

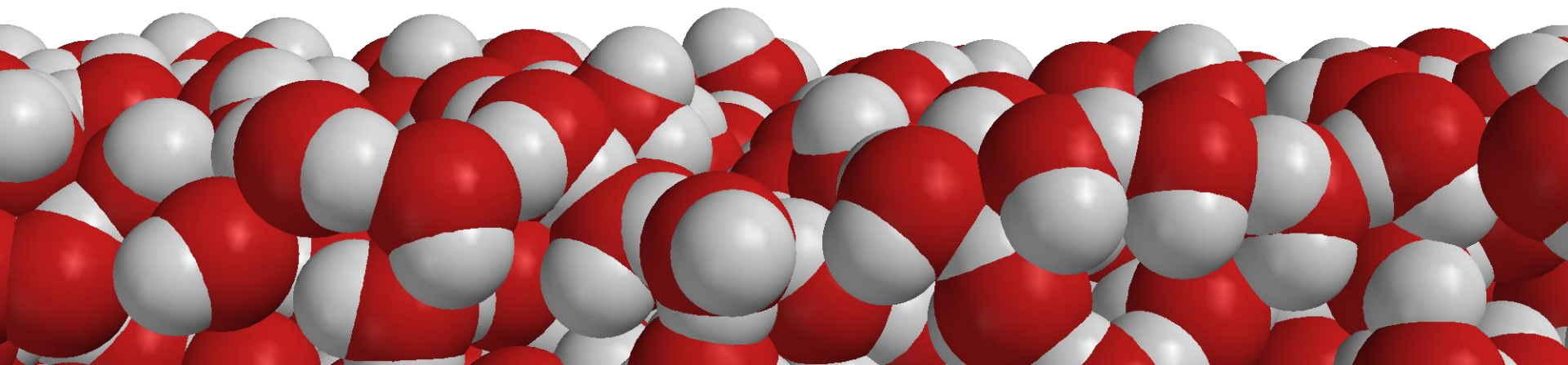
Working with **ODYSSEY**  
Molecular Explorer

## in the Science Classroom

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Irvine, California 92612

*support@wavefun.com*



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Molecular Modeling

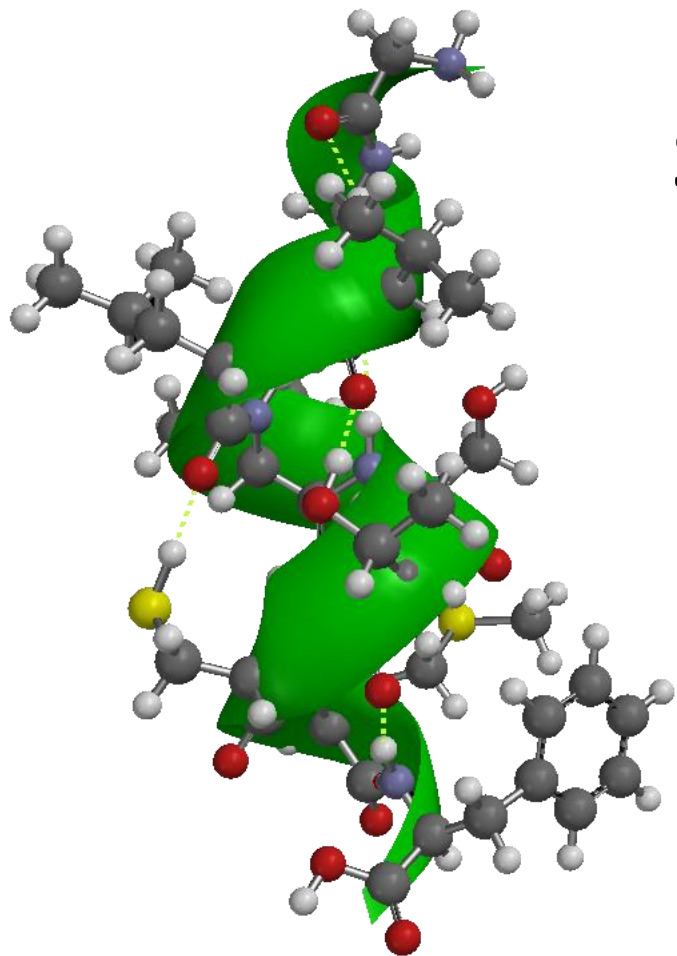
# Using Science to Teach Science

# What Is **ODYSEY** ?

Molecular Explorer

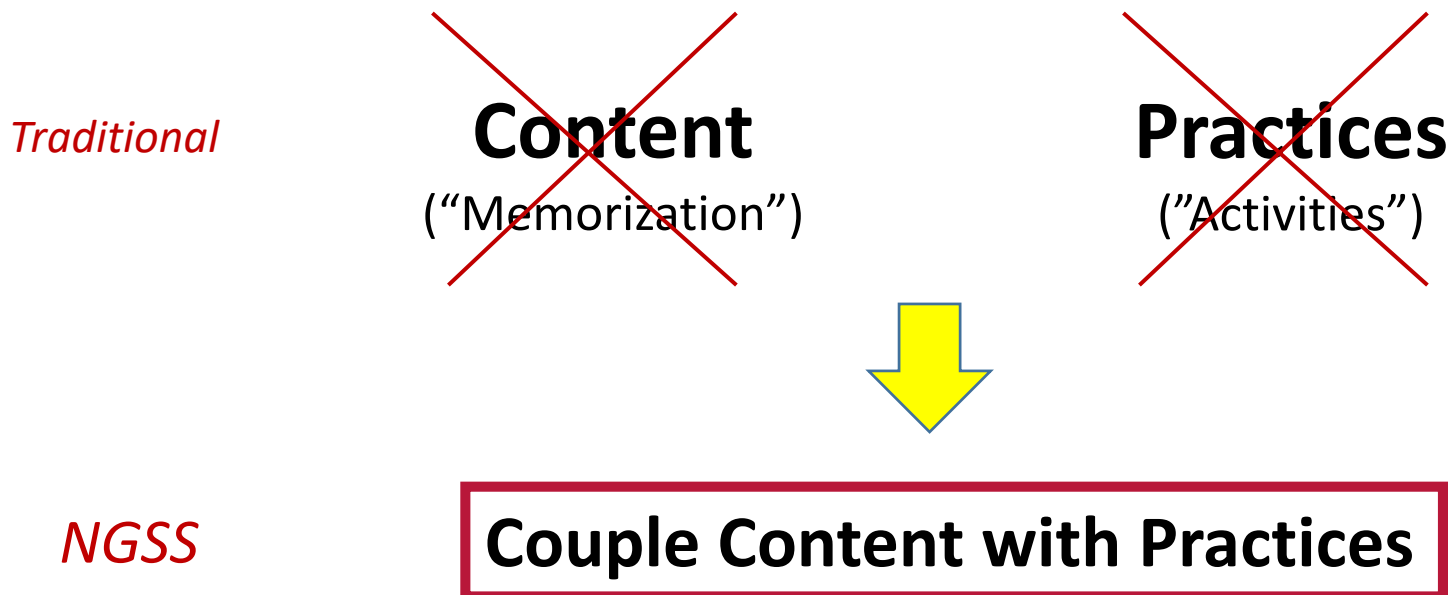
## How Is It Unique ?

