Teaching Chemistry

with ODYSSEY Molecular Explorer

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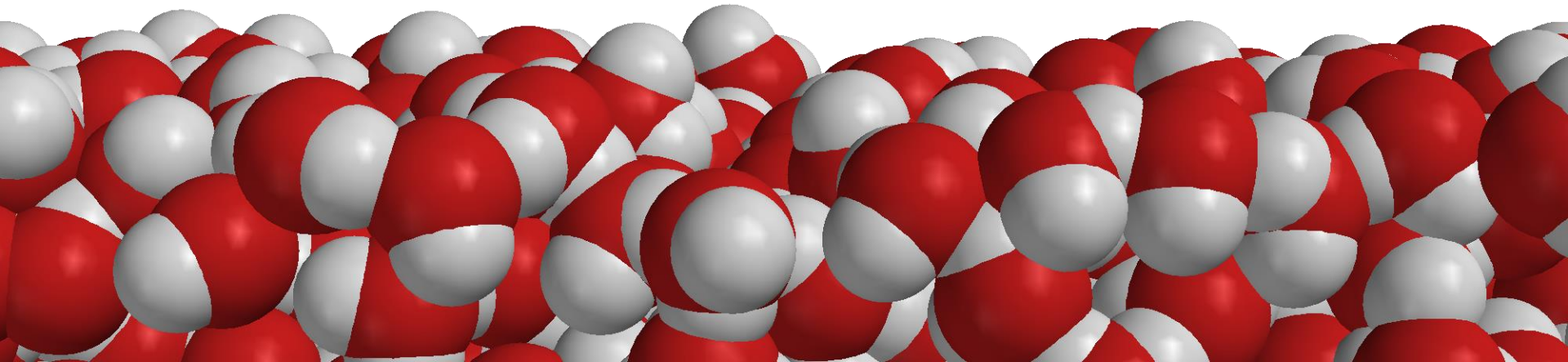


In This Document…

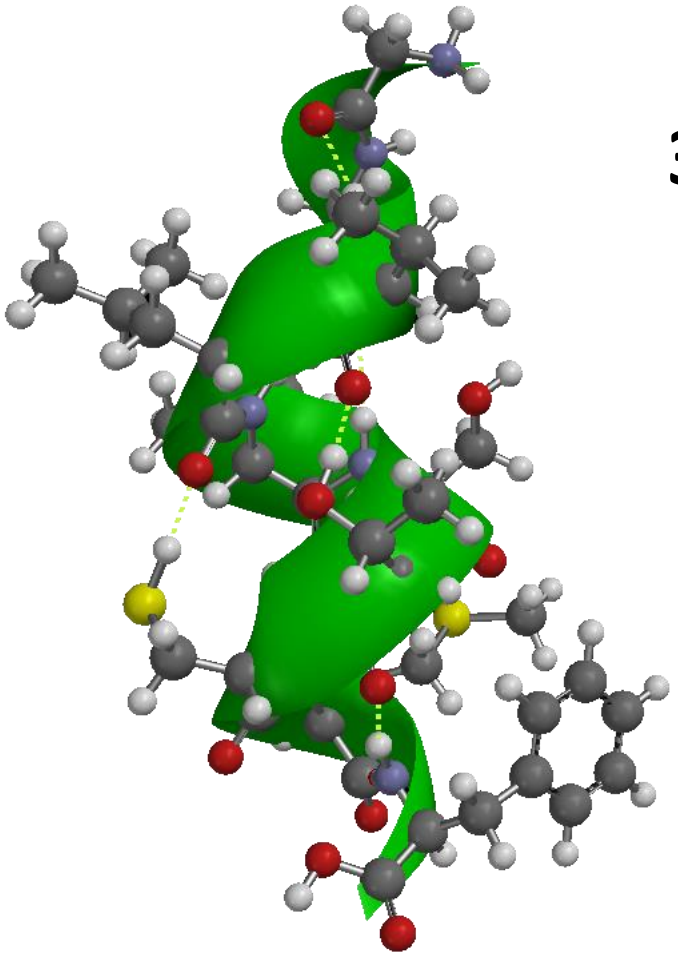
ODYSSEY
Molecular Explorer

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

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**

Instructor Computer (Lecture)

Lab Computers

Student-Owned Computers

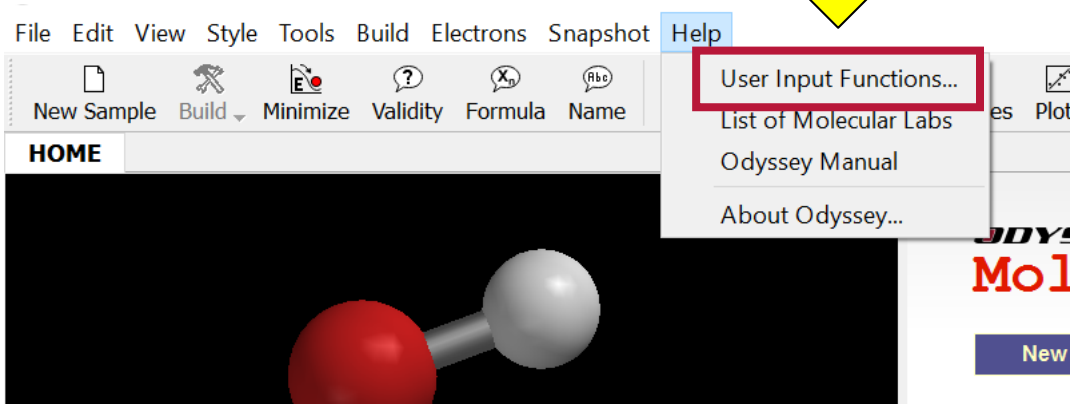
ODYSSEY Molecular Explorer

User Input Functions

Touchscreen, Trackpad, Mouse

How Do I Manipulate the Models?

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



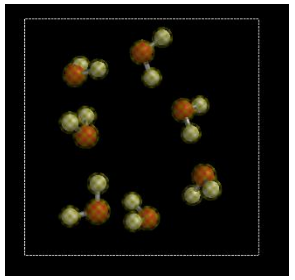
Main 3D Functions

- **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)

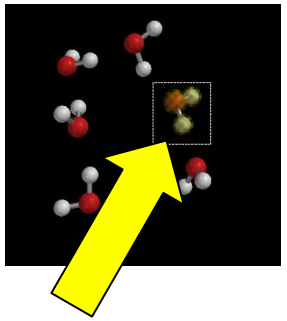
Further options are available, especially for older computers
→ Consult ***User Input Functions…*** in the **Help** menu

Models with Multiple Molecules

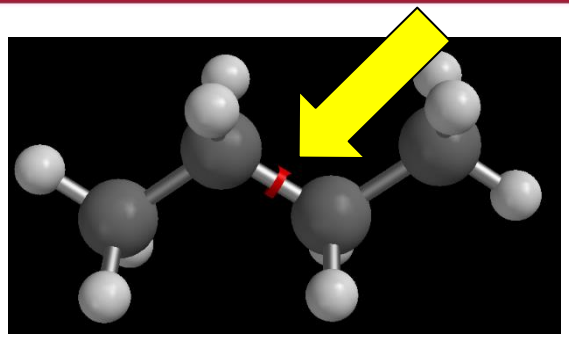
- CTRL key not held down → Rotate / Translate **Entire** Model (= All Molecules)



- **CTRL key held down** → Rotate / Translate **Selected** Molecule Only



Manipulating a Selected Bond



- **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)

ODYSSEY Molecular Explorer

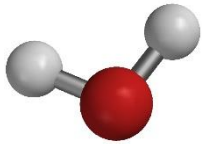
Visualization

Model Styles and Other Display Options

What Style Should I Choose?

