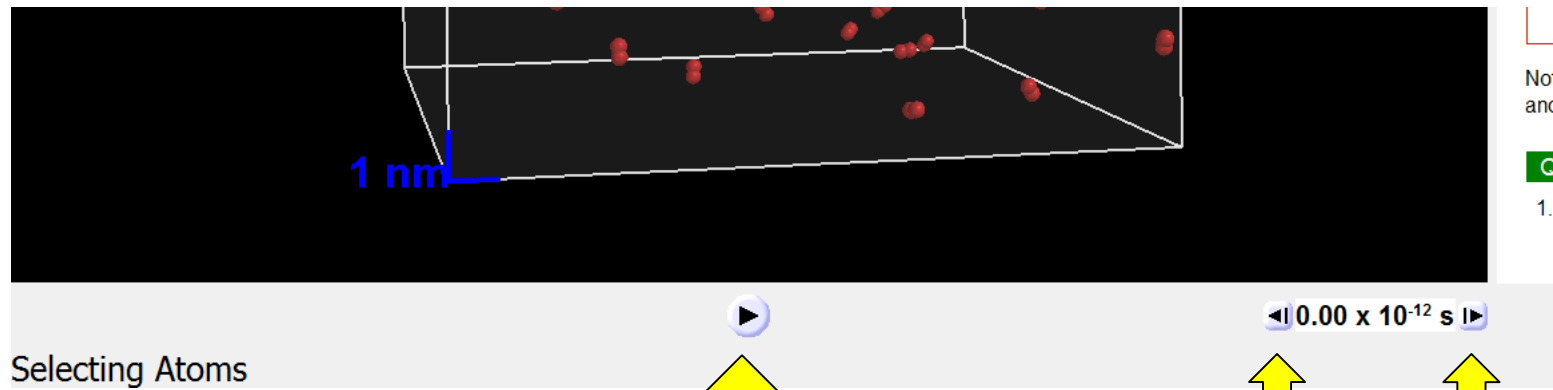
- Dipole Arrows**
(Combine with the **Hide** style)
→ *Dipole-dipole forces*

- Hydrogen Bonds**
(Combine with the **Tube** style)
→ *Hydrogen bonding forces*



Dynamics

Starting and Controlling Simulations



Go/Stop Toggle
(Continuous Simulation)

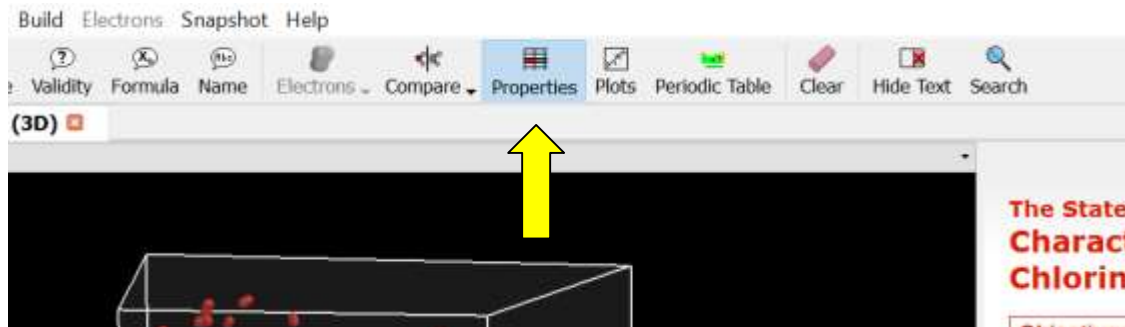
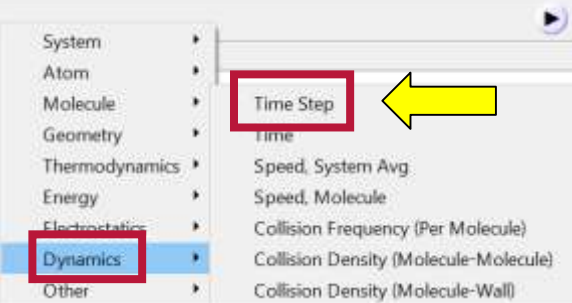
Go Back / Go Forward
(Step-by-Step)