### 3D Visualization & Simulation

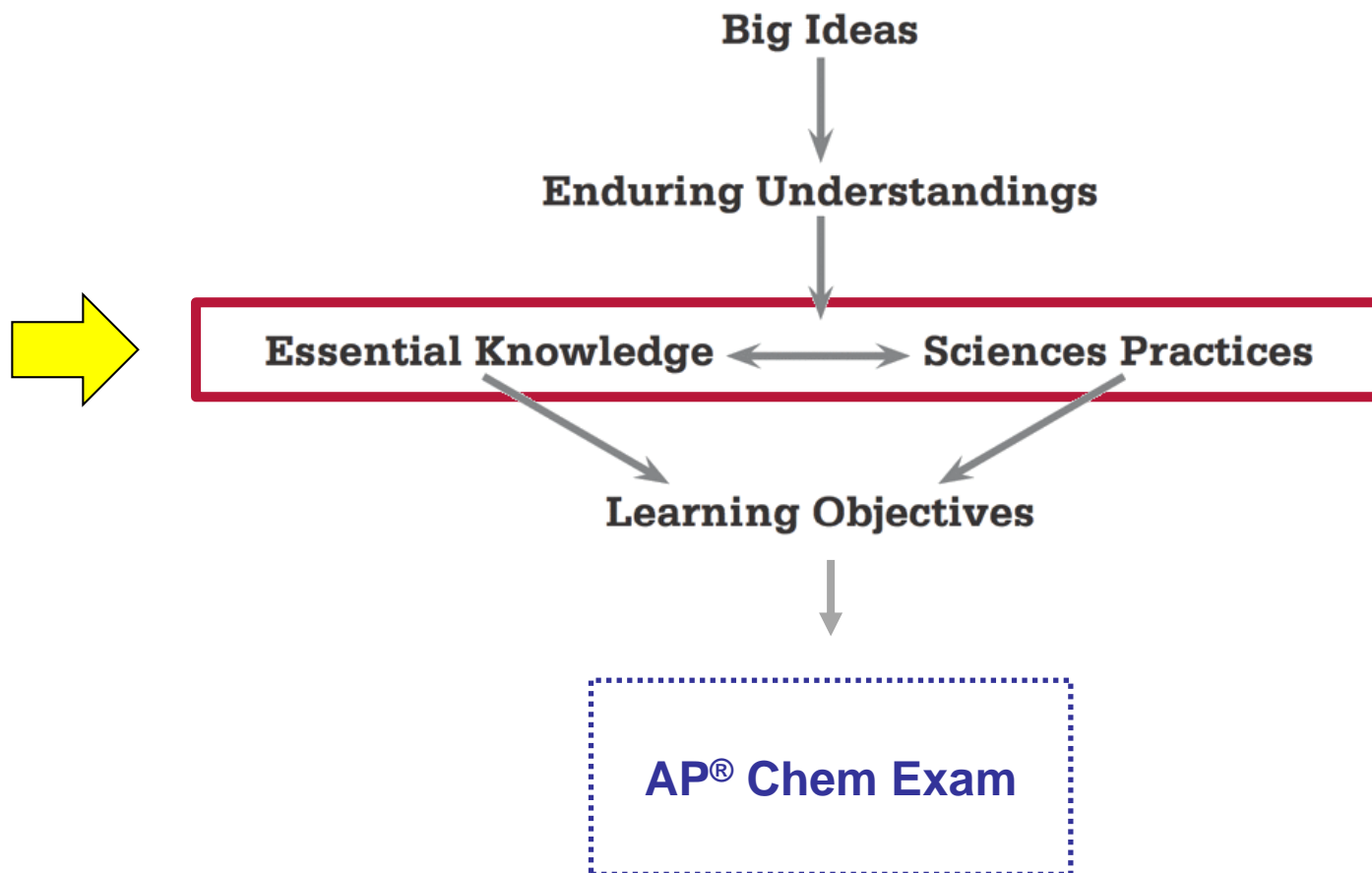


- a) **At the Molecular Level...Always**
- b) **Very Science-Based...Always**  
(Closely Related to “Real”  
Molecular Modeling Programs)
- c) **Explorable...Always**

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



Knowledge + Skill = Exam Question

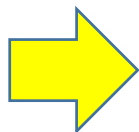


\*AP<sup>®</sup> is a trademark registered and/or owned by the College Board, which was not involved in the production of, and does not endorse, this product.

# How Can **ODYSSEY** Molecular Explorer Be Used?

- **Direct Demonstrations**

("The Molecular Perspective")



- **Inquiry/Exploration**

(Ask Leading Questions!)

- **Computer Lab Experiments**

(Complement Wet Lab)

- **Take-Home Labs**

- **Enrichment**

- **Self-Study**

*Teacher Computer*

*Classroom  
Computers*

*Student  
Computers*

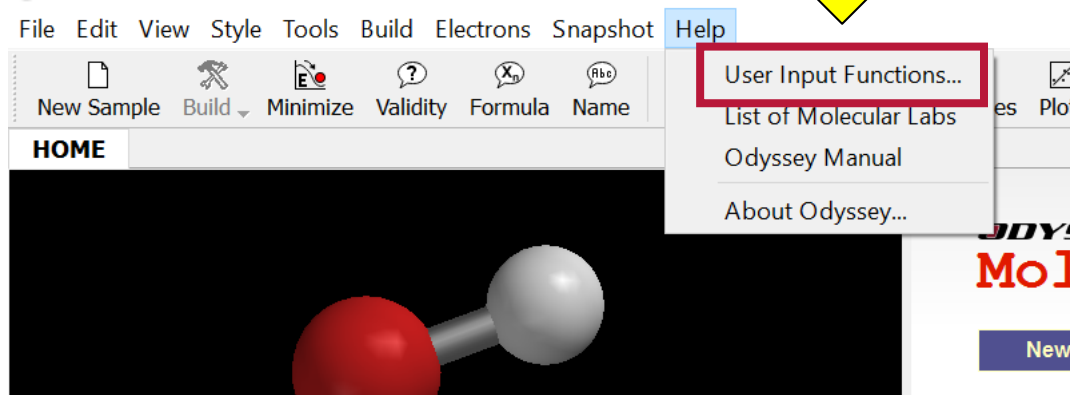
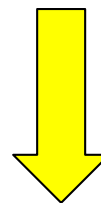
User Input Functions

**Touchscreen, Trackpad, Mouse**



**In-Program Reference:**  
***Help* Menu**

(Tailored for Windows/Macintosh)