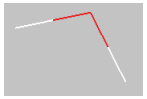
- Start with **Space Filling** — it shows what things "really look like"
  - Molecular shape
  - Packing in solids and liquids
  - Emptiness of gases

- 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



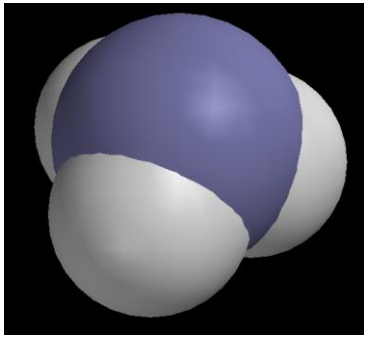
→ **Ball and Spoke** is the default style for the build panels

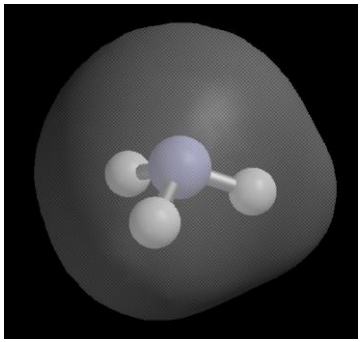
→ Use **Space Filling** for gases…or you will hardly see anything !

Custom Visualization (I)

Molecular Shape / Polarity

- **Space Filling** style — Approximate Shape

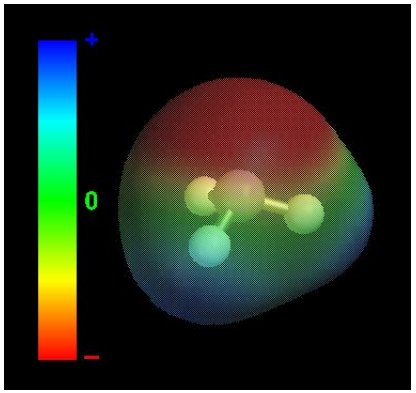




- **Outer Surface** — True Shape

  (Electron Cloud, ~98% of the total density)

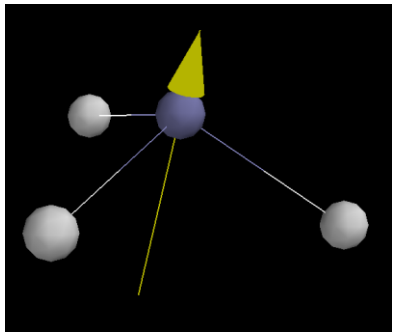
- **Polarity Map** — True Shape + Polarity

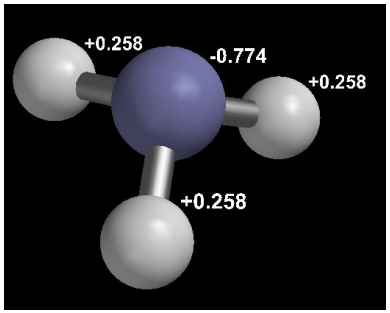


ODYSSEY Molecular Explorer — Custom Visualization (II)

Molecular Shape / Polarity

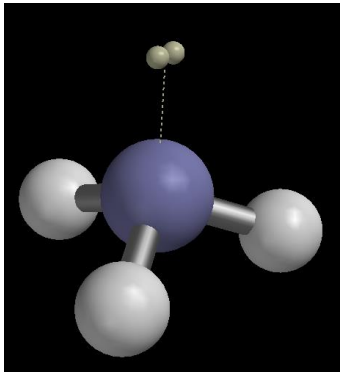
- **Dipole Arrow(s)** —
  Combine with **Ball and Wire**
  (or **Wire**) style





- **Charge Labels** — Atomic Partial Charges

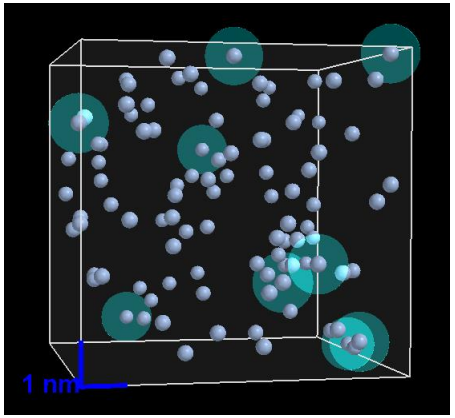
- **Lone Pairs** — Cartoon Representation

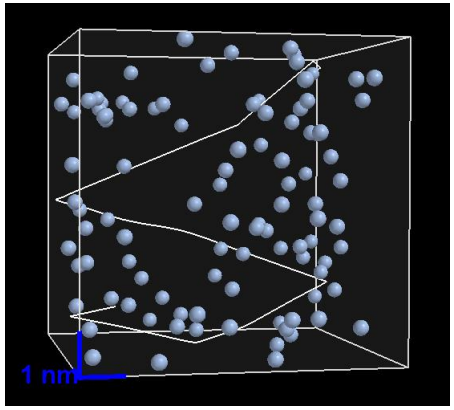


Custom Visualization (IV)

Gas Laws / Kinetic Theory

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



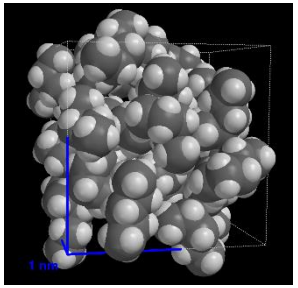


- **Trails** — *Right-click* on an atom and select **Set Trail**

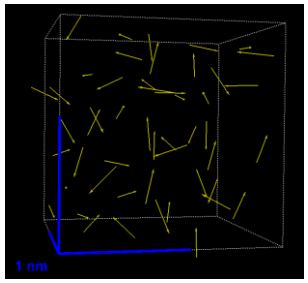
Custom Visualization (III)

Intermolecular Forces

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



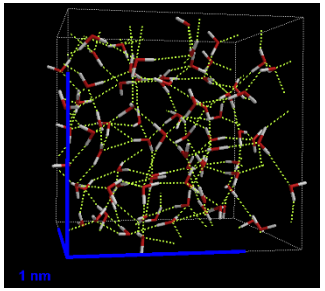
C_5H_{12} (*l*)



CH_2Cl_2 (*l*)

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

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



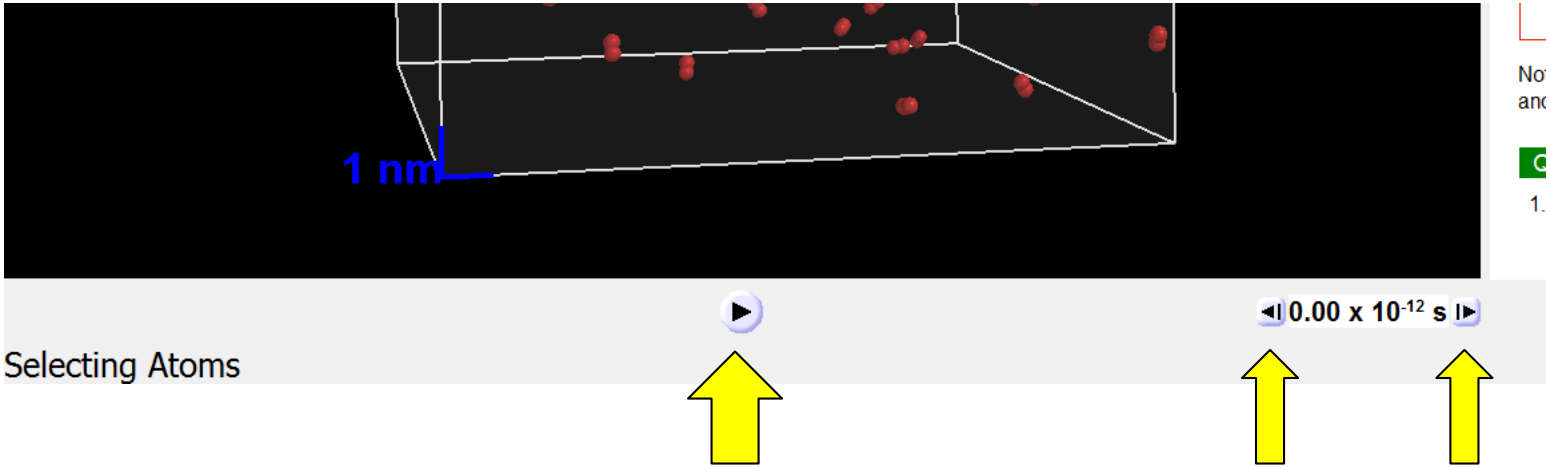
H_2O (*l*)

ODYSSEY
Molecular Explorer

Dynamics

Starting and Controlling Simulations

Molecular Dynamics (I)



Go/Stop Toggle
(Continuous Simulation)

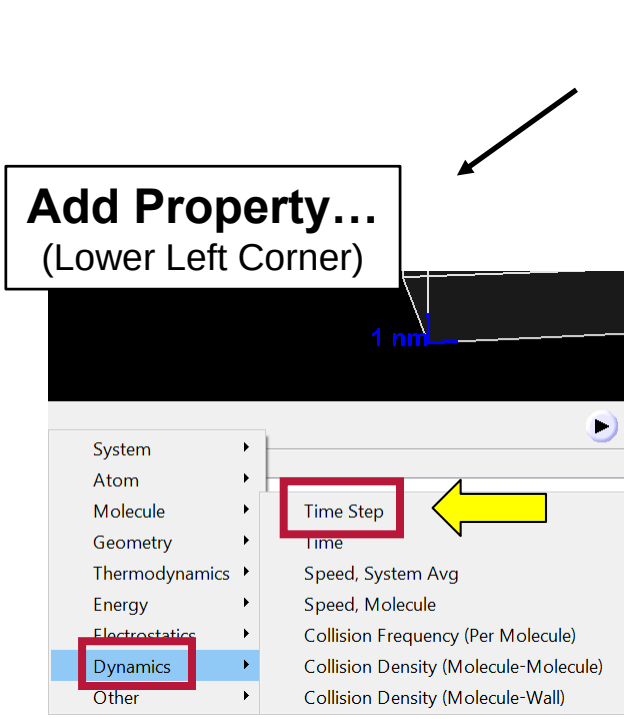
Go Back / Go Forward
(Step-by-Step)

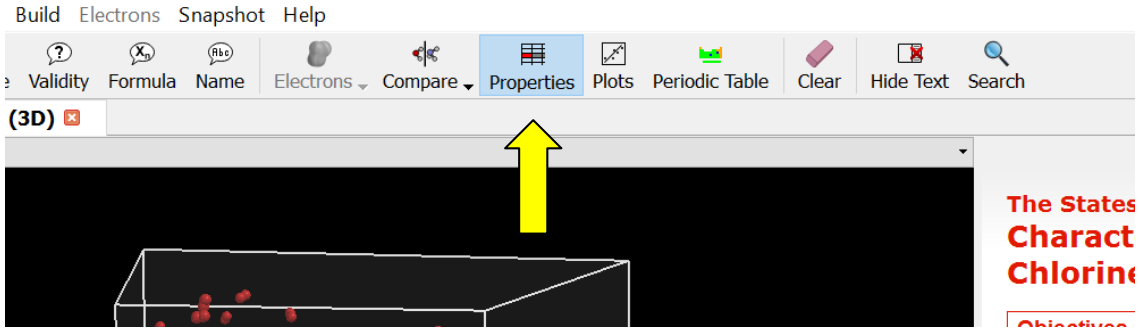
Time Scales

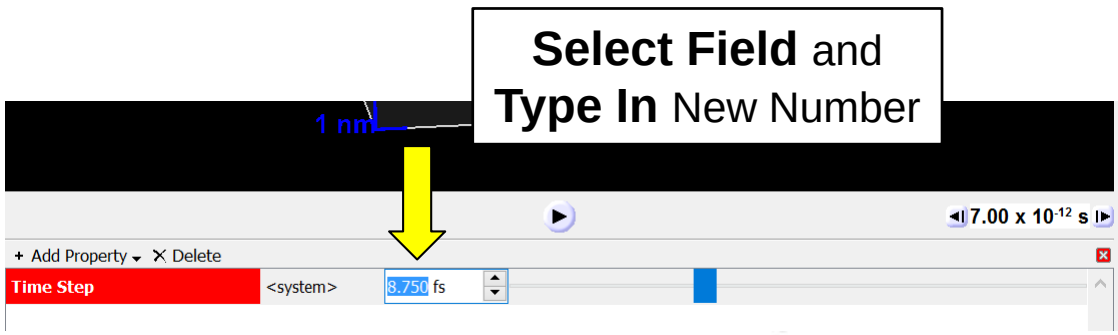
- ~10^{-15} s (femtoseconds) ← Actual Molecular Time Step (as assigned by the program)
- ~10^{-12} s (picoseconds) ← Typical "Step-by-Step" Interval
- ~10^{-9} s (nanoseconds) ← Maximum Length of Simulations (long simulations of hours duration)

Molecular Dynamics (II)

Slowing Down (and Speeding Up)







Molecular Dynamics (III)

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”)

