3-D Molecular Designs
...where molecules become real ™

MSOE UNIVERSITY Center for BioMolecular Modeling

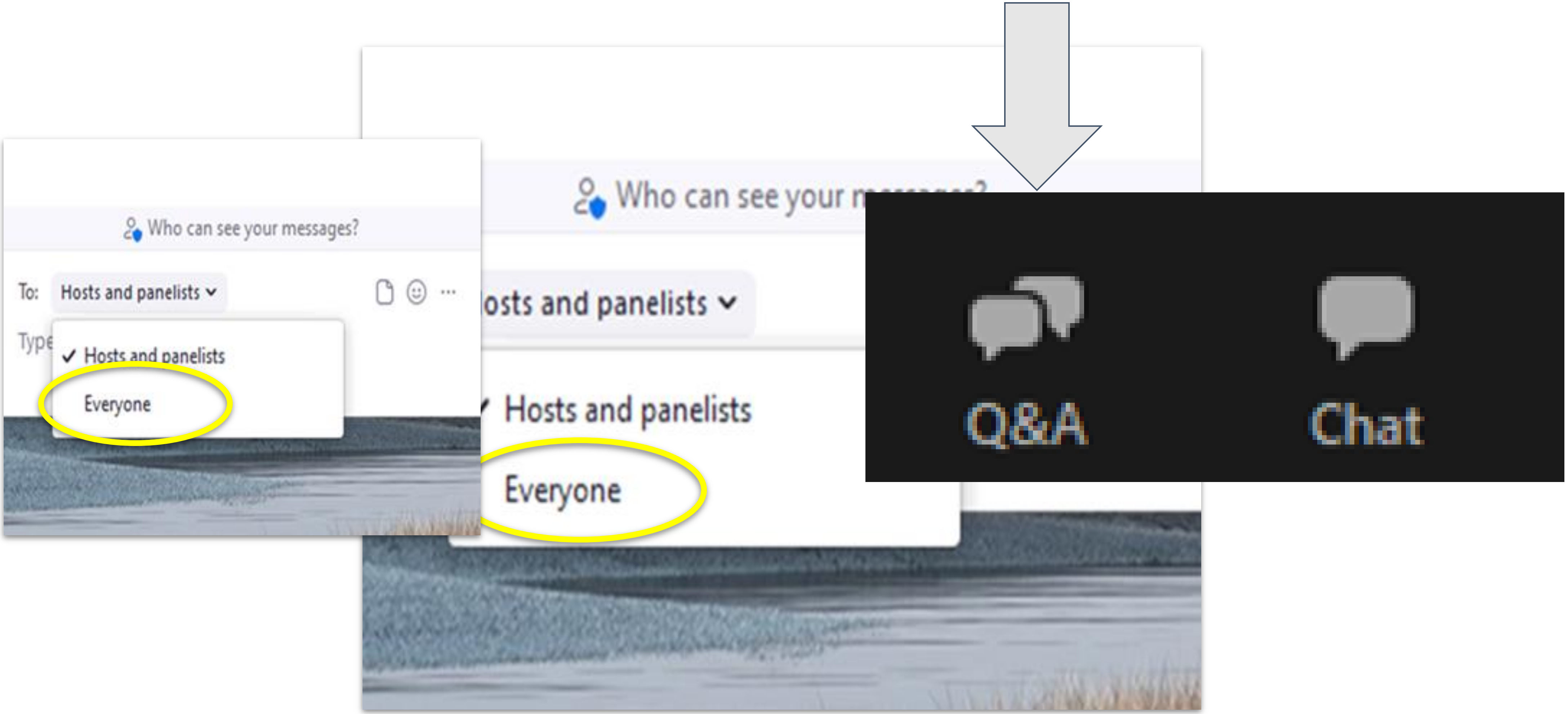
MODELING MARVELS

2022 EDUCATORS WEBINARS

- **MATTHEW KERN, M.Sc.**
  From Particles to Properties: Bridging Scales with Water Kit® Models
- **TIM HERMAN, PhD**
  Exploding Frog Eggs & Discovery of Aquaporin

WATER CHEMISTRY WEBINAR

TUESDAY | FEB 22 6:30 - 8 PM CST


Who can see your messages?
To: Hosts and panelists
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Hosts and panelists
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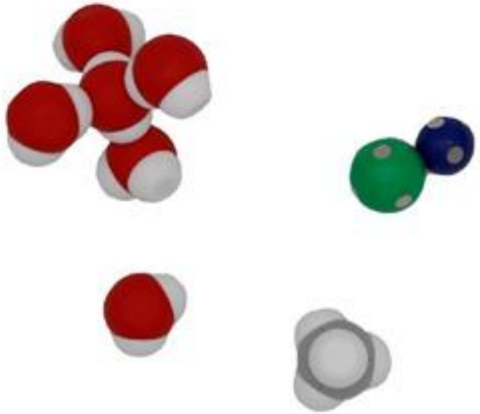
Hosts and panelists
Everyone
Q&A
Chat

Water Student Modeling Pack



Water Kit©

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WATER CHEMISTRY WEBINAR

TUESDAY | FEB 22 6:30 - 8 PM CST

PRESENTER:

MATTHEW KERN, M.Sc.

**Walworth Barbour American International School,
Even Yehuda, Israel**

From Particles to Properties: Bridging Scales with Water Kit® Models

MODELING MARVELS
2022 EDUCATORS WEBINARS

Workshop Learning Goals

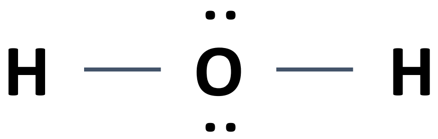
- ☑ Describe strategies for using Water Student Modeling Pack/Water Kit® models to explain structure-property relationships.
- ☑ Explain how Water Student Modeling Pack/Water Kit® models can be used to describe the atomic composition of simple molecules and extended structures (NGSS MS-PS-1).
- ☑ Use Water Student Modeling Pack/Water Kit® models to compare the structure of water at the bulk scale to infer the strength of electrical forces between particles (NGSS HS-PS1-3).
- ☑ Identify where to find additional resources for aligning Water Student Modeling Pack/Water Kit® models with your curriculum and integrating the models into instruction.

Water Kit® Assembly Instructions

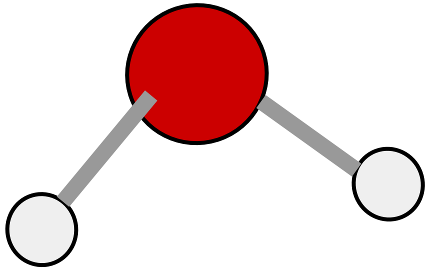
Atomic Composition and Models of Water Molecules

H_2O

Molecular formula



Lewis structure



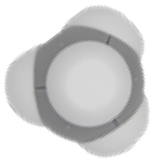
Ball-and-stick model

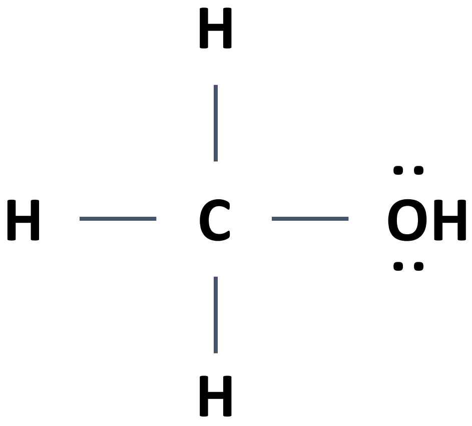
Space-fill model

Modeling Other Simple Molecules

?