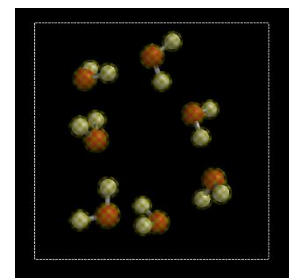
- ❑ **Rotate**
  - Drag (Touchscreen)
  - **Left** Button + Drag (Trackpad / Mouse)
  
- ❑ **Translate**
  - **Long** Press + Drag (Touchscreen)
  - **Right** Button + Drag (Win Touchpad / Mouse)
  - **⌘** + **Button** + Drag (Mac Trackpad)
  
- ❑ **Zoom**
  - **Pinch** (Touchscreen / Trackpad)
  - **Scroll Wheel** (Mouse)

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

☐ CTRL key not held down



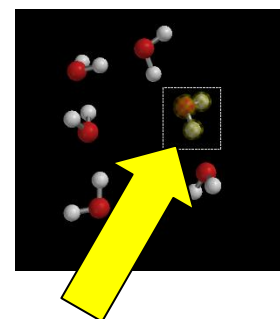
Rotate / Translate  
**Entire** Model  
( = All Molecules)

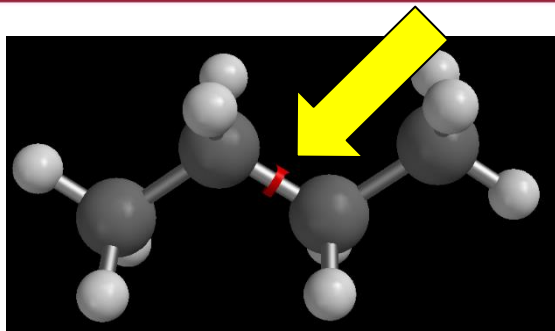


☐ **CTRL key** held down



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

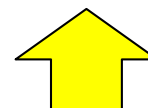
- ❑ **ALT key held down** →

**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**

## What Style Should I Choose?

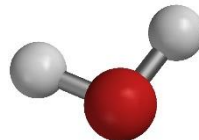
☐ Start with **Space Filling** — it shows what things “really look like”

- 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

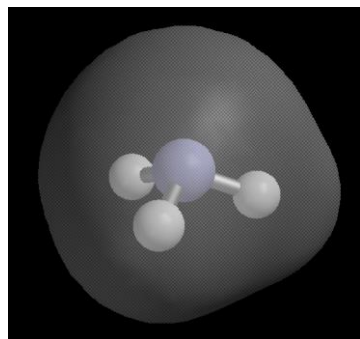
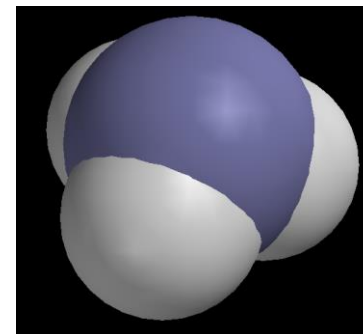


→ **Ball and Spoke** is the default style for the build panels

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

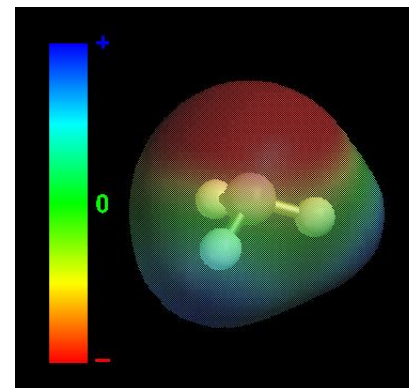
### Molecular Shape / Polarity

- ☐ **Space Filling** style — Approximate Shape



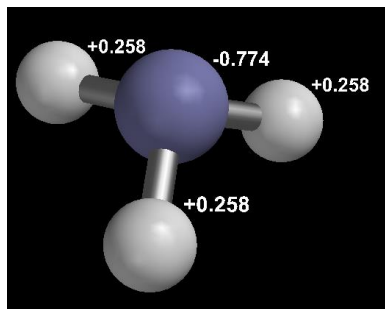
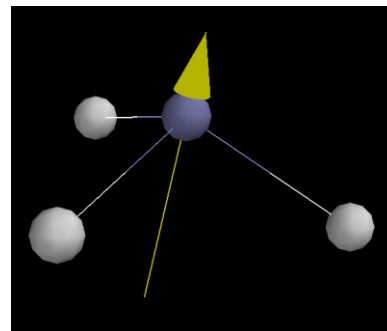
- ☐ **Outer Surface** — True Shape  
(Electron Cloud, ~98% of the total density)

- ☐ **Polarity Map** — True Shape + Polarity



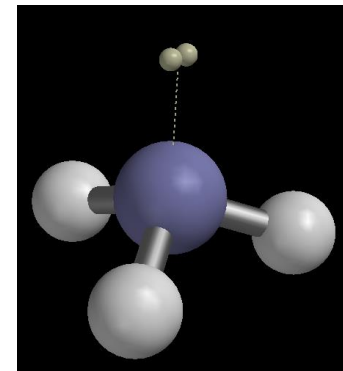
## Molecular Shape / Polarity

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



- ☐ **Charge Labels** — Atomic Partial Charges

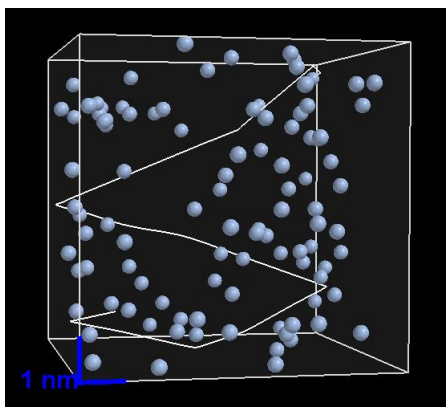
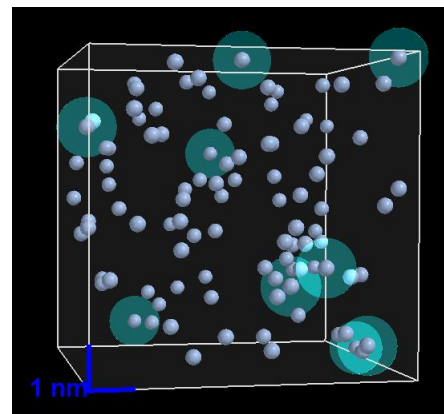
- ☐ **Lone Pairs** — Cartoon Representation





### Gas Laws / Kinetic Theory

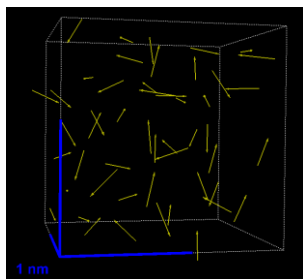
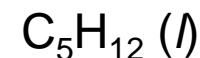
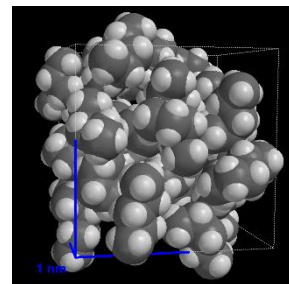
- ❑ **Collisions** —  
select **Molecule-Wall**  
→ Concept of “Pressure”