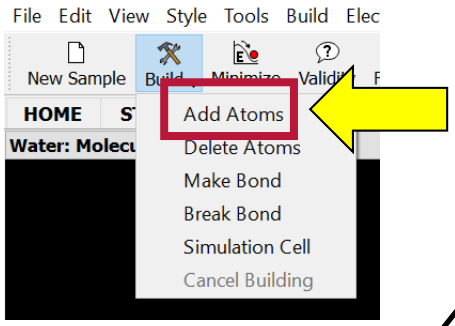
ODYSSEY
Molecular Explorer

Building

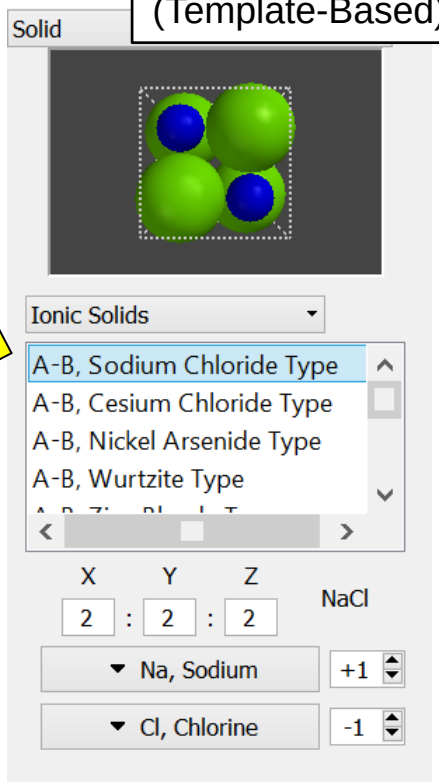
From Molecules to Simulation Cells

Simple Building

Molecules, Solids

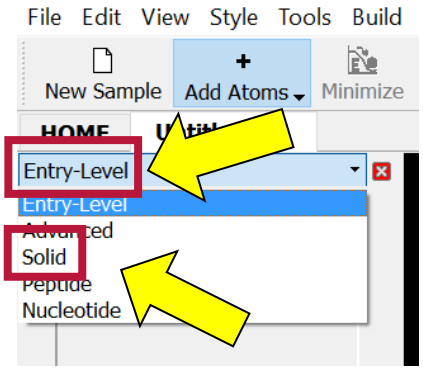


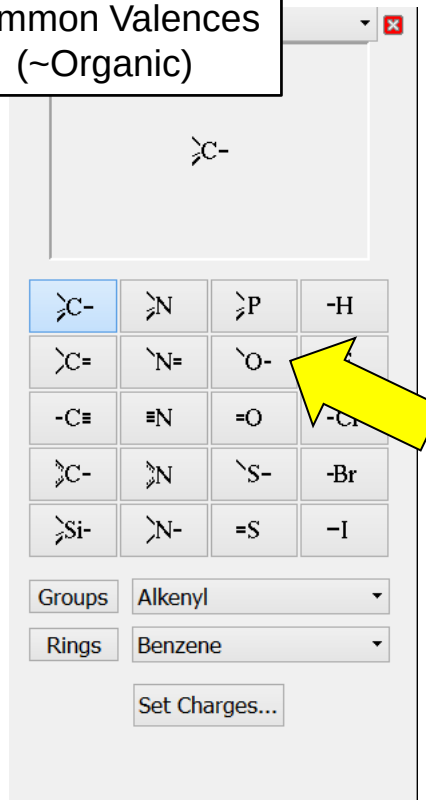
Solid
(Template-Based)



NaCl

Entry-Level
Common Valences
(~Organic)

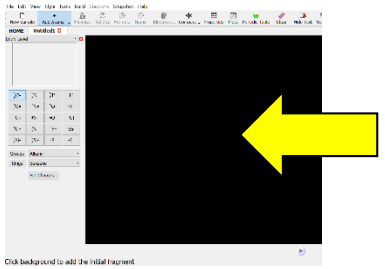


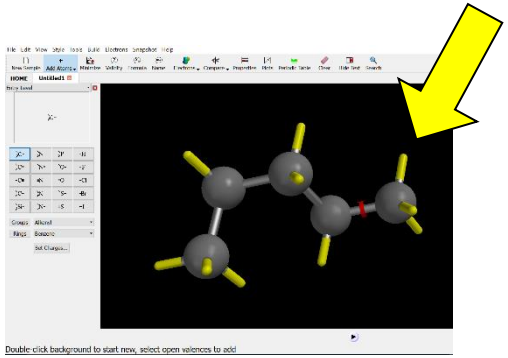


H_2O

ODYSSEY Molecular Explorer — Molecule Building (I)

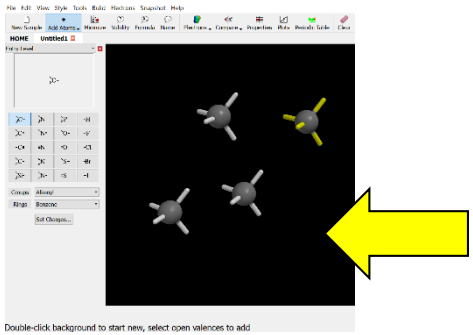
- Initial single click on background
  → Start molecule (first building block)

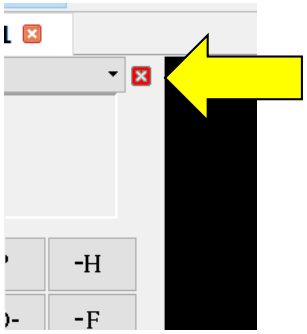




- **Single** click on yellow spoke (free valence)
  → Continue with the *same* molecule

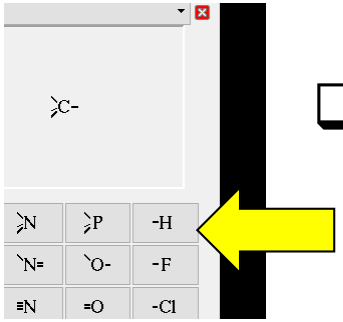
- **Double**-click on background
  → Start *new* (additional) molecule



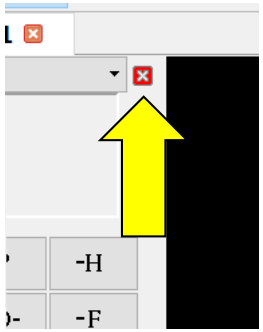


- Close the build panel with its **Close** button
  (Starting a simulation ▶ will also close the build panel)

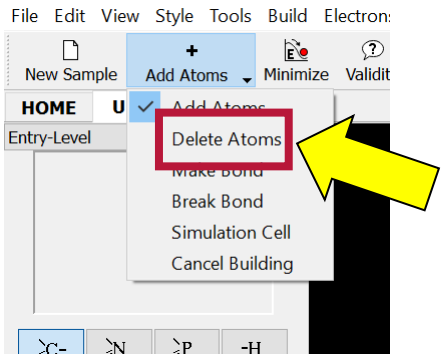
ODYSSEY Molecular Explorer — Molecule Building (II)



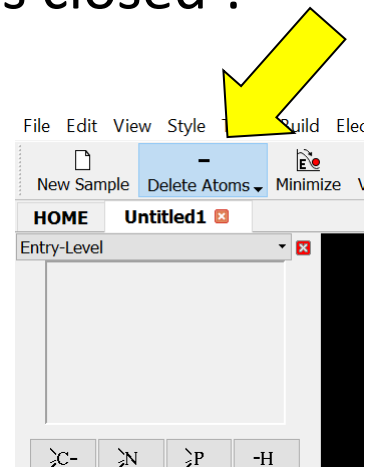
- **Hydrogens** can be added manually…



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



- **Deleting** is modal
  → Will <u>keep deleting</u> until returning to “Add Atoms”



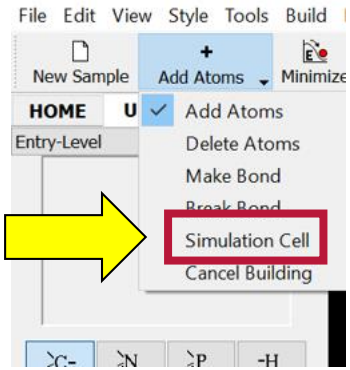
- Always **Minimize** (or run a simulation ▶) when done building!