Time Scales

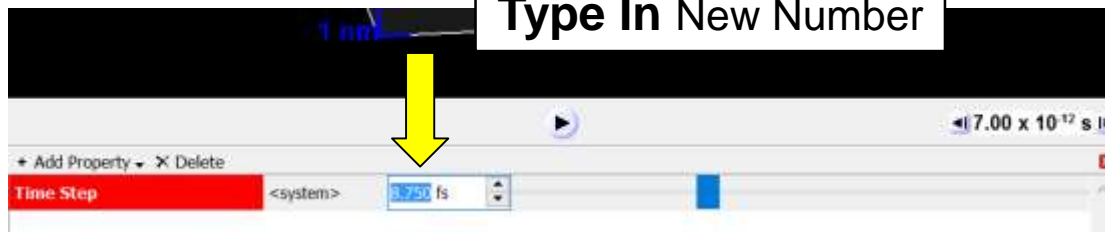
- ~10⁻¹⁵ s (femtoseconds) ← Actual Molecular Time Step
(as assigned by the program)
- ~10⁻¹² s (picoseconds) ← Typical “Step-by-Step” Interval
- ~10⁻⁹ s (nanoseconds) ← Maximum Length of Simulations
(long simulations of hours duration)

Slowing Down (and Speeding Up)

Add Property...
(Lower Left Corner)



**Select Field and
Type In New Number**



Slowing Down (and Speeding Up)

Smaller Time Step

Larger Time Step

Number of Computational Steps

Per Minute of Wall-Clock Time (!) Stays the Same

Simulation Effectively
Slows Down

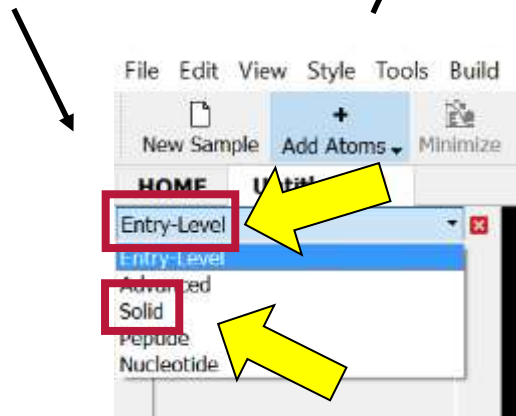
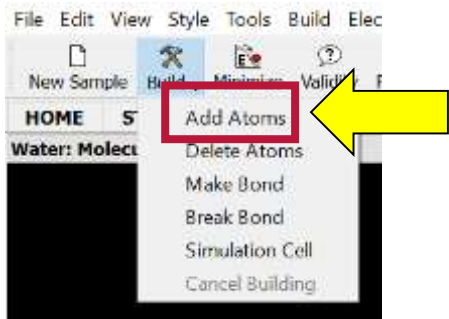
Simulation Effectively
Speeds Up

Can always **reduce**
the time step size...

...but should **not** significantly increase
step size or may provoke a numerical
instability (and possibly program crash)
(→ automatically assigned time step is already “large”)

Building
From Molecules to Simulation Cells

Molecules, Solids



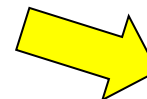
Entry-Level
Common Valences
(~Organic)

Common Valences (~Organic)

>C-	>N	>P	-H
>C=	>N=	>O-	-Cl
$\text{-C}\equiv$	=N	=O	-C
>C-	>N	\`S-	-Br
>Si-	>N-	=S	-I

Groups Alkenyl
Rings Benzene
Set Charges...

NaCl



H₂O



Solid
(Template-Based)

Solid

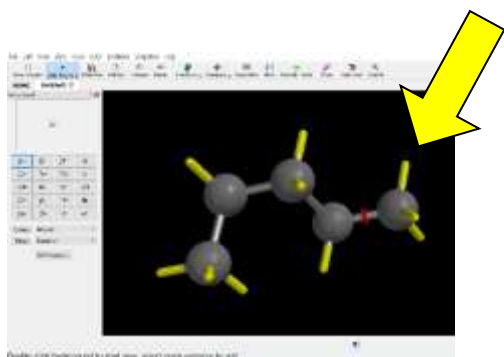
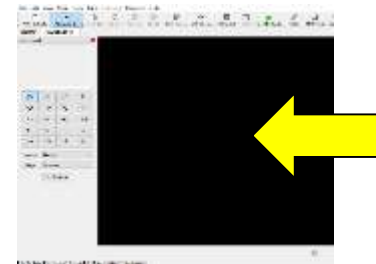
Ionic Solids

- A-B, Sodium Chloride Type
- A-B, Cesium Chloride Type
- A-B, Nickel Arsenide Type
- A-B, Wurtzite Type