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

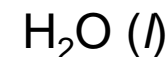
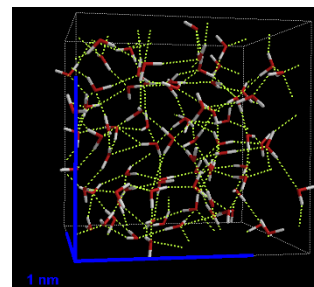
## Intermolecular Forces

- ☐ **Space Filling** style  
→ *Dispersion forces*



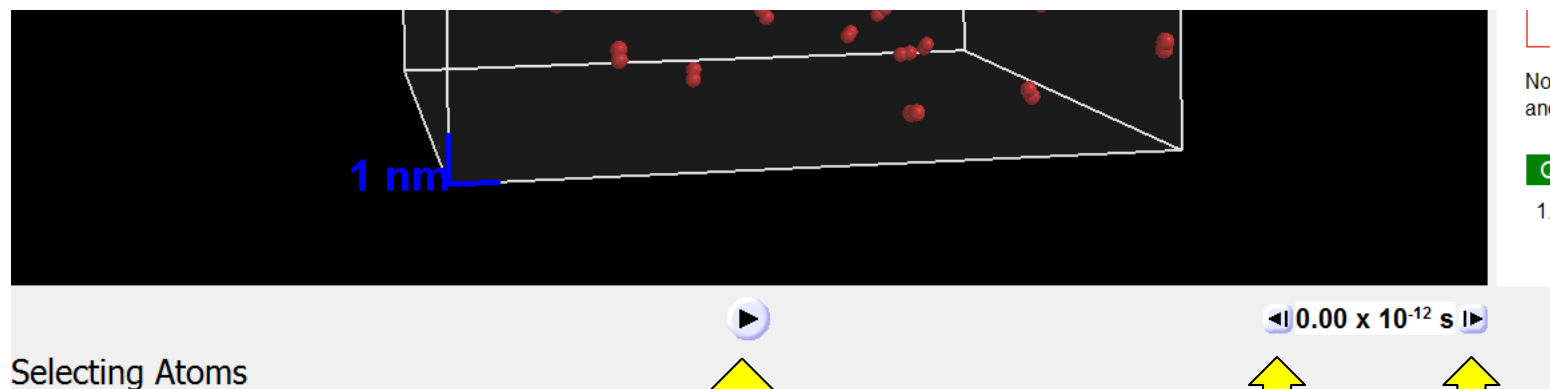
- ☐ **Dipole Arrows**  
(Combine with the **Hide** style)  
→ *Dipole-dipole forces*

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



Dynamics

# Starting and Controlling Simulations



**Go/Stop Toggle**  
(Continuous Simulation)

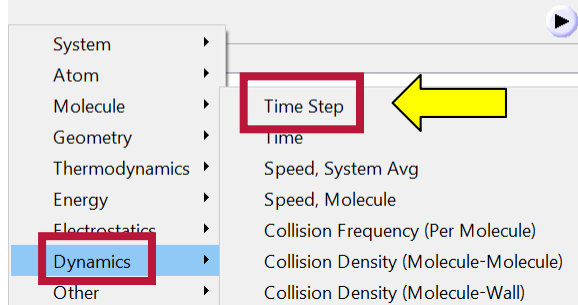
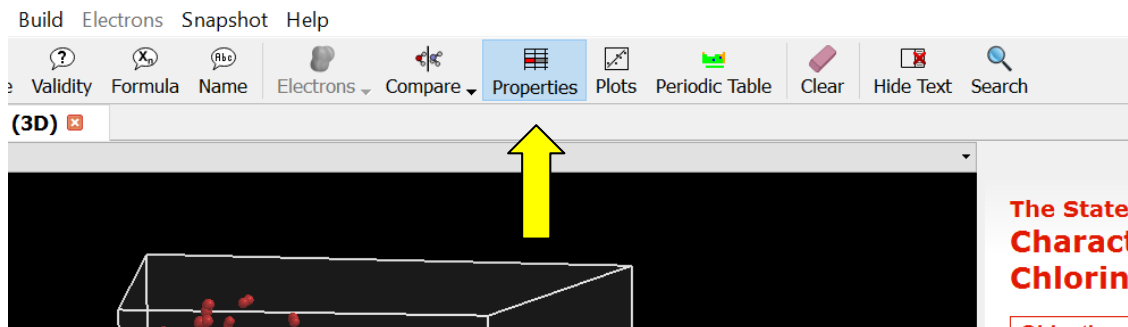
**Go Back / Go Forward**  
(Step-by-Step)

## Time Scales

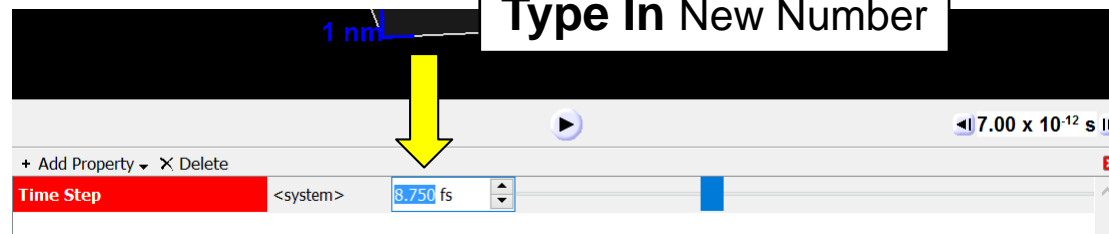
- |                                  |   |
|----------------------------------|---|
| $\sim 10^{-15}$ s (femtoseconds) | ← Actual Molecular Time Step<br>(as assigned by the program)            |
| $\sim 10^{-12}$ s (picoseconds)  | ← Typical “Step-by-Step” Interval                                       |
| $\sim 10^{-9}$ s (nanoseconds)   | ← Maximum Length of Simulations<br>(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**

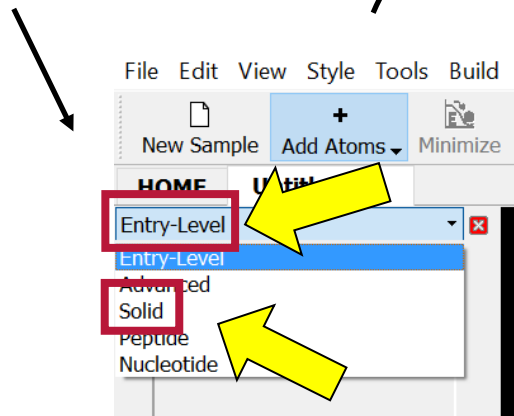
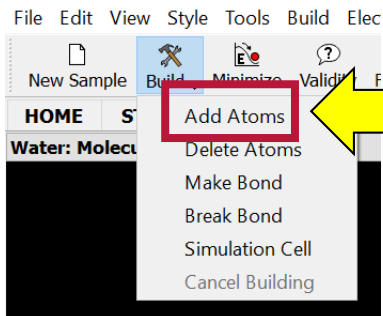
Simulation Effectively  
**Speeds Up**