Building of Gases and Liquids (I)

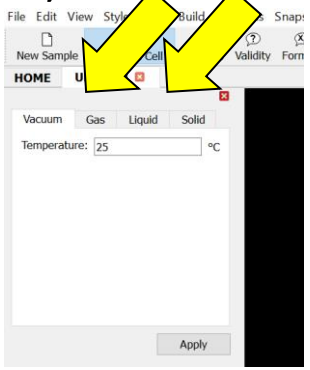
- Must build molecule first

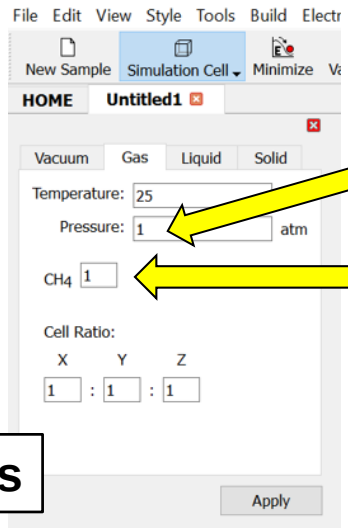
  (Mixture: need one molecule for each of the components)

- Then use *Simulation Cell* panel



Gas or Liquid

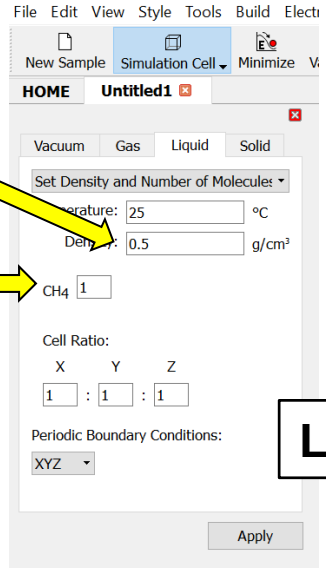




Pressure

Density

# of Molecules



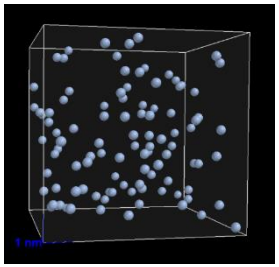
Gas

Liquid

Building of Gases and Liquids (II)

- Don't exceed ~1,000 atoms* total
  …or things may get very slow!

**atoms*, not molecules



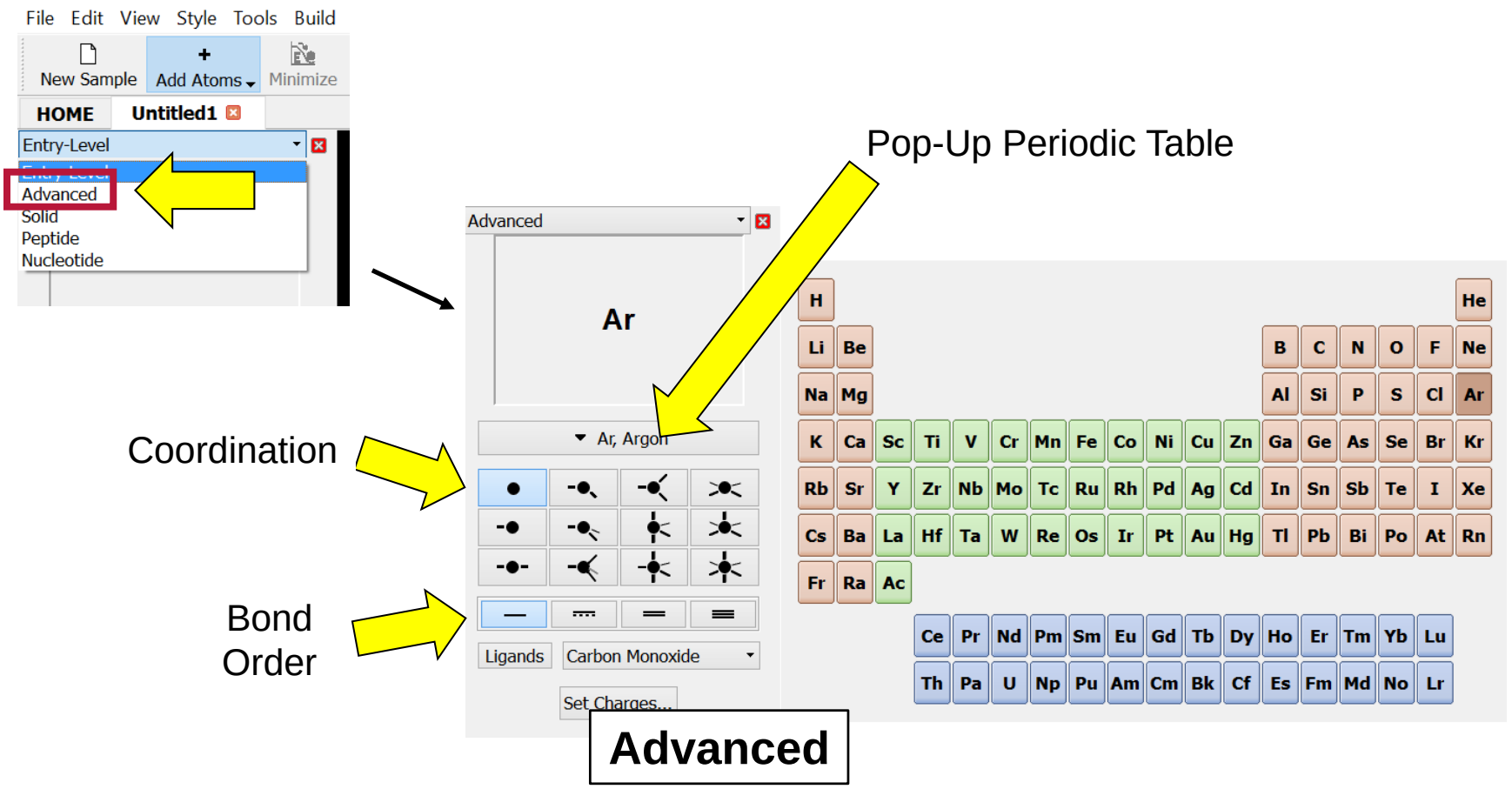
- *Argon* is excellent for
  Gas Laws / Kinetic Theory
  (computationally "cheap")