Methane
(CH_4)

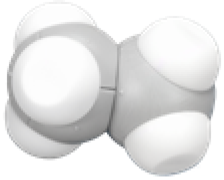




Methanol
(?)

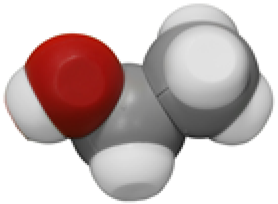
?

Ethane
(C_2H_6)

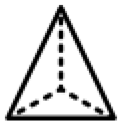


?

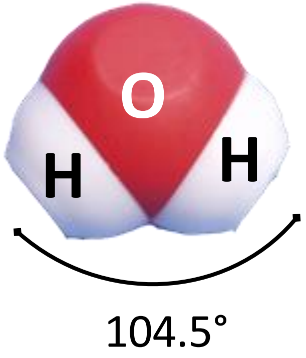
Ethanol
(C_2H_5OH)

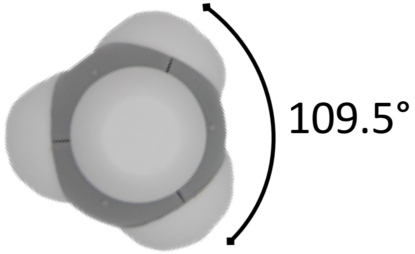


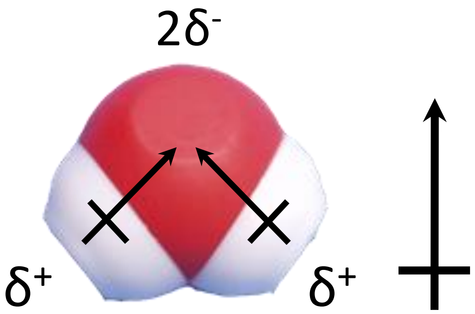
Closer Look at Molecular Structure

- **Tetrahedral** *electron* geometry 
- **Bent** *molecular* geometry
- Why is angle between hydrogen atoms 104.5° in water instead of 109.5°, like in methane?
- Electronegativities: H = 2.20; O = 3.44

  ΔEN 0.4 - 1.8 → Polar covalent bond
- Bond and molecule dipole moments







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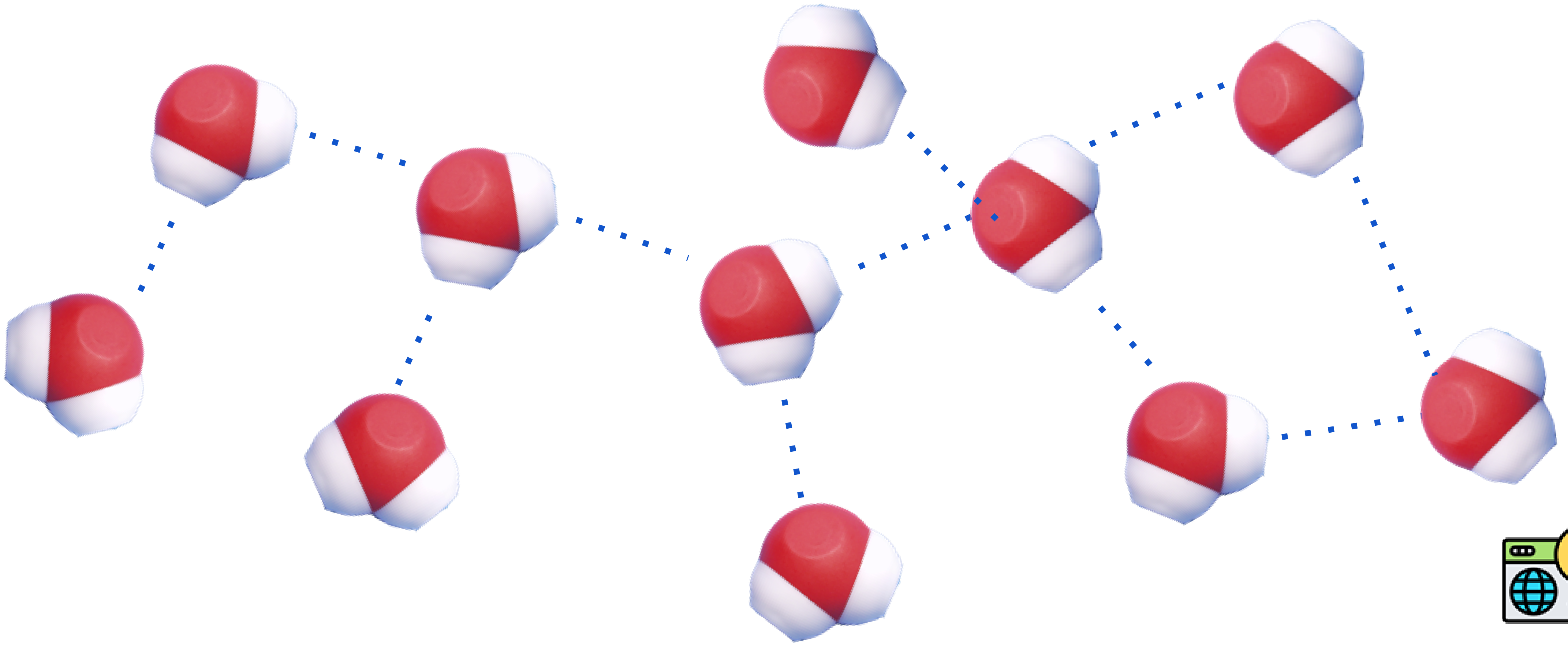
Why is water a **liquid** at room temperature?

Molecule	Molecular Formula	Number of atoms	Molar Mass ($g \cdot mol^{-1}$)	State at 20℃
Ethane	C_2H_6	8	30.07	gas
Ethanol	C_2H_5OH	9	46.07	liquid
Methane	CH_4	5	16.04	gas
Methanol	CH_3OH	6	32.04	liquid
Water	H_2O	3	18.02	liquid

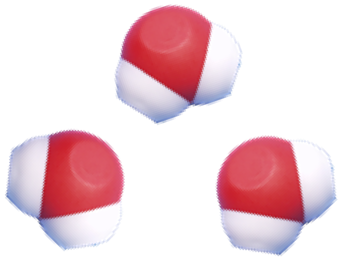
Intermolecular attractions (hydrogen bonds) consequence of polarity



[Water Kit® Basic lessons]

Examine the data in the table. How would you explain the *differences* in the surface tensions of the liquids?

Interface	Surface Tension (mN·m^{-1}) at 20°C
Acetone—Air	25.20
Benzene—Air	28.88
Toluene—Air	28.40
Methanol—Air	22.70
Ethanol—Air	22.10
Octane—Air	21.62
Water—Air	72.80



If heat is continually applied, why doesn't the temperature of a water sample increase linearly (e.g. ↗)? Explain using models.

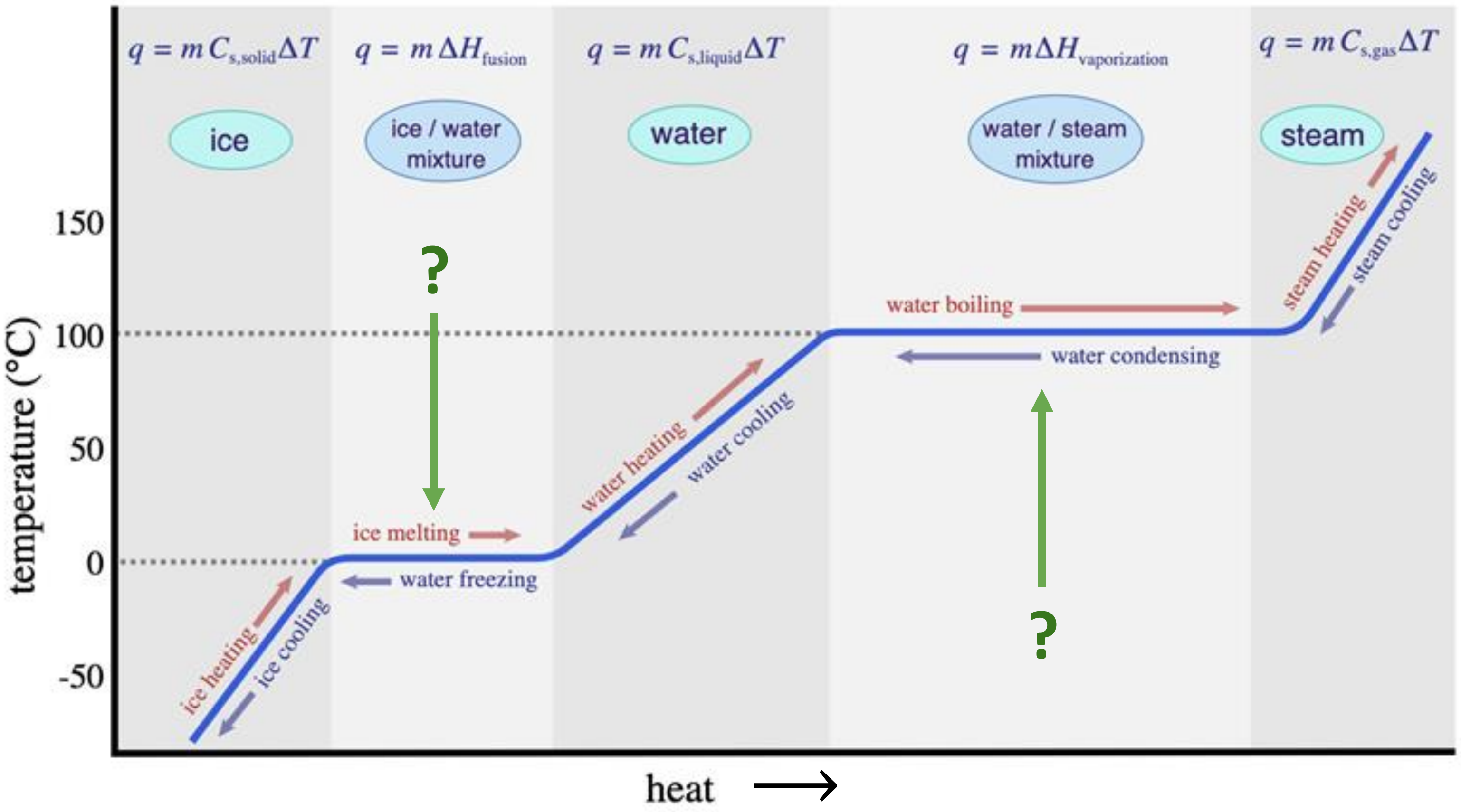


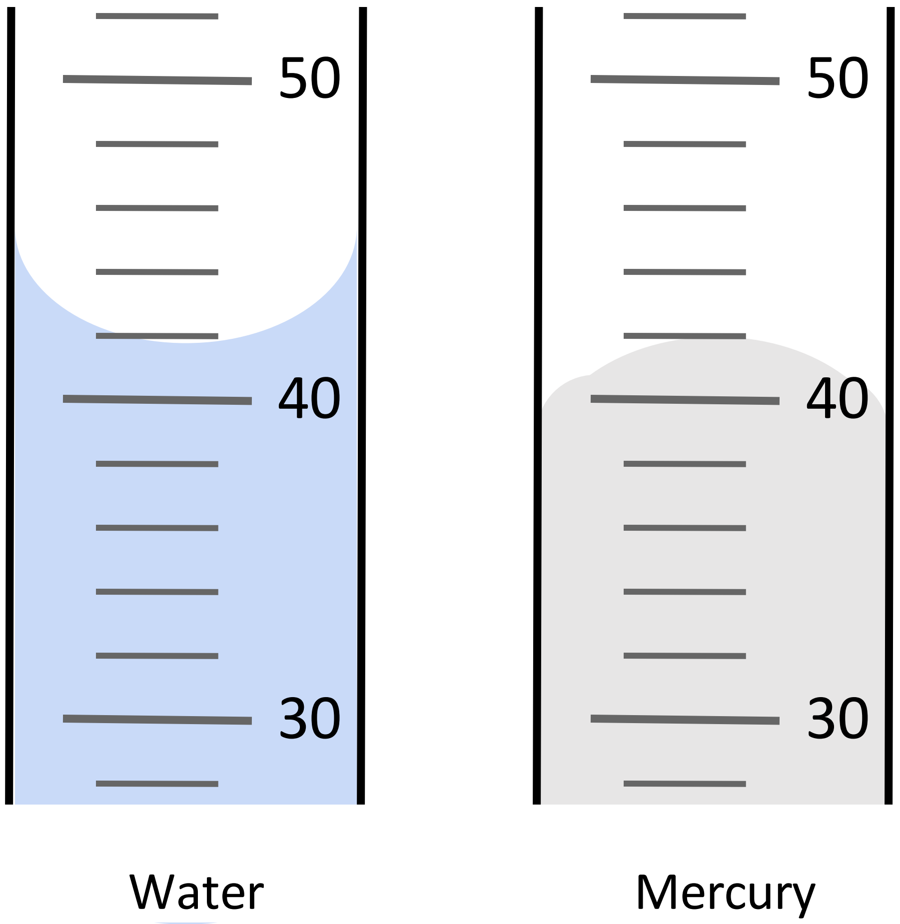
Image source: chembook, by Paul McCord

Additional properties that could be explored

Compound, Formula	Specific Heat Capacity ($J\ g^{-1}\ K^{-1}$)	Heat of Vaporization ($J \cdot mol^{-1}$)	Vapor Pressure (kPa) at 20℃
Acetone, C_3H_6O	2.15	29,100	24.66
Ethanol, C_2H_6O	2.44	38,560	5.95
Octane (gasoline), C_8H_{18}	2.22	34,410	1.33
Methanol, CH_3OH	2.14	35,210	11.90
Water, H_2O	4.18	40,660	2.33

Why does water form a meniscus?

- Meniscus = curved surface at liquid—air interface
- Support your claim with evidence from the models
- Why does water have *concave* (◡) meniscus while mercury has *convex* (◠) meniscus?



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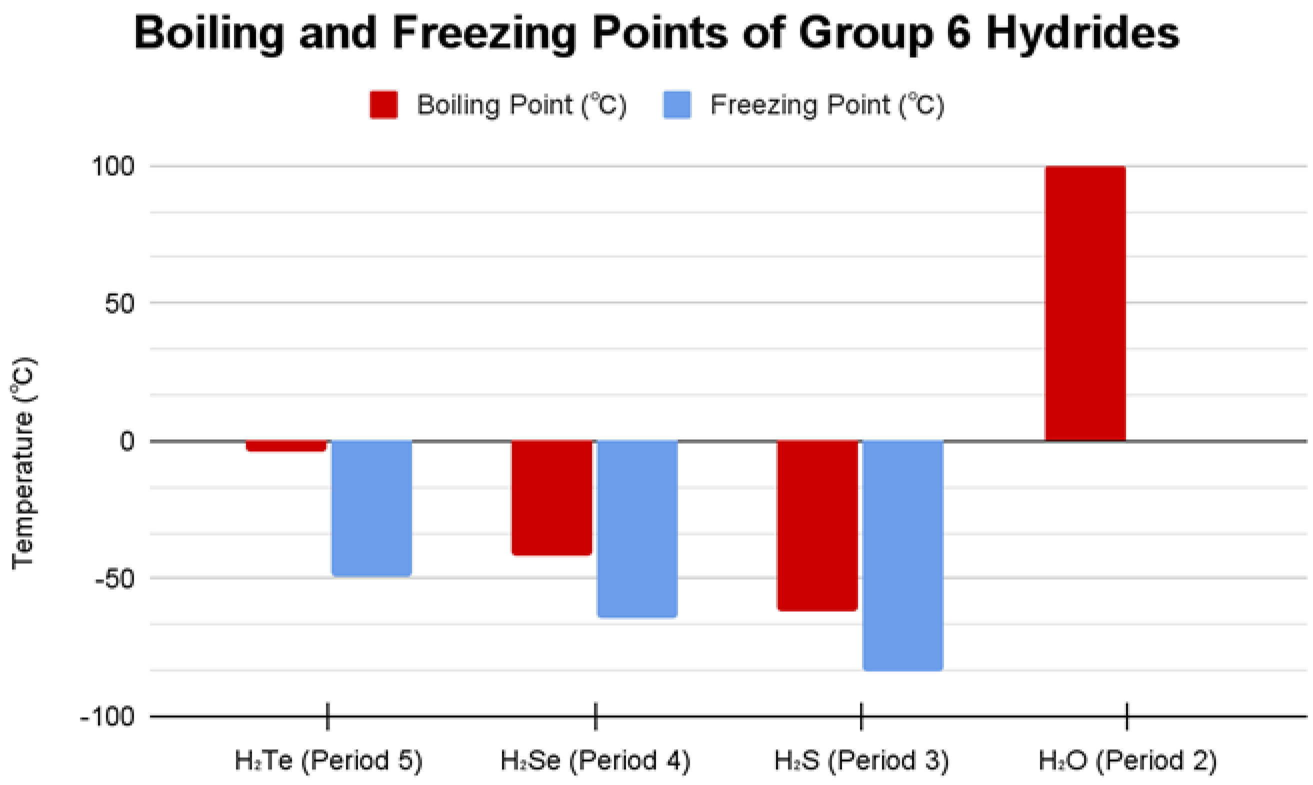
Examine the model below. What do you notice about the relative boiling and freezing points of water?



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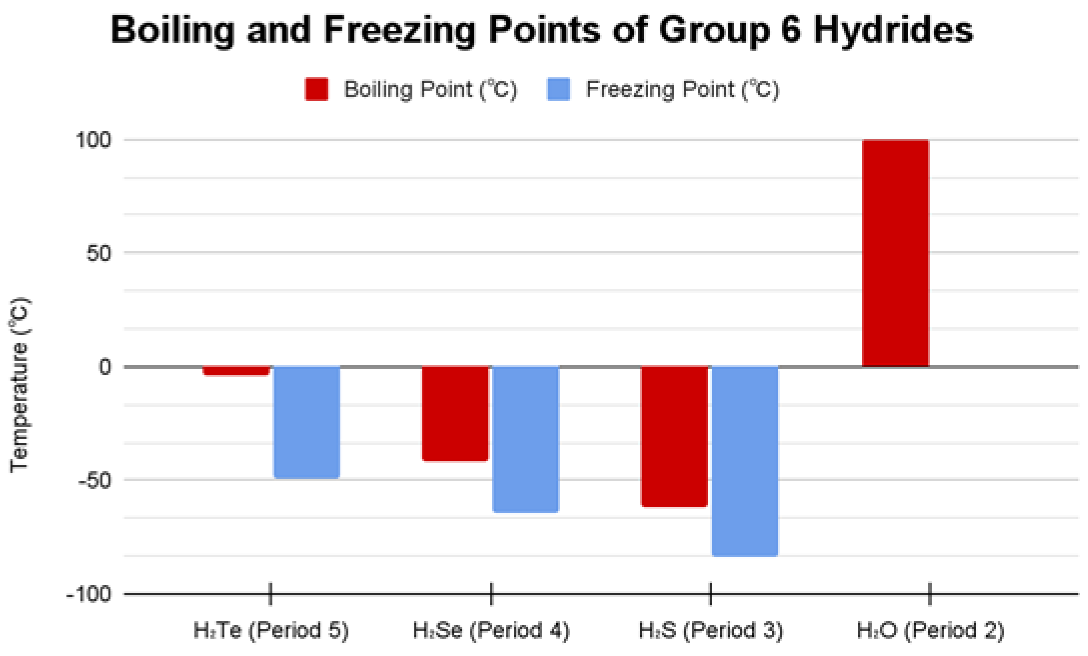


$\Delta EN = 0.1$ $\Delta EN = 0.35$ $\Delta EN = 0.38$ $\Delta EN = 1.24$

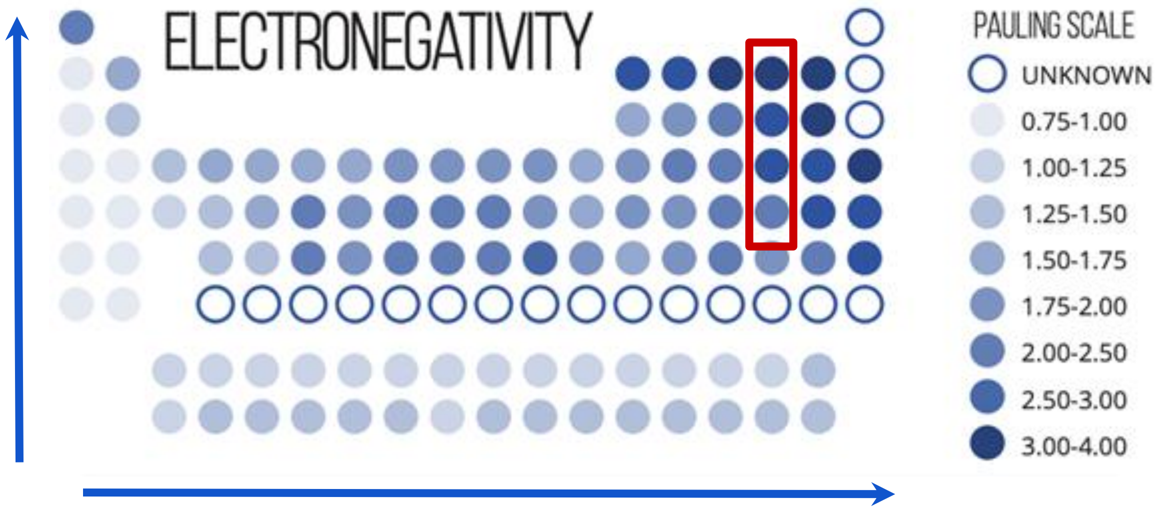
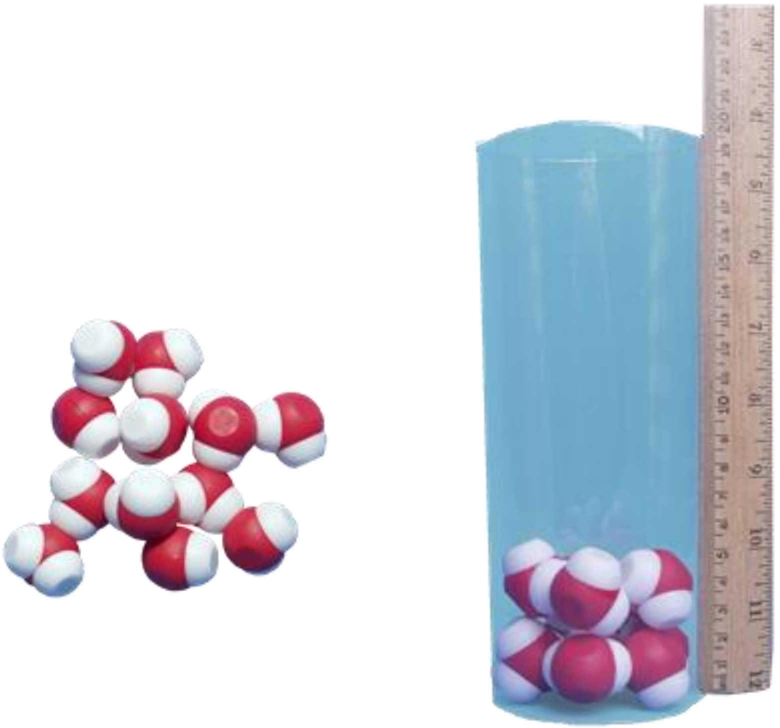


Image source: Compound Interest

Why can water, in its solid state, float on itself in the liquid state?

ρ = mass/volume



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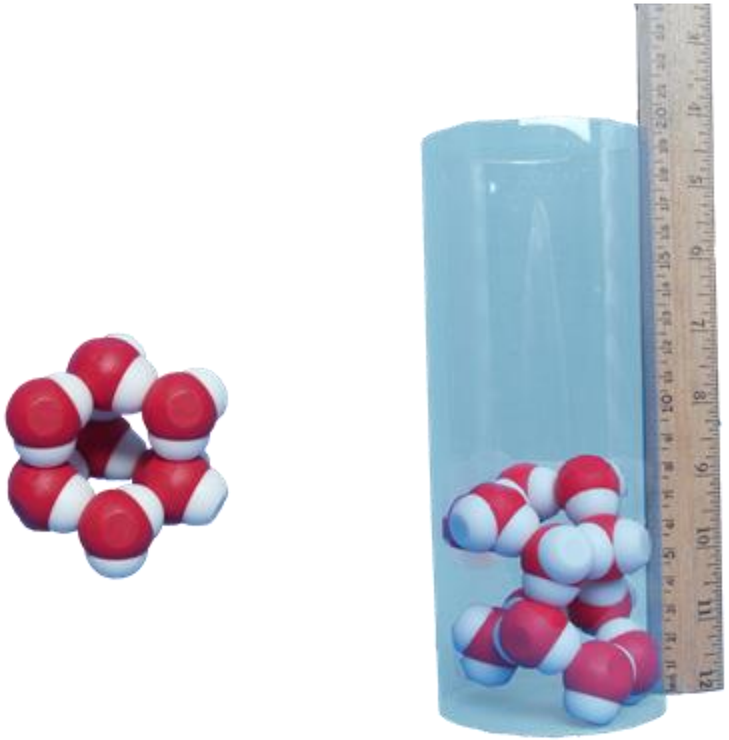
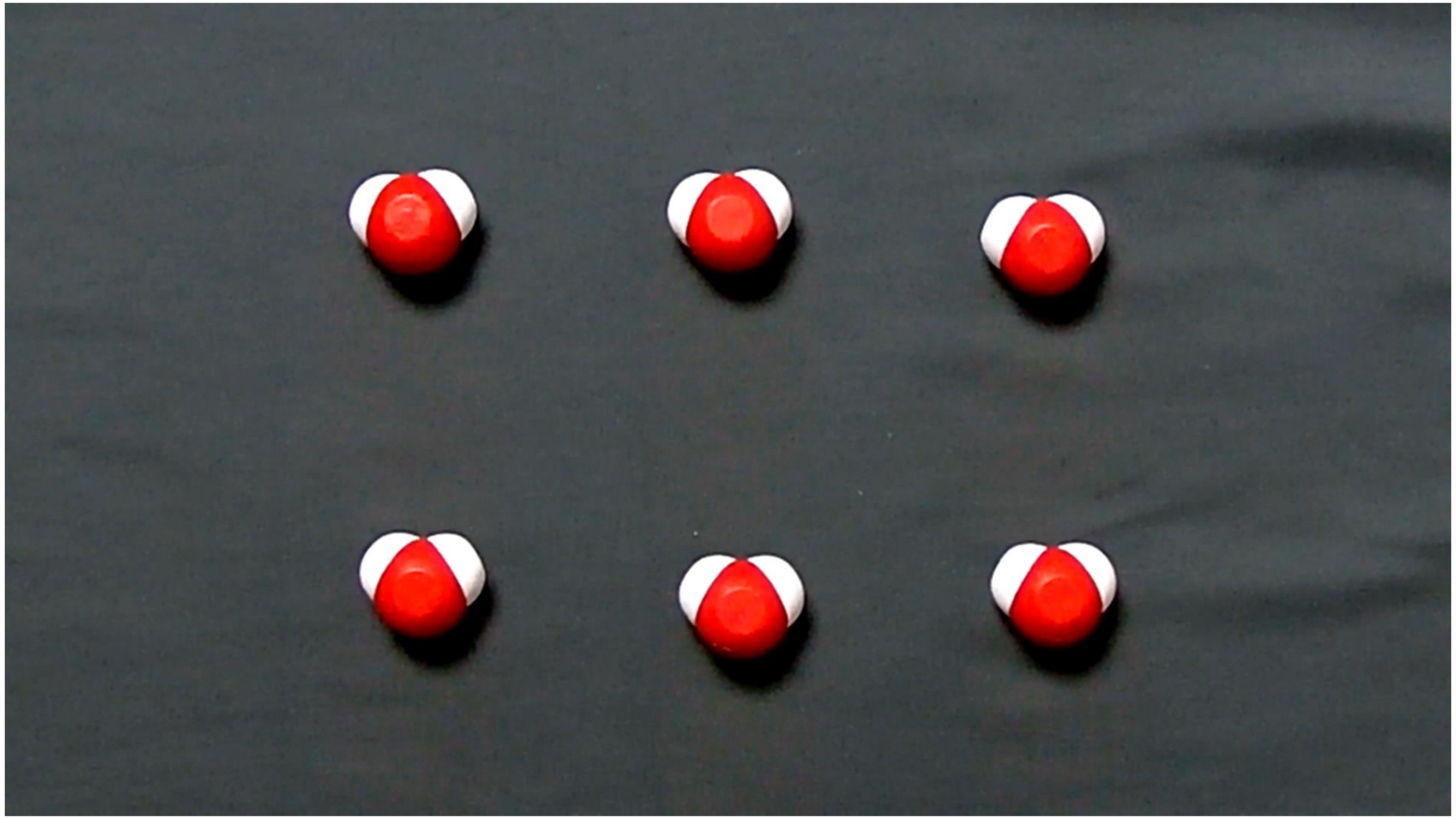
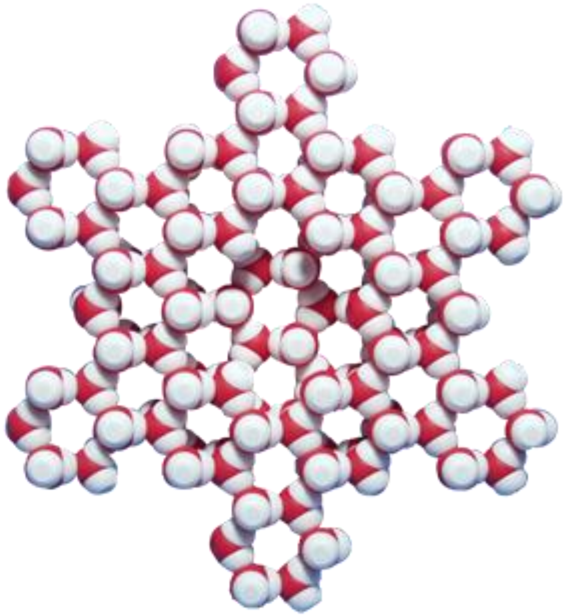


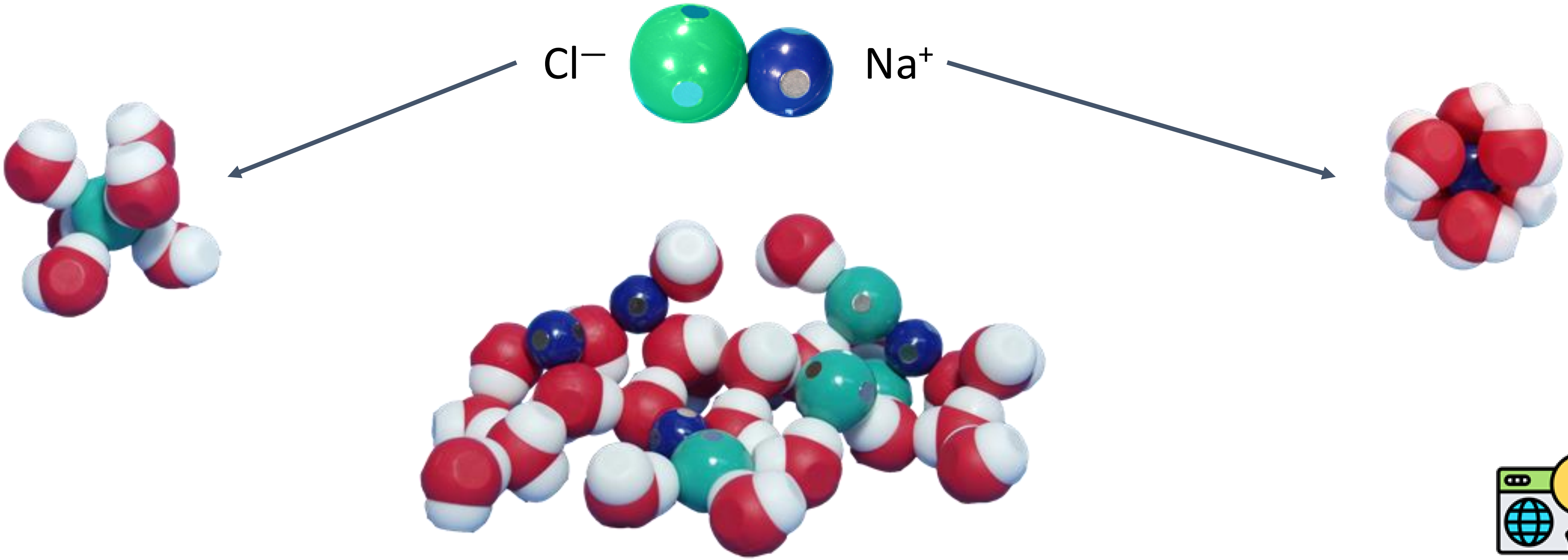
How do you build a hexagonal ice crystal?





Water Kit® Patterns in Crystal Structures

Why is water such a common solvent?



Water Kit® Basic lessons

Why is chloride ion represented LARGER than the sodium ion?

$Cl^- > Na^+$

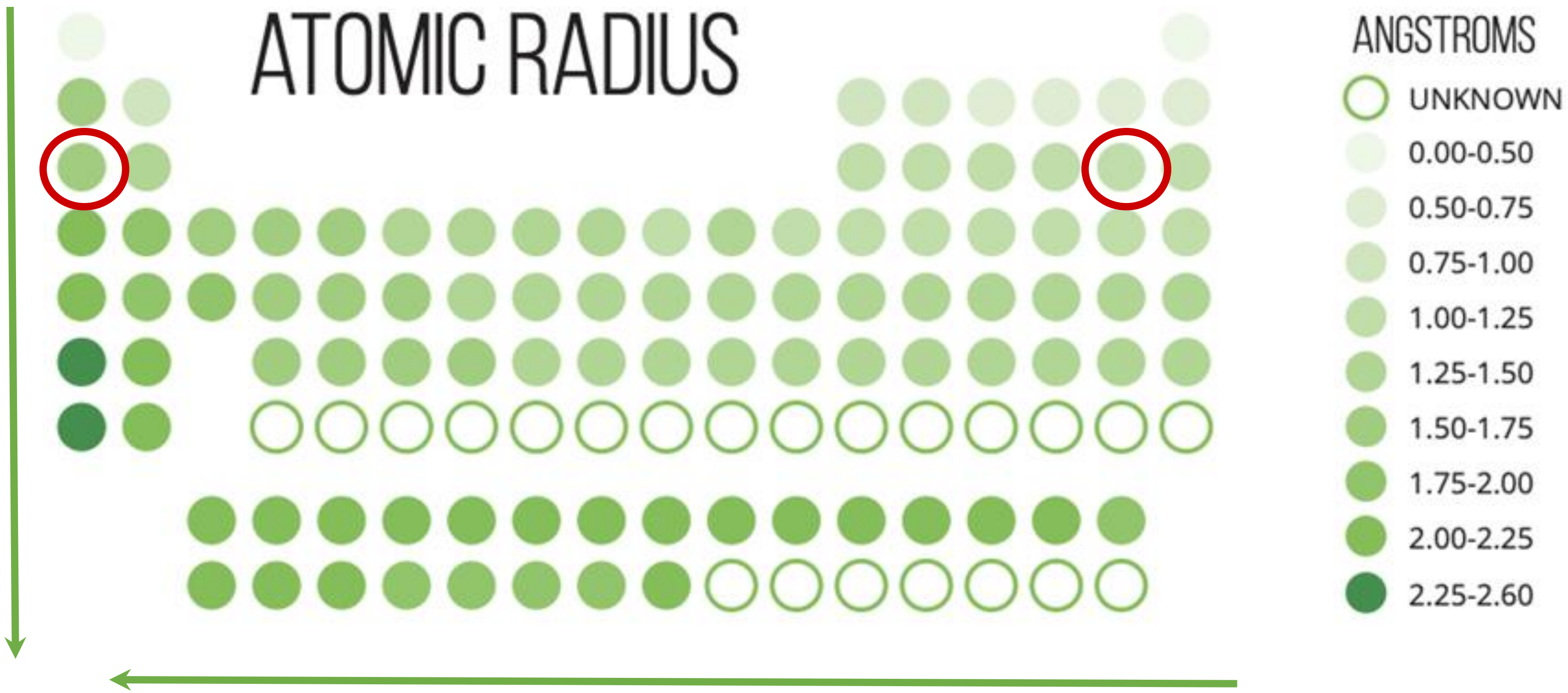


Image source: Compound Interest

Why can water act as both an **acid** AND a **base**?

Brønsted-Lowry acid: Any species that can *donate* a proton (H^+)

Brønsted-Lowry base: Any species that can *accept* a proton (H^+)

$2H_2O\ (l) \rightleftharpoons H_3O^+\ (aq) + OH^-(aq)$

How could you model the *autoionization* of water?

pH = $-\log[H_3O^+]$; In neutral solution, $[H_3O^+] = [OH^-]$

How could you model an acidic solution? Basic solution?

Water Kit® pH lesson

Strengths of Models	Limitations of Models
?	?

Strengths of Models

- Models are color-coded to differentiate between atoms
- Models illustrate relative sizes of particles
- Geometry of models reflects geometry of real molecules
- Attraction between magnets provides kinesthetic sense of bonding/electrostatic (Coulombic) interactions
- Interactions between particles can be modeled

Limitations of Models

- Models do not represent subatomic particles
- Atoms have no color in reality
- Water molecules are not “hard” structures
- Electron clouds are not static
- Electron cloud probability not represented
- Oscillation of covalent bonds not evident
- Models do not show that hydrogen atoms bond to form H_2

- Kit content and assembly instructions
- Lessons
- Animations
- Videos
- Connections to NGSS
- Additional online resources

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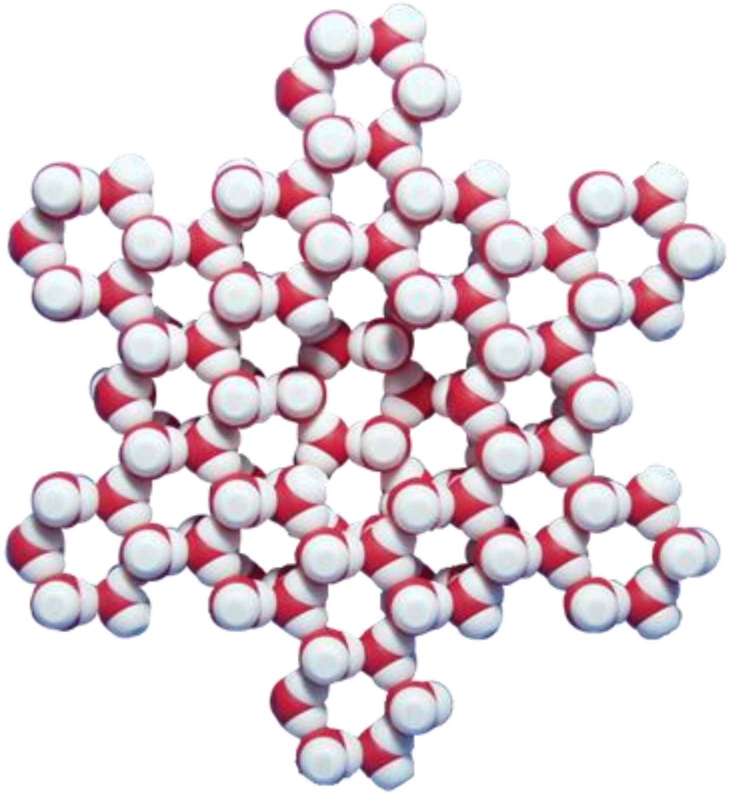
Questions? Ideas? Suggestions? Comments?



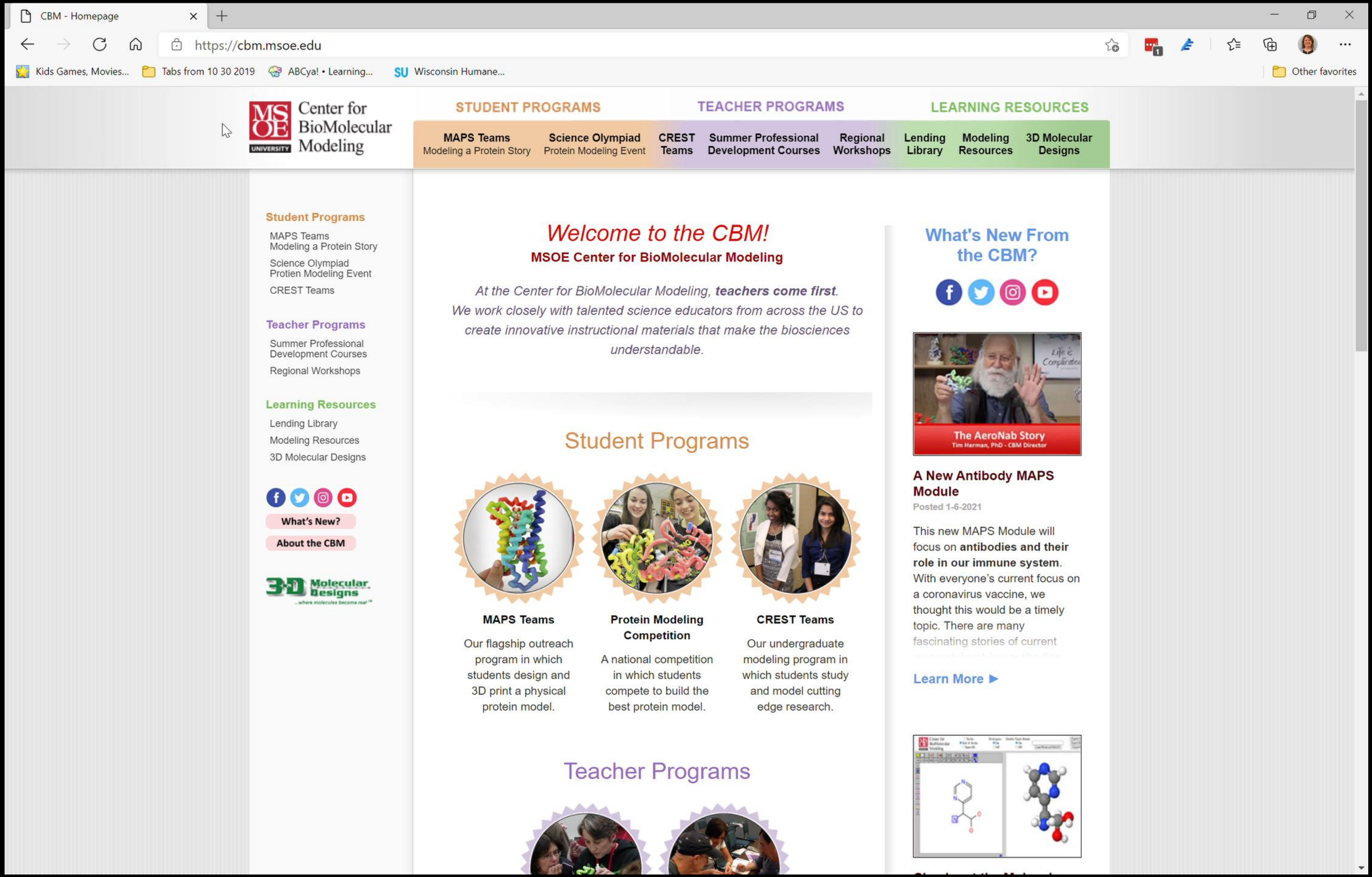
Workshop NGSS Connections

SEPs	CCCs	DCIs
Developing and Using Models Develop a model to predict and/or describe phenomena.	**Scale, Proportion, and Quantity** Time, space, and energy phenomena can be observed at various scales using models to study systems that are too large or too small.	**PS1.A: Structure and Properties of Matter** Substances are made from different types of atoms, which combine with one another in various ways. Atoms form molecules that range in size from two to thousands of atoms. Solids may be formed from molecules, or they may be extended structures with repeating subunits (e.g., crystals).

Workshop NGSS Connections

SEPs	CCCs	DCIs
Constructing Explanations and Designing Solutions Construct and revise an explanation based on valid and reliable evidence obtained from a variety of sources (including students' own investigations, models, theories, simulations, peer review) and the assumption that theories and laws that describe the natural world operate today as they did in the past and will continue to do so in the future.	**Patterns** Different patterns may be observed at each of the scales at which a system is studied and can provide evidence for causality in explanations of phenomena.	**PS1.A: Structure and Properties of Matter** The periodic table orders elements horizontally by the number of protons in the atom's nucleus and places those with similar chemical properties in columns. The repeating patterns of this table reflect patterns of outer electron states. **PS1.B: Chemical Reactions** The fact that atoms are conserved, together with knowledge of the chemical properties of the elements involved, can be used to describe and predict chemical reactions.

Have you heard of the Model Lending Library?



- Borrow kits and models for 2 weeks.
- There is no charge for borrowing models
- All you pay is return shipping ($20-$40)
- Models are available to:
  - Elementary School
  - Middle School
  - High School
  - College Educator
  - and more!

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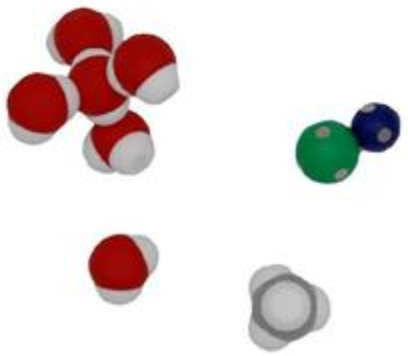
THANK YOU FOR ATTENDING!

Kits and models used in this session:



Purchase kits at www.3dmoleculardesigns.com

Use discount code WEBINAR20 to receive 20% off most items in our catalog.

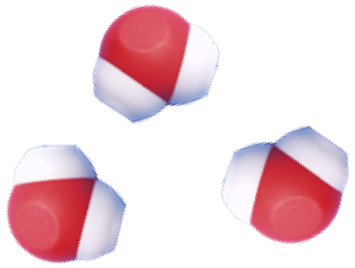
Student Modeling Packs are not eligible for discount.

Examine the data in the table below. What do you notice about water's boiling and freezing points?

Compound, Formula	Boiling Point (℃)	Freezing Point (℃)
Hydrogen polonide, H_2Po	31.6	-35.3
Hydrogen telluride, H_2Te	-4	-49
Hydrogen selenide, H_2Se	-42	-64
Hydrogen sulfide, H_2S	-62	-84
Water, H_2O	100	0

Why can liquid water absorb so much heat energy before increasing in temperature?

Compound, Formula	Specific Heat Capacity ($J\ g^{-1}\ K^{-1}$)
Acetone, C_3H_6O	2.15
Ethanol, C_2H_6O	2.44
Octane (gasoline), C_8H_{18}	2.22
Methanol, CH_3OH	2.14
Water, H_2O	4.18



Why is pure water a *poor* conductor of electricity?