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

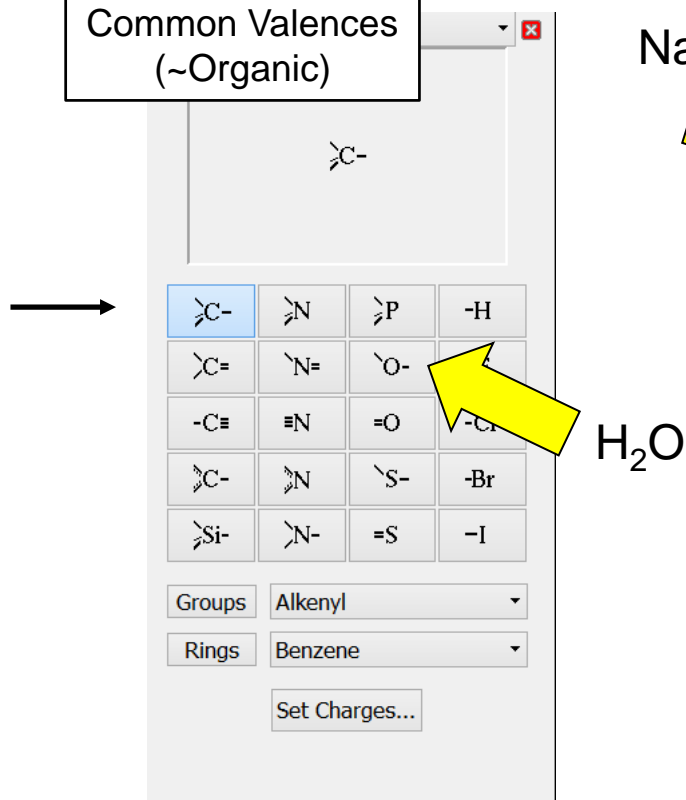
...but should **not** significantly increase  
step size or may provoke a numerical  
instability (and possibly program crash)  
(→ automatically assigned time step is already “large”)

Building  
**From Molecules to Simulation Cells**

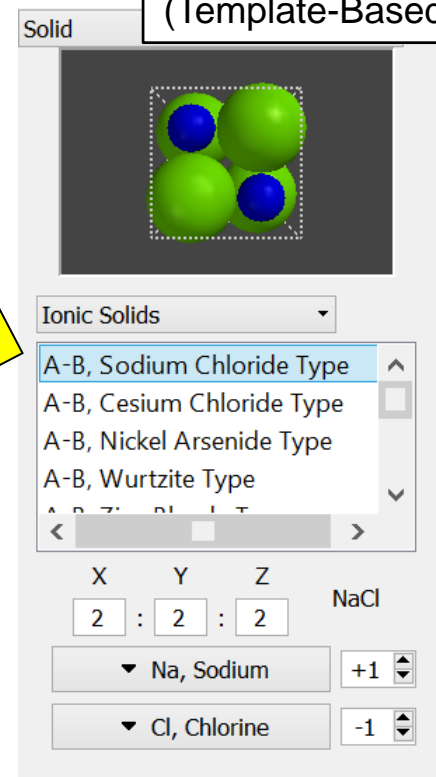
## Molecules, Solids



**Entry-Level**  
Common Valences  
(~Organic)

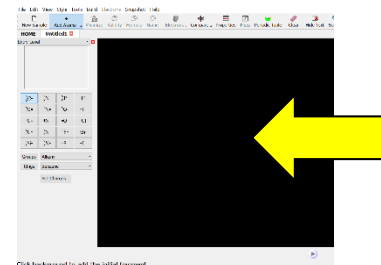


**Solid**  
(Template-Based)

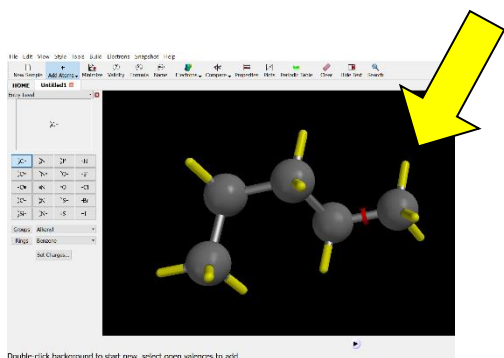




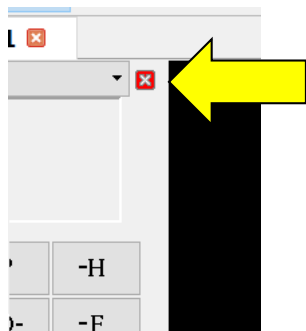
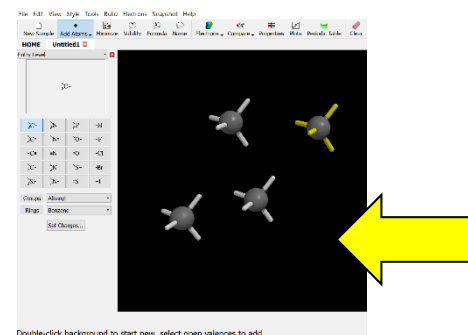
- ❑ Initial single click on background  
→ Start molecule (first building block)



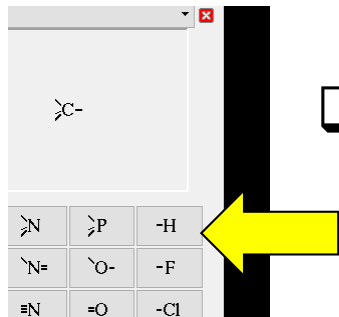
- ❑ **Single** click on yellow spoke (free valence)  
→ Continue with the *same* molecule



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

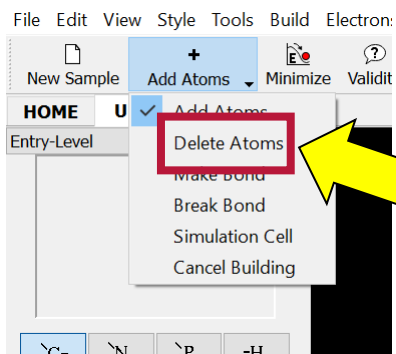


- ❑ Close the build panel with its **Close**  button  
(Starting a simulation  will also close the build panel)

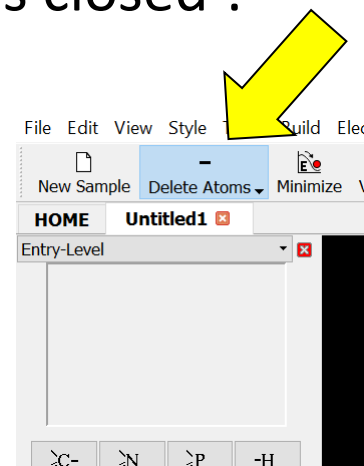




☐ **Hydrogens** can be added manually...