- 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^3 instead of 1.0 g/cm^3)
  → More mobility, faster equilibrium

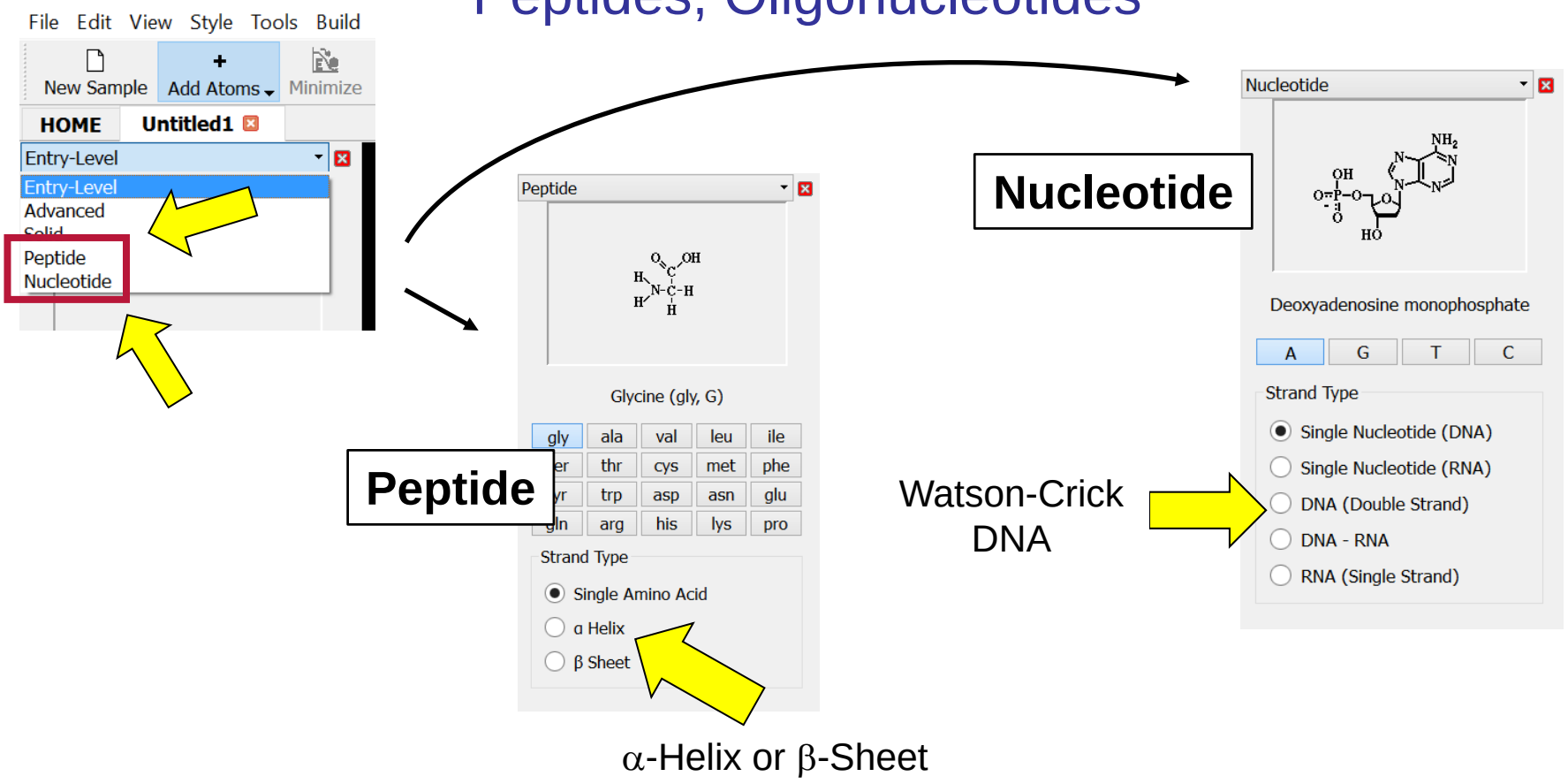
Advanced Building

Unusual Bond Orders, Inorganic Compounds, Complexes



Biopolymer Building

Peptides, Oligonucleotides



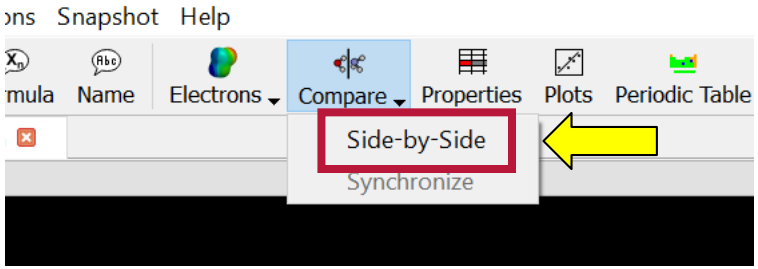
- Don't exceed ~30 amino acids / ~30 base pairs
  …or things may get very slow!