X Y Z NaCl
2 : 2 : 2

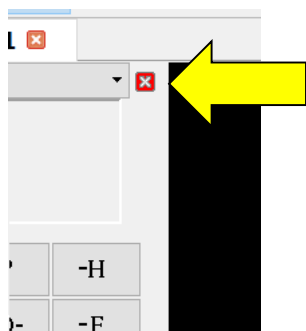
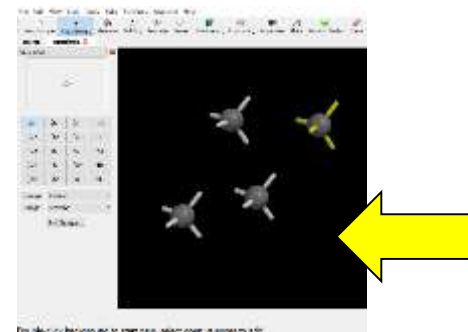
Na, Sodium +1
Cl, Chlorine -1


- ❑ Initial single click on background
→ Start molecule (first building block)

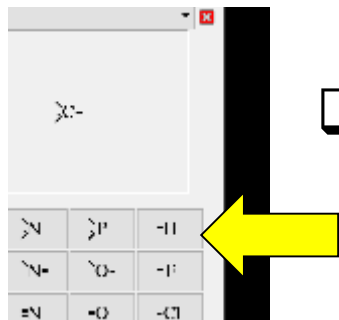


- ❑ **Single** click on yellow spoke (free valence)
→ Continue with the *same* molecule

- ❑ **Double**-click on background
→ Start *new* (additional) molecule

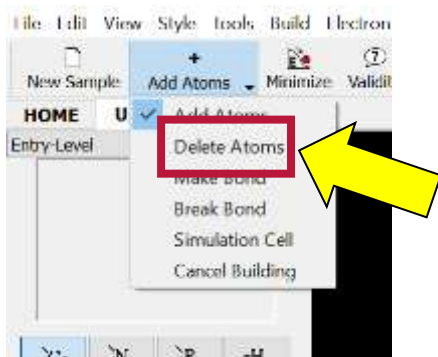
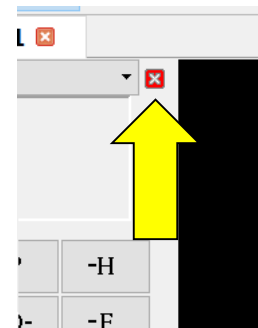


- ❑ Close the build panel with its **Close**  button
(Starting a simulation  will also close the build panel)

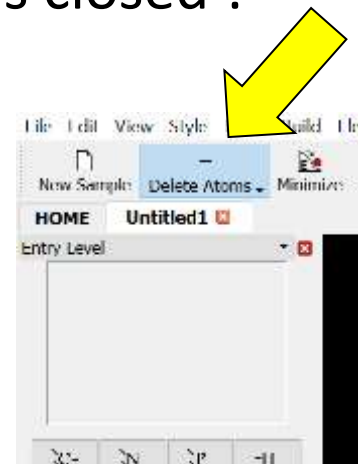




☐ **Hydrogens** can be added manually...

...or are filled in automatically as soon as the build panel is closed !



☐ **Deleting is modal**
→ Will keep deleting until returning to "Add Atoms"

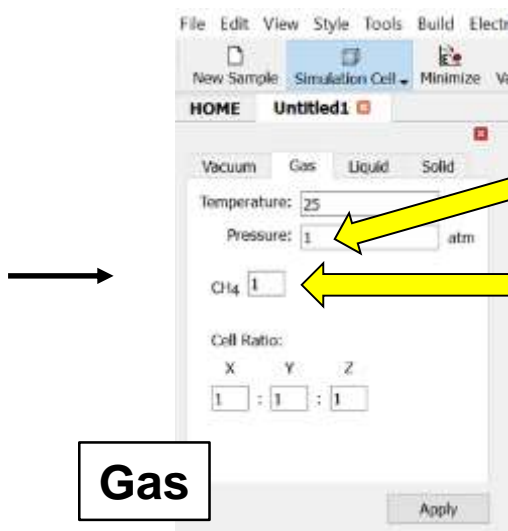
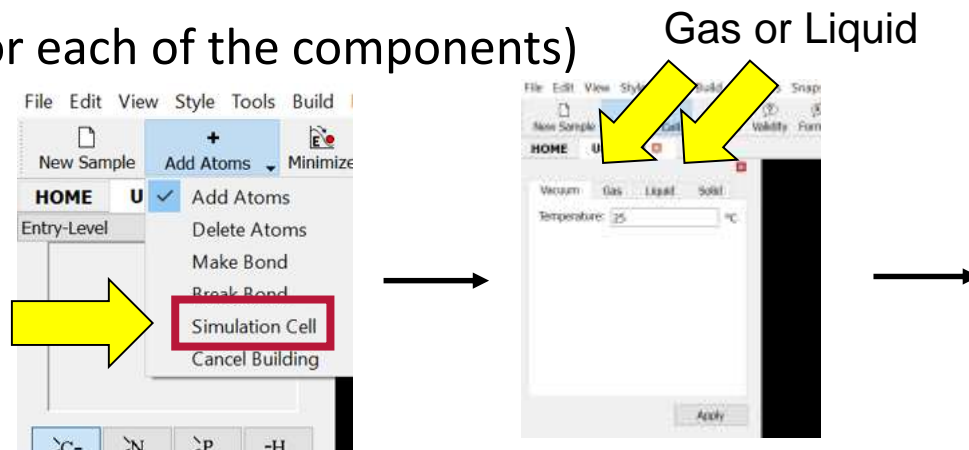


☐ Always **Minimize**  (or run a simulation ) when done building!

- ❑ Must build molecule first

(Mixture: need one molecule for each of the components)

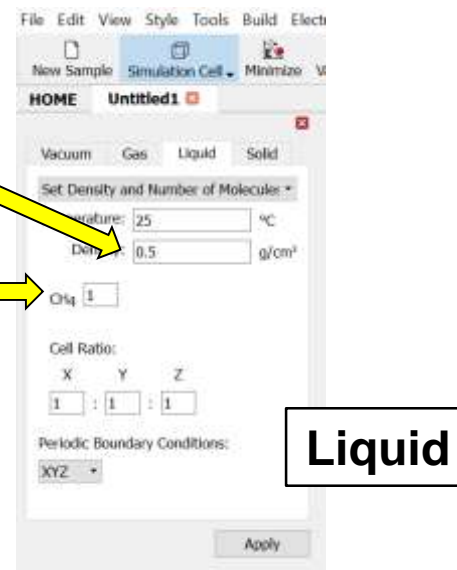
- ❑ Then use *Simulation Cell* panel



Pressure

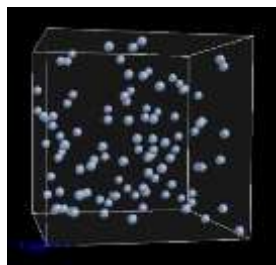
Density

of Molecules



- ❑ Don't exceed $\sim 1,000$ atoms* total
...or things may get very slow!

—————
*atoms, not molecules



- ❑ *Argon* is excellent for
Gas Laws / Kinetic Theory
(computationally “cheap”)

- ❑ Build Gases at ~ 10 atm (rather than ~ 1 atm)
→ More collisions, “better” (faster) equilibrium
- ❑ Build Liquids at slightly reduced density
(such as 0.9 g/cm^3 instead of 1.0 g/cm^3)
→ More mobility, faster equilibrium

Unusual Bond Orders, Inorganic Compounds, Complexes

The screenshot shows the software interface with the 'Entry-Level' dropdown menu open, highlighting the 'Advanced' option. A yellow arrow points from 'Advanced' to the 'Advanced' window. The 'Advanced' window displays 'Ar' (Argon) and a 'Pop-Up Periodic Table' with various elements highlighted in green and blue. A yellow arrow points from the 'Pop-Up Periodic Table' to the 'Advanced' window. Below the 'Advanced' window, there are three yellow arrows pointing to different sections: 'Coordination' points to a grid of coordination icons, 'Bond Order' points to a grid of bond order icons, and a box labeled 'Advanced' points to the 'Advanced' window itself.