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



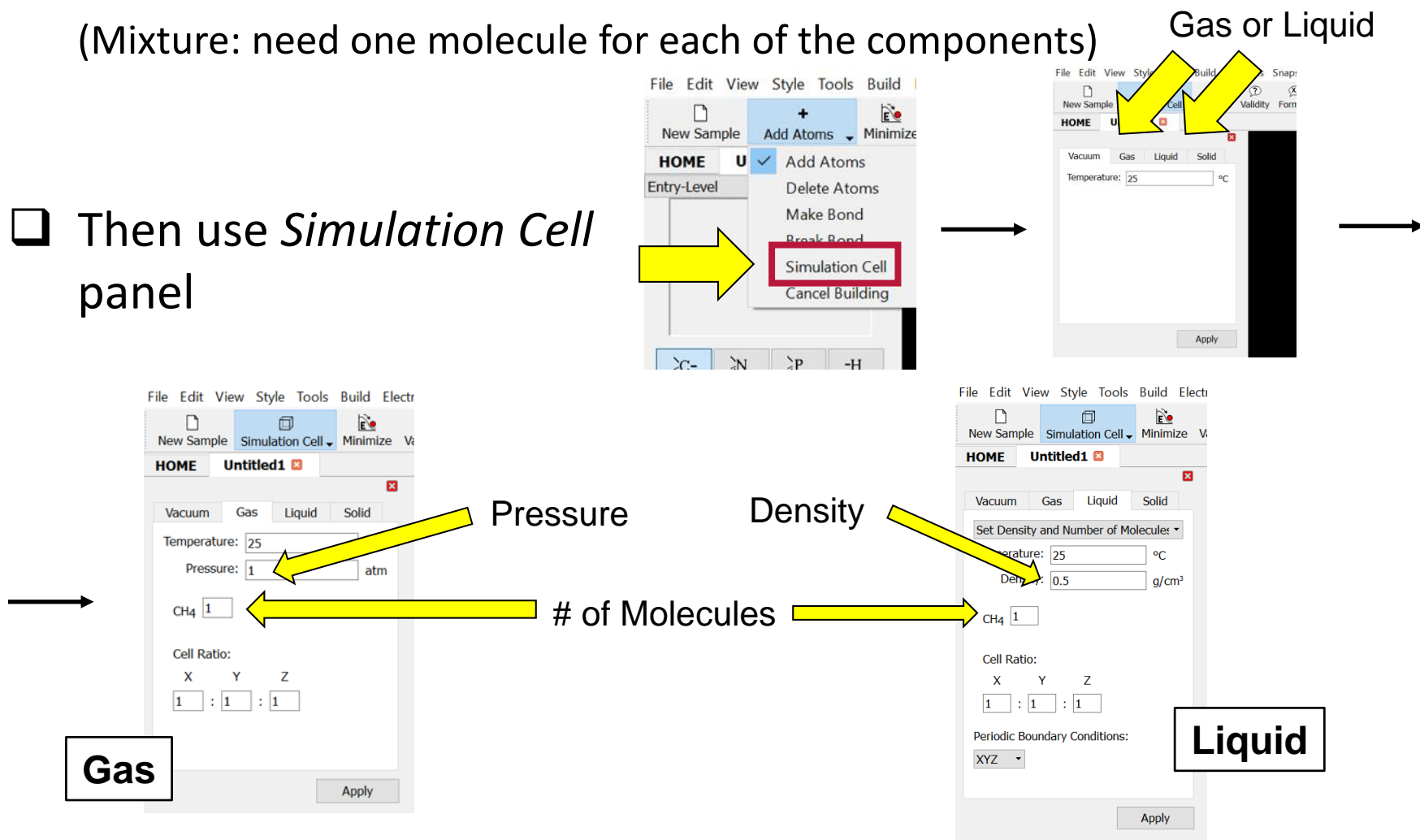
☐ **Deleting is modal**  
→ Will keep deleting until returning to “Add Atoms”



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

- ❑ Must build molecule first  
(Mixture: need one molecule for each of the components)

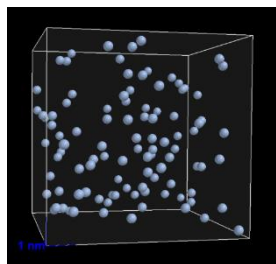
- ❑ Then use *Simulation Cell* panel



- ❑ Don't exceed ~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<sup>3</sup> instead of 1.0 g/cm<sup>3</sup>)  
→ More mobility, faster equilibrium

## Unusual Bond Orders, Inorganic Compounds, Complexes

File Edit View Style Tools Build

New Sample Add Atoms Minimize

HOME Untitled1

Entry-Level

Advanced

Solid

Peptide

Nucleotide

Coordination

Bond Order

Advanced

Pop-Up Periodic Table

Ar

Ar, Argon

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

Ligands Carbon Monoxide

Set Charges...

Advanced

## Peptides, Oligonucleotides

The interface shows the 'HOME' tab with 'Untitled1' open. The 'Build' menu is open, showing 'Entry-Level', 'Advanced', 'Solid', 'Peptide', and 'Nucleotide'. The 'Peptide' panel displays the chemical structure of glycine and a list of amino acids (gly, ala, val, leu, ile, ser, thr, cys, met, phe, tyr, trp, asp, asn, glu, gln, arg, his, lys, pro). The 'Strand Type' section has 'Single Amino Acid' selected. The 'Nucleotide' panel displays the chemical structure of deoxyadenosine monophosphate and options for strand type (Single Nucleotide (DNA), Single Nucleotide (RNA), DNA (Double Strand), DNA - RNA, RNA (Single Strand)).