ODYSSEY Molecular Explorer

Comparing

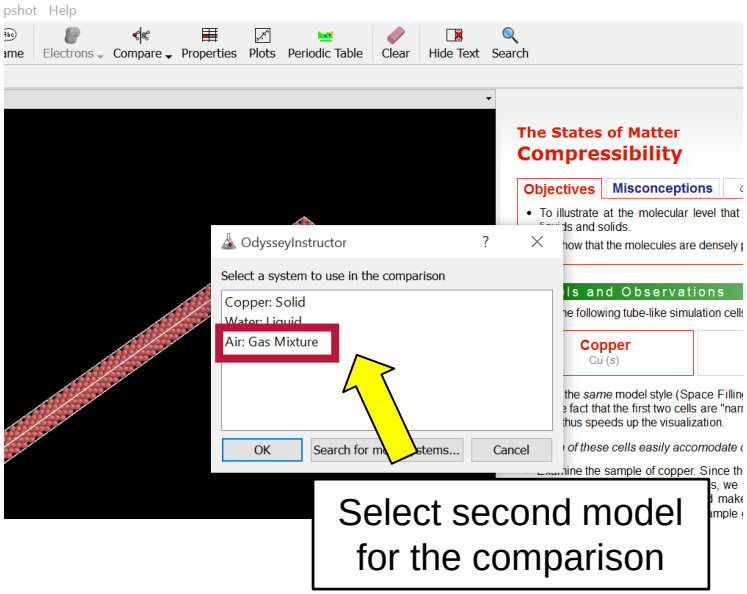
Showing Models Side-by-Side

Comparing Two Models from the Same Lab

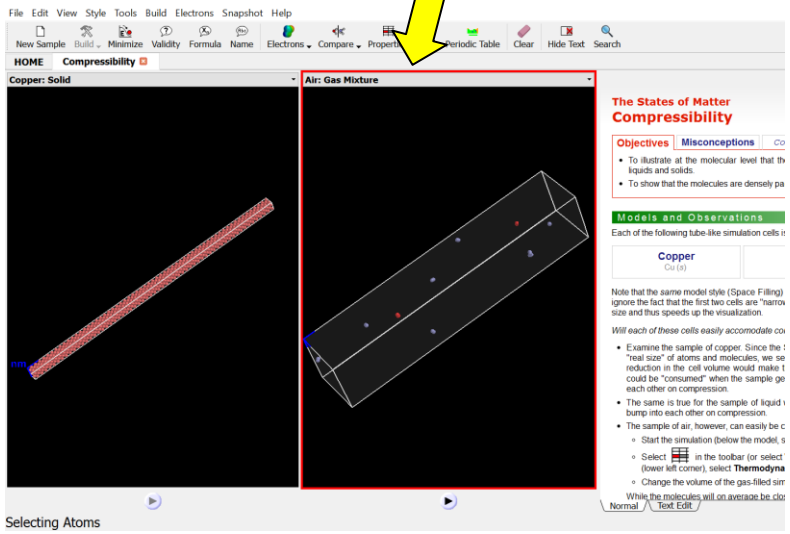


Models can be manipulated individually

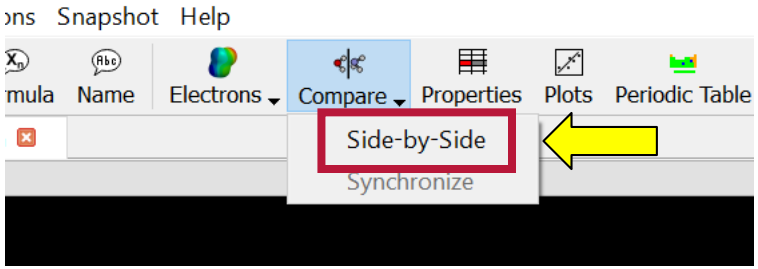
Choose “active” model (has **red frame** around it) by selecting its background



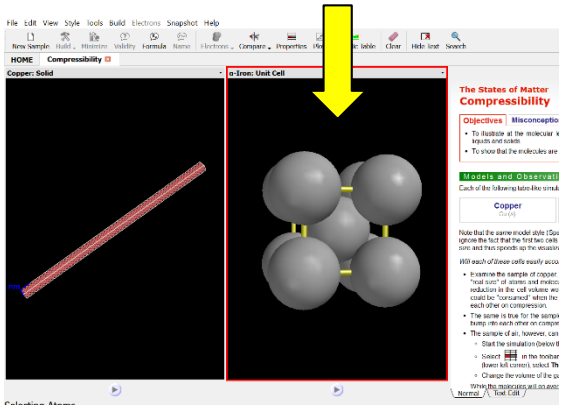
Select second model for the comparison

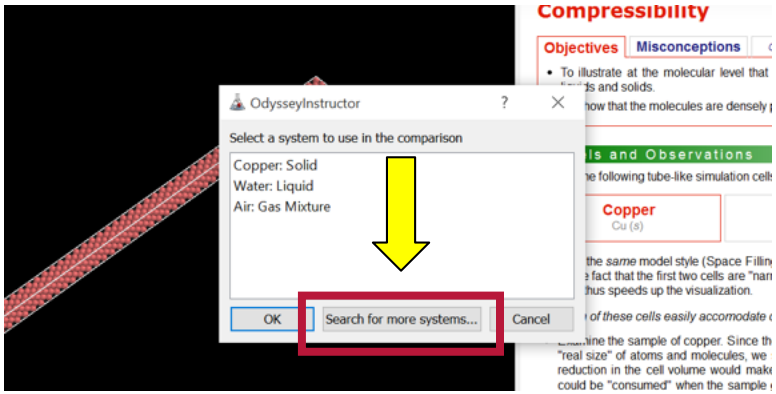


Getting the Comparison Model via Search

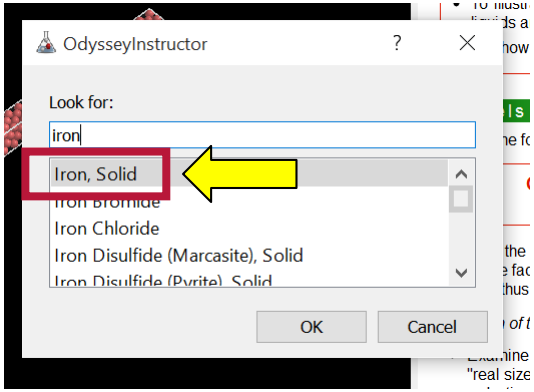


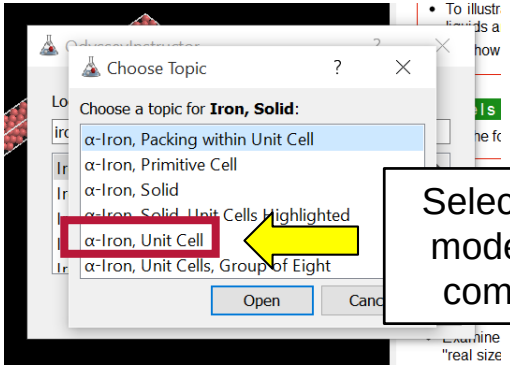
Second model initially shown on same scale (zoom is required)





Available for comparison: ~1,800 models

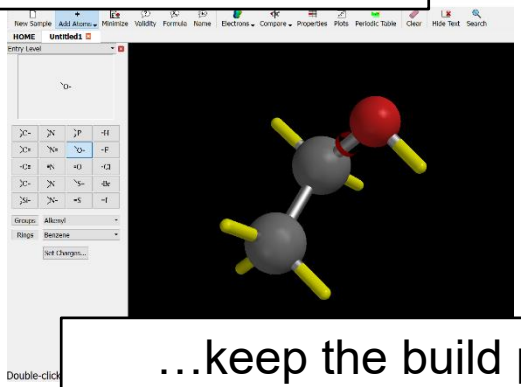




Select second model for the comparison

Comparing Two User-Built Models (I)

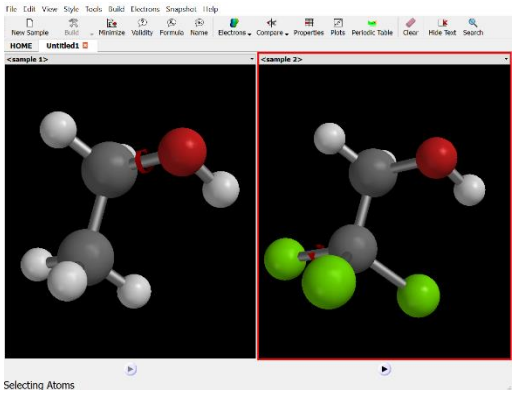
Build the first model…



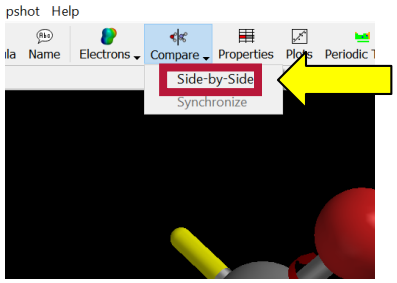
…keep the build panel **open!**
(if already closed, you **must** reopen it with *Build* → *Add Atoms*)