File Edit View Style Tools Build

New Sample Add Atoms Minimize

HOME Untitled1

Entry-Level

Advanced

Solid

Peptide

Nucleotide

Pop-Up Periodic Table

Ar

Ar, Argon

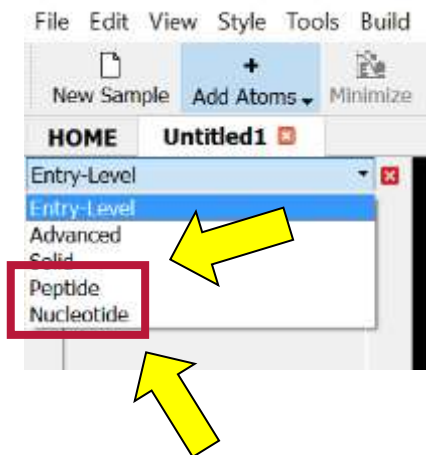
Coordination

Bond Order

Advanced

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

Peptides, Oligonucleotides

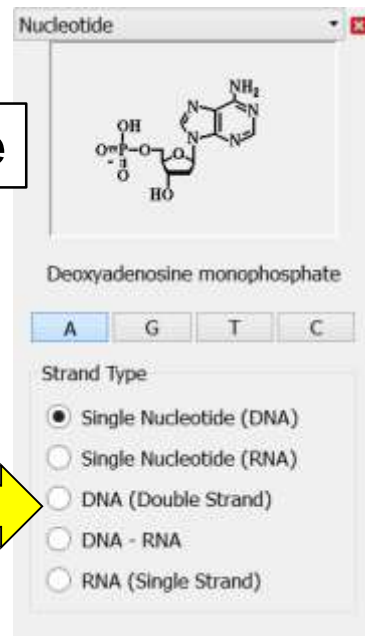


Peptide



α -Helix or β -Sheet

Nucleotide

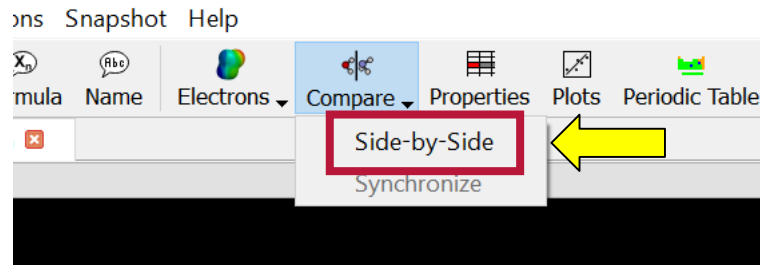


Watson-Crick
DNA

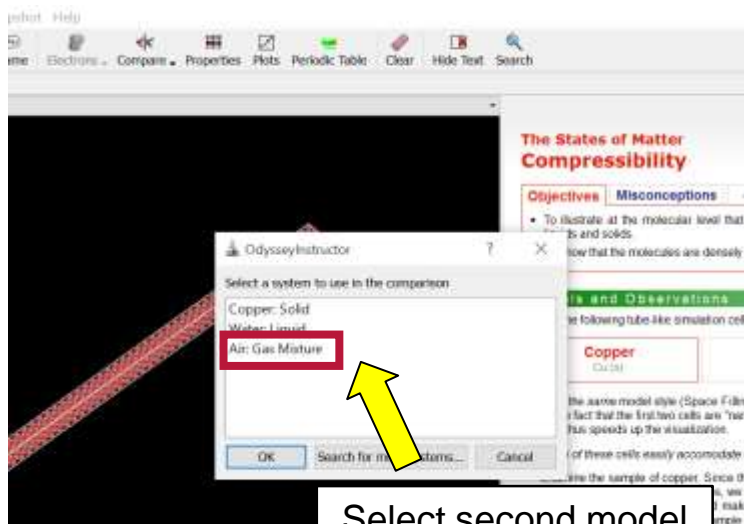
- ❑ Don't exceed ~30 amino acids / ~30 base pairs
...or things may get very slow!

Comparing
Showing Models Side-by-Side

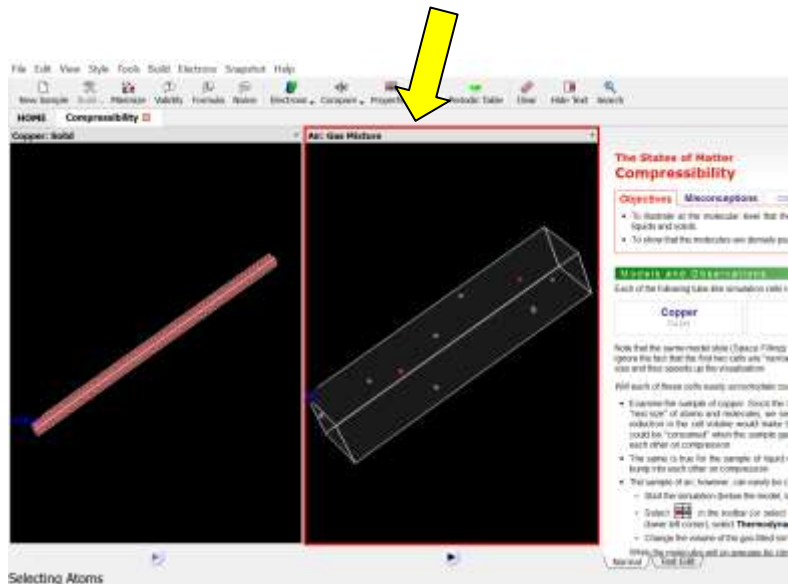
Comparing Two Models from the Same Lab



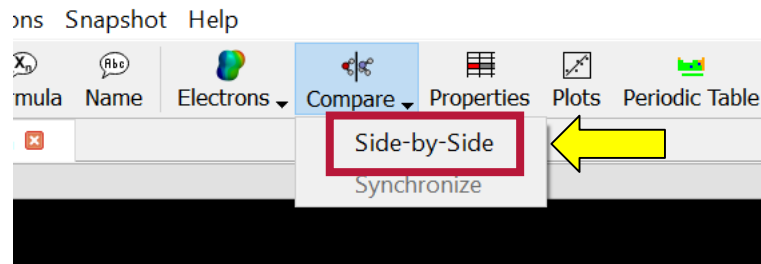
Models can be manipulated individually
Choose "active" model (has **red frame** around it) by selecting its background



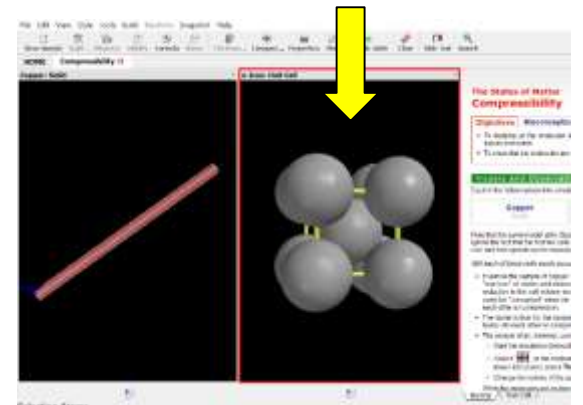
Select second model for the comparison



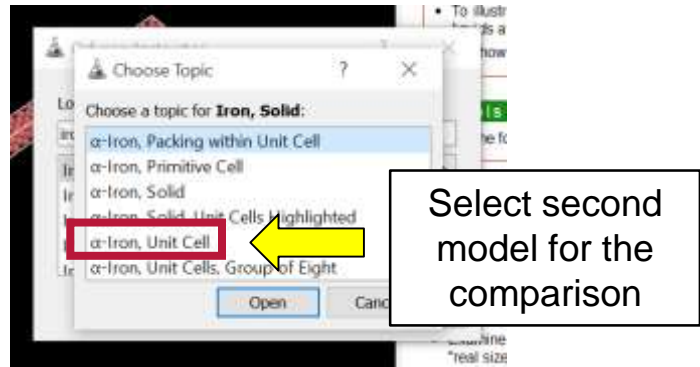
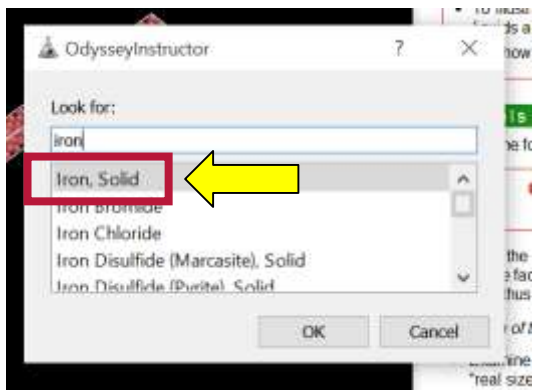
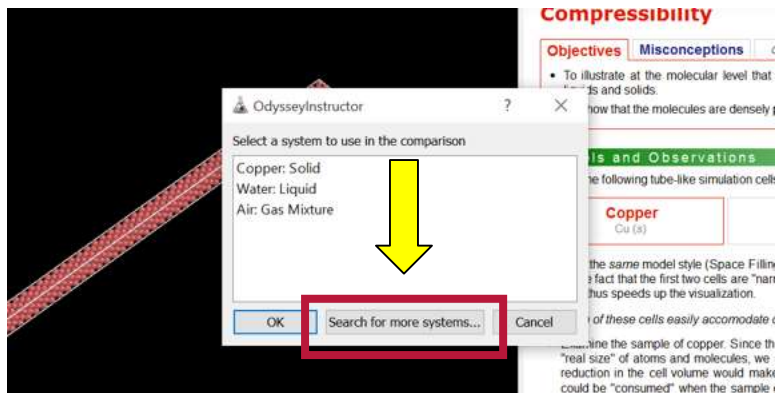
Getting the Comparison Model via Search



Second model initially shown on same scale (zoom is required)

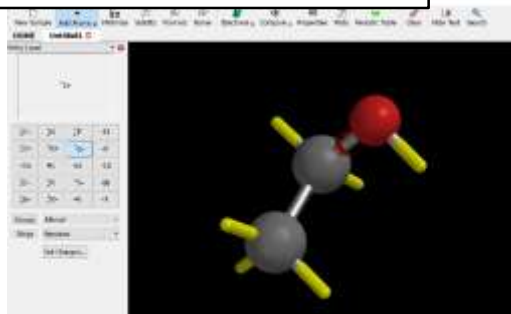


Available for comparison:
~1,800 models

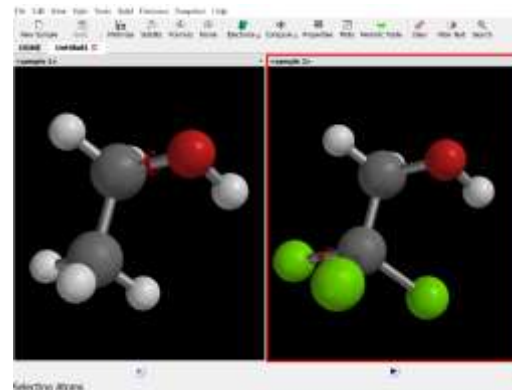


Select second model for the comparison

Build the first model...

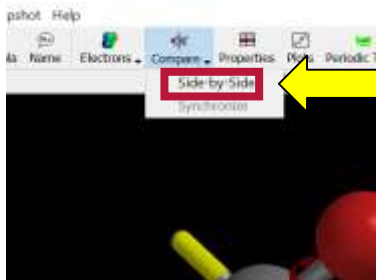


- Suitable even for...
- simulation **cells**
 - independent **dynamics** of both systems
 - independent **electron** cloud calculations

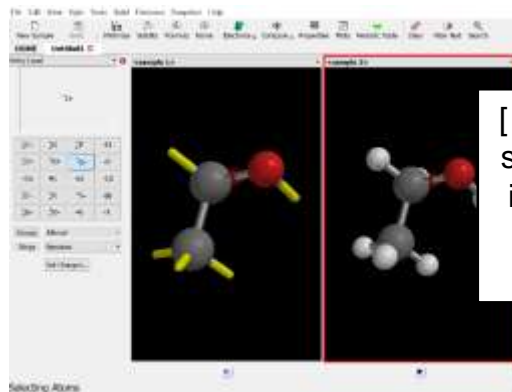
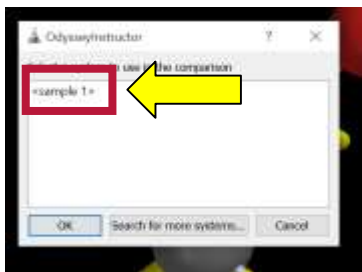


...keep the build panel **open!**
(if already closed, you **must** reopen it with *Build* → *Add Atoms*)

Modify the second model, finally close the build panel
(Note: Cannot reopen panel once closed)



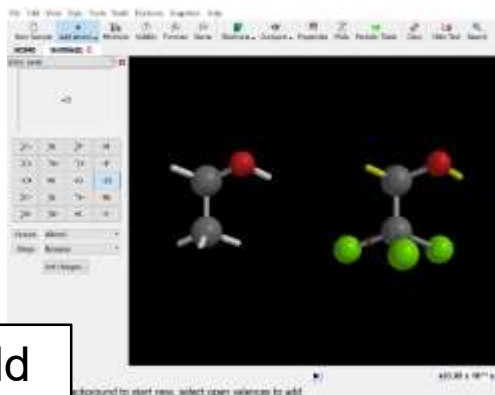
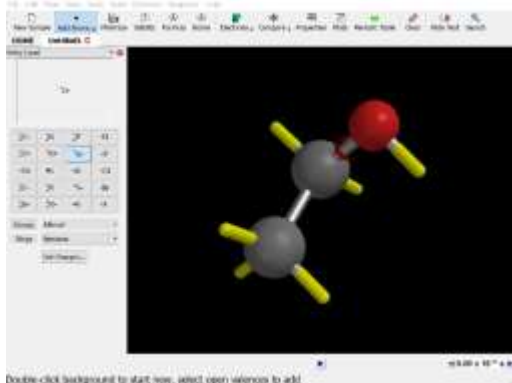
Duplication Step



[The hydrogens of the second model will turn into yellow spokes as soon as a building block is selected]

Alternate Method

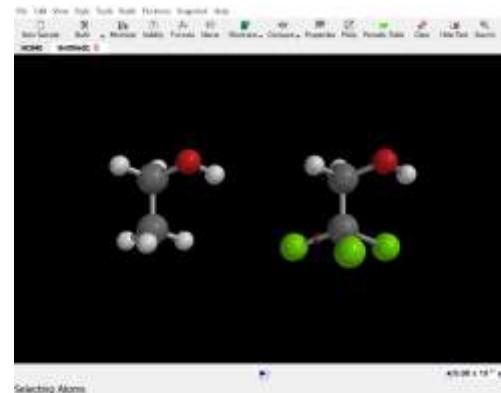
Build the first molecule...



...and simply add another molecule to the **same** model (double-tap/double-click on background to start the second molecule)

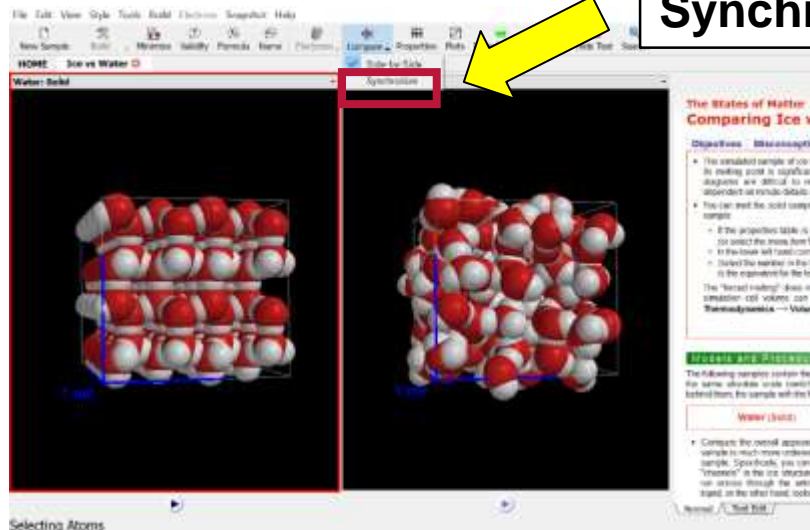
Close the build panel

- Comparison of two simulation cells not possible
- Dynamics applies to the interacting **dimer** (!) of molecules, not the two molecules independently
- Electron cloud calculated for the **dimer** (!) of molecules, not the two molecules independently



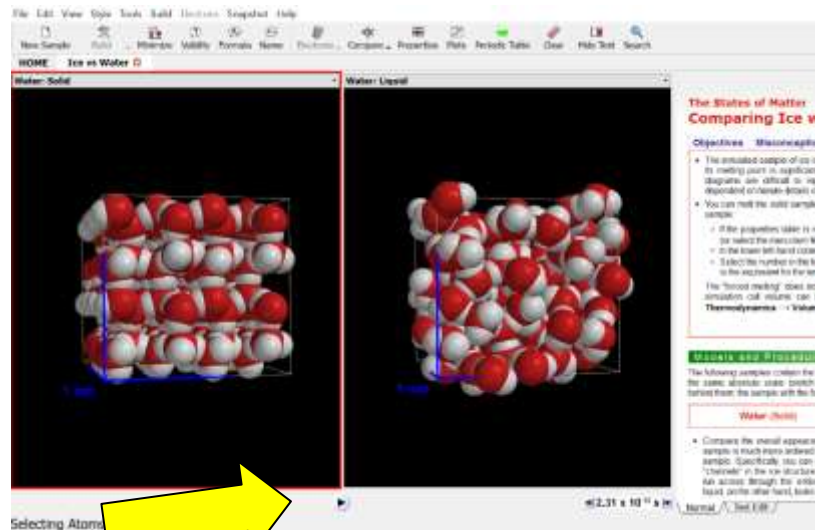
Running Two Simulations at Once

Synchronize option



Calculating the dynamics of two systems at once invariably probes the limits of computational power → expect slow simulations

Selecting Atoms



Selecting Atoms

One dynamics toggle controls both simulations (simulations progress at the same speed)