**Peptide**

**Nucleotide**

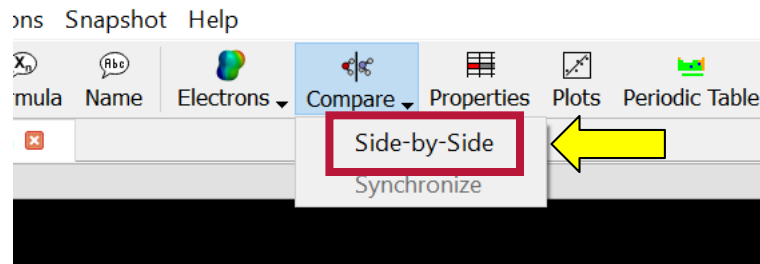
Watson-Crick DNA

$\alpha$ -Helix or  $\beta$ -Sheet

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

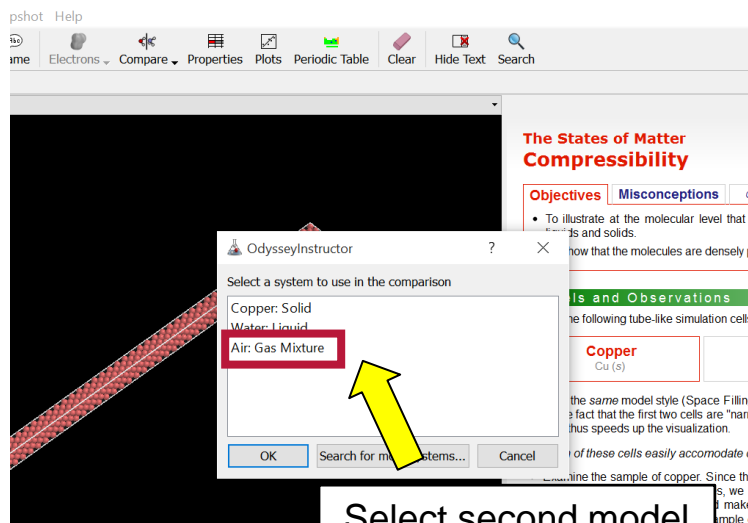
Comparing  
**Showing Models Side-by-Side**

# Comparing Two Models from the Same Lab

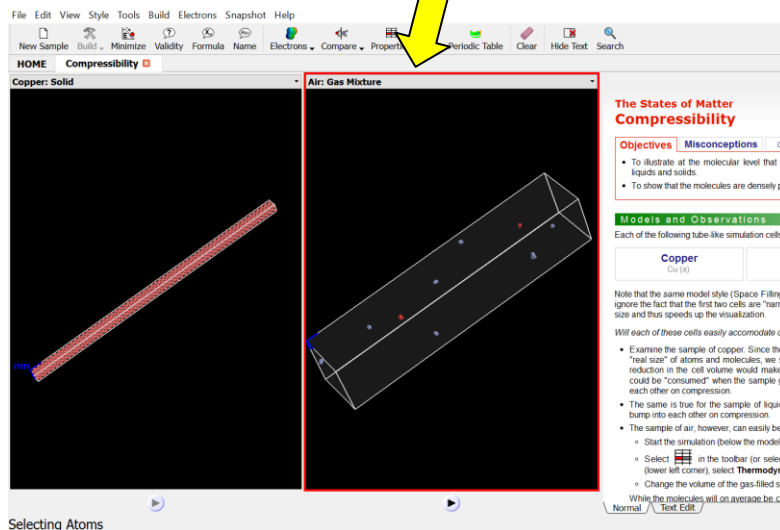


Models can be manipulated individually

Choose “active” model (has **red frame** around it) by selecting its background

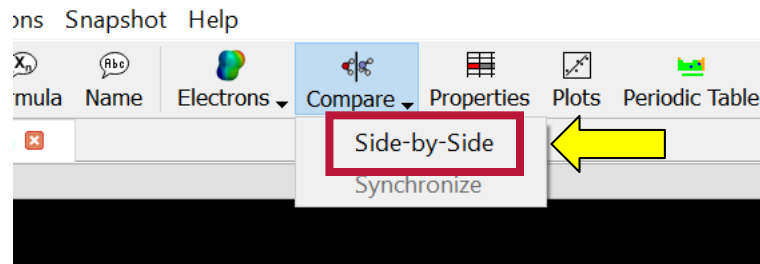


Select second model for the comparison

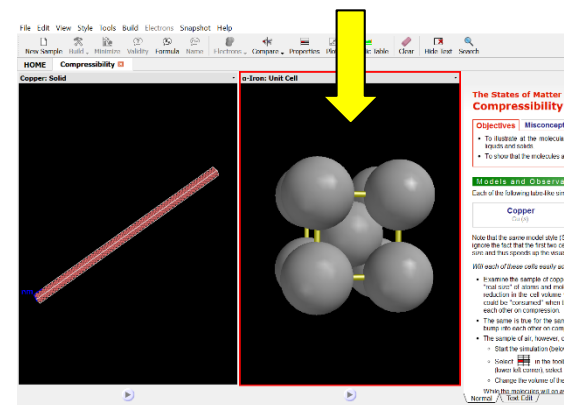




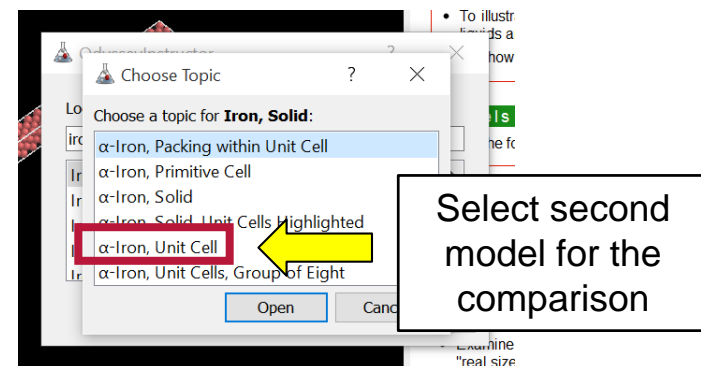
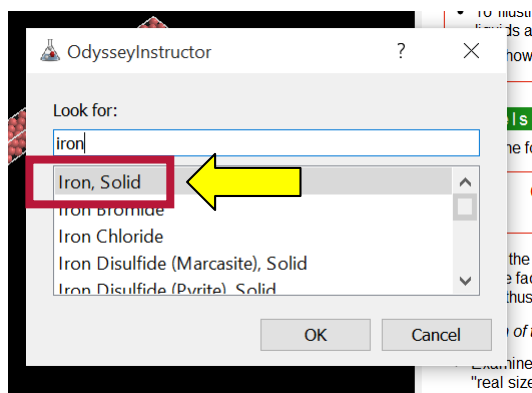
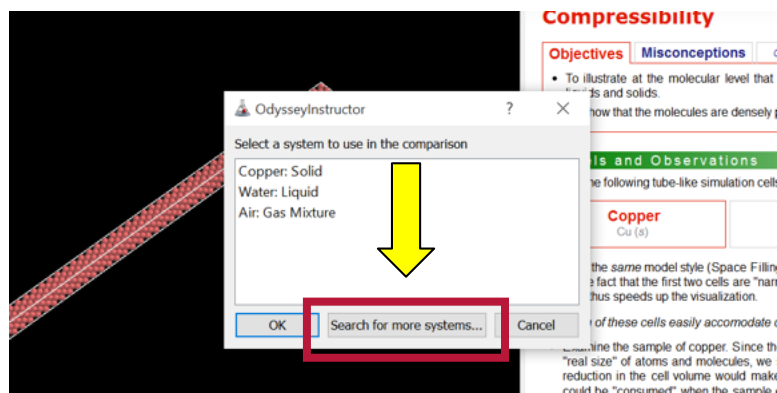
# Getting the Comparison Model via Search



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

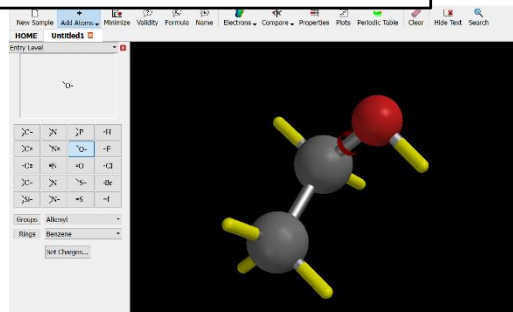


Available for comparison:  
~1,800 models



# Comparing Two User-Built Models (I)

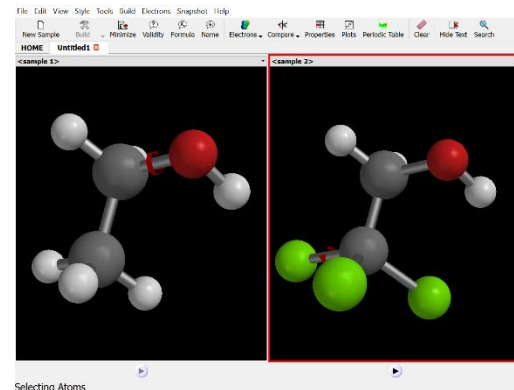
Build the first model...



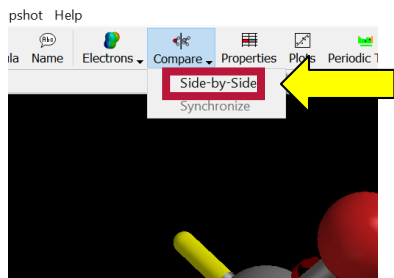
Suitable even for...

- ☐ simulation **cells**
- ☐ independent **dynamics** of both systems
- ☐ independent **electron** cloud calculations

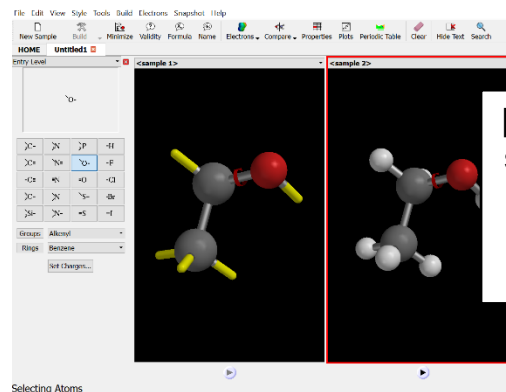
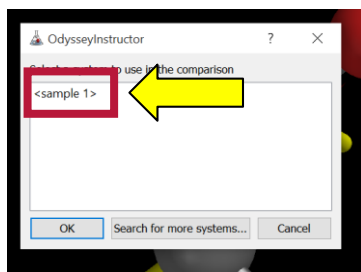
...keep the build panel **open!**  
(if already closed, you **must** reopen it with *Build* → *Add Atoms*)



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



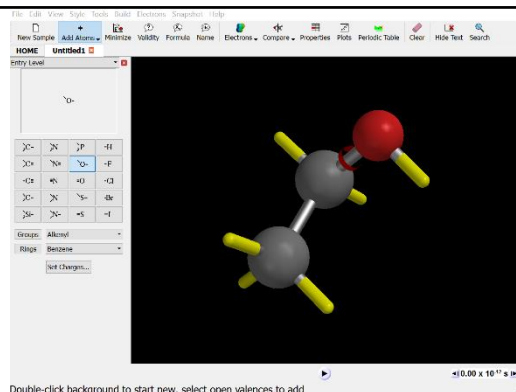
Duplication  
Step



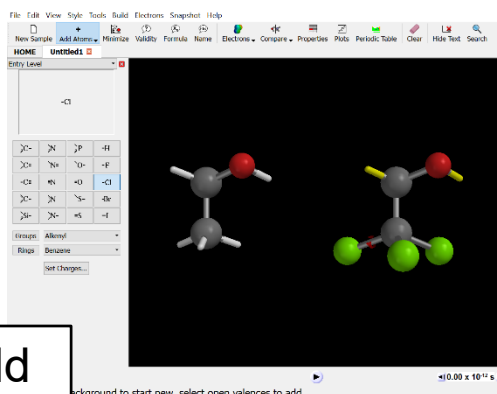
[ The hydrogens of the second model will turn into yellow spokes as soon as a building block is selected ]

## Alternate Method

Build the first molecule...

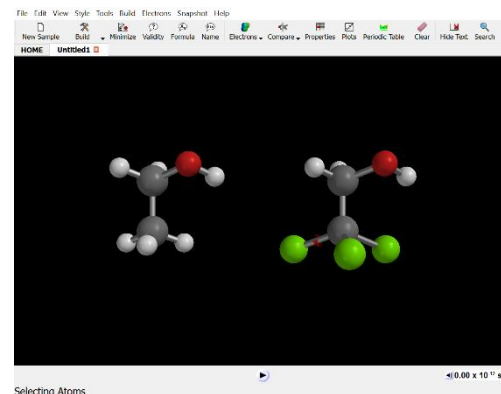


...and simply add another molecule to the **same** model (double-tap/double-click on background to start the second molecule)



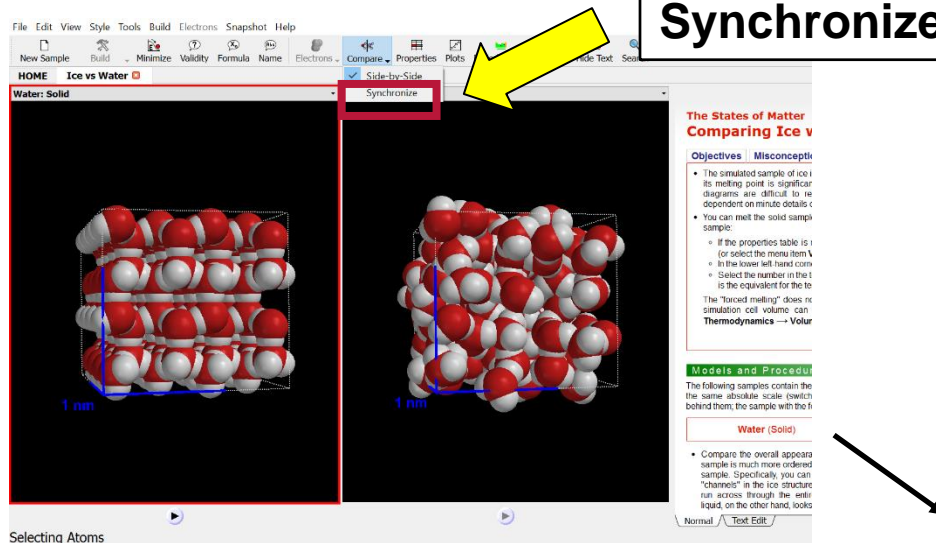
Close the build panel

- ☐ 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

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