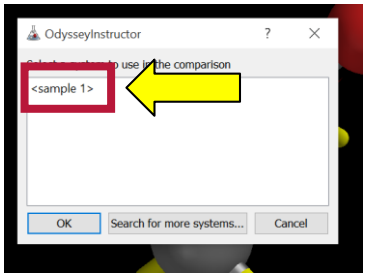
Suitable even for…

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

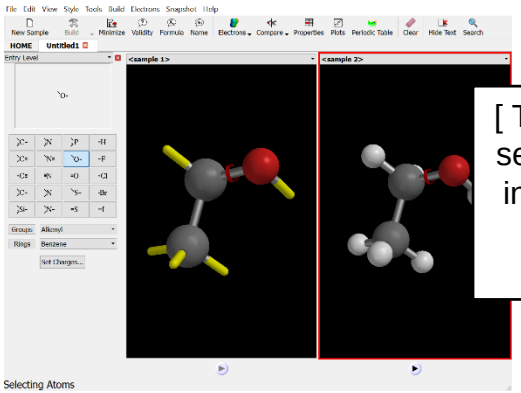


Modify the second model, finally close the build panel
(*Note:* Cannot reopen panel once closed)





Duplication Step

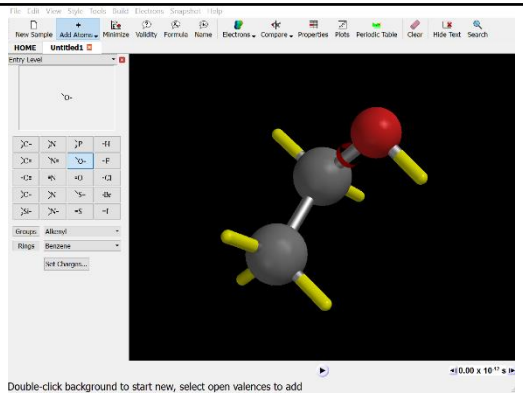


[The hydrogens of the second model will turn into yellow spokes as soon as a building block is selected]

ODYSSEY Molecular Explorer — Comparing Two User-Built Models (II)

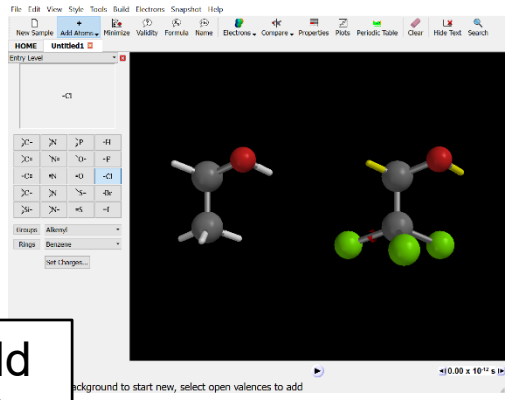
Alternate Method

Build the first molecule…

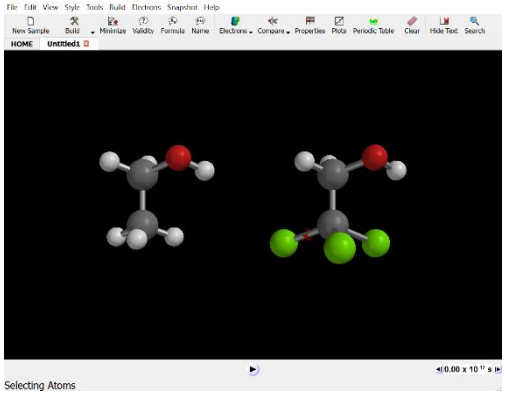


…and simply add another molecule to the **same** model

(double-tap/double-click on background to start the second molecule)



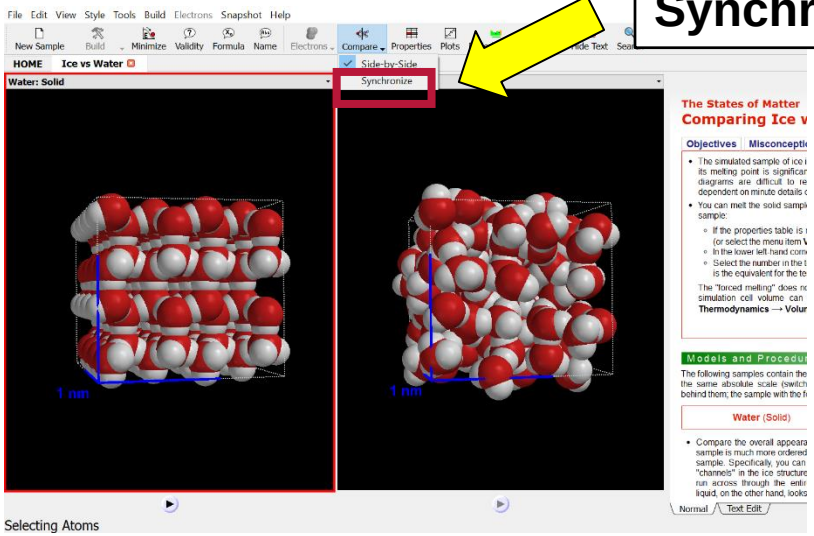
Close the build panel



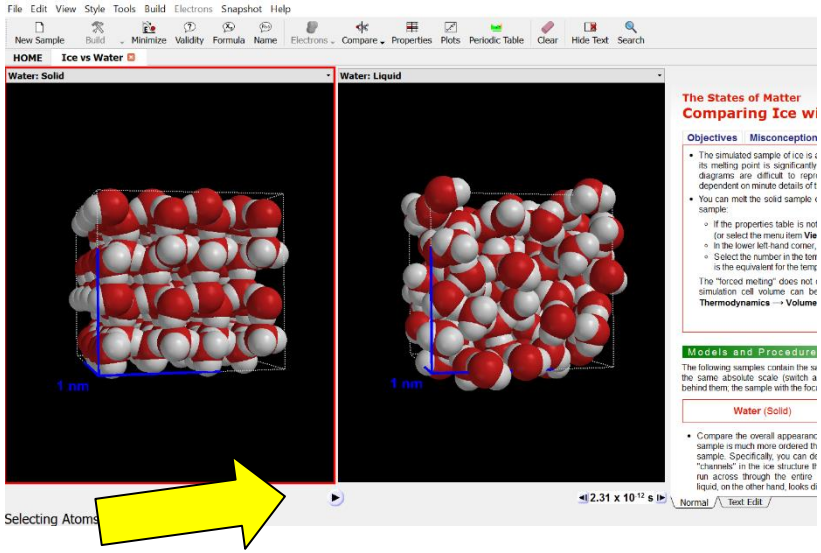
- ❑ Comparison of two simulation cells not possible
- ❑ Dynamics applies to the interacting **dimer** (!) of molecules, not the two molecules independently
- ❑ Electron cloud calculated for the **dimer** (!) of molecules, not the two molecules independently

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)