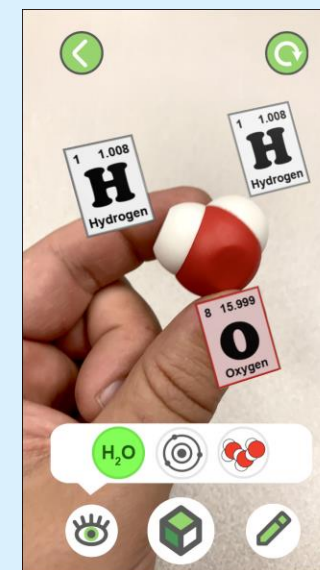




Mark Hoelzer, MFA
3D Molecular Designs

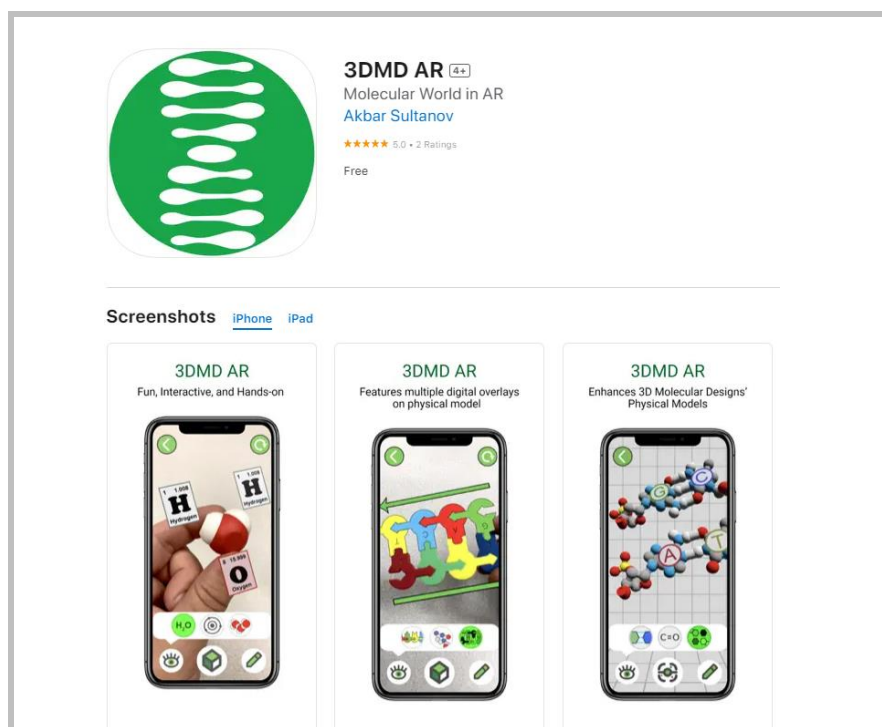
Enhancing Molecular Models with Augmented Reality (AR)



Before we dive in. . .

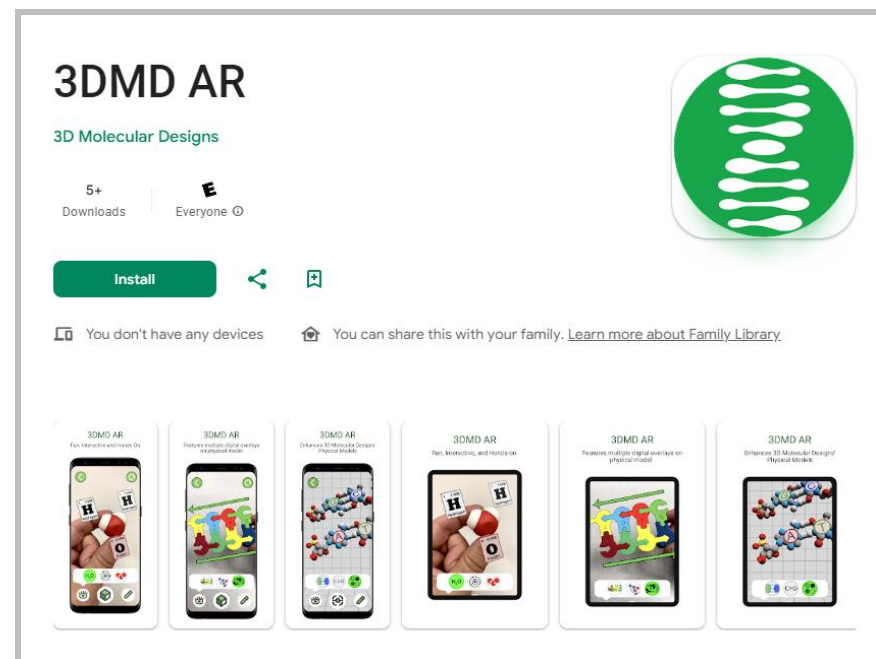
Apple App Store (iPhone/iPad)

<https://apps.apple.com/us/app/3dmd-ar/id6450119774>

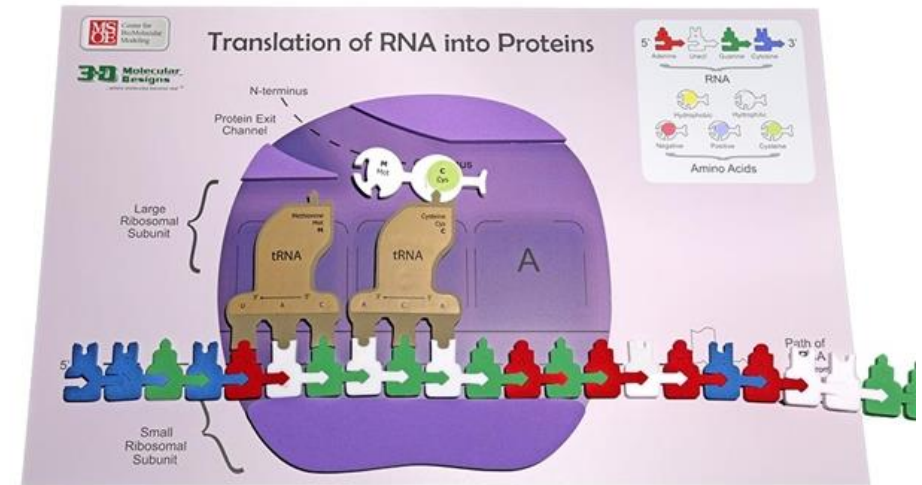


Google Play Store (Android)

<https://play.google.com/store/apps/details?id=com.ThreeDMolecularDesigns.ThreeDMDAR>



3D Molecular Designs makes **Physical Models** of molecules and proteins



Physical Models have inherent strengths and limitations



Strengths:

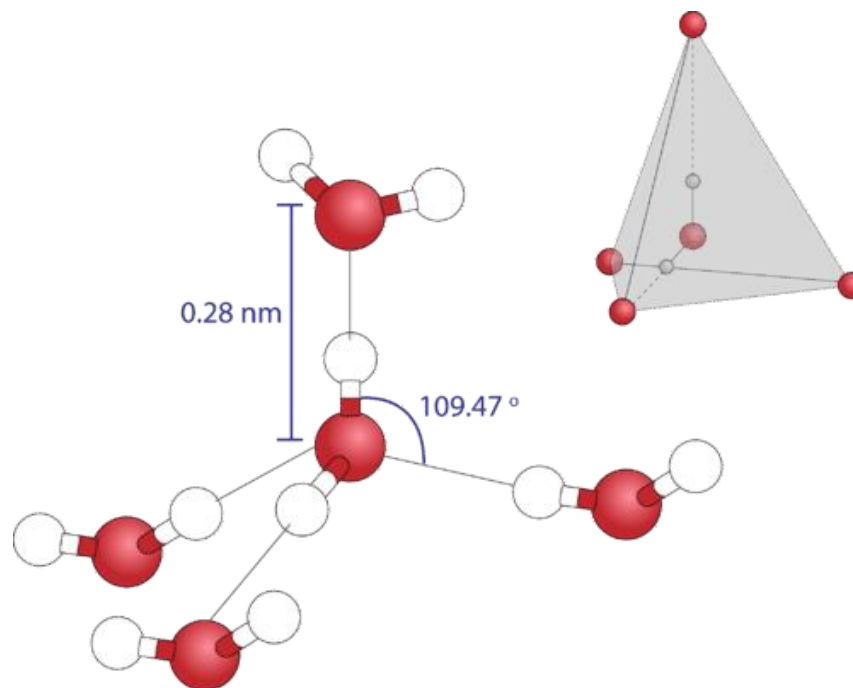
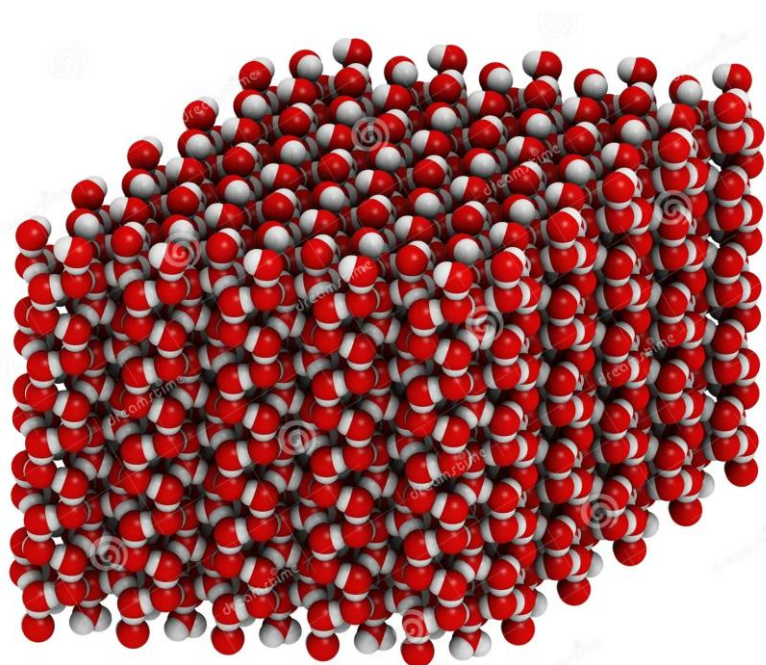
- focus attention
- tangible and tactile
- self exploration

Limitations:

- Static color schemes
- challenge to animate
- production limitations



Interactive Digital Media (IDM) has inherent strengths and limitations



Strengths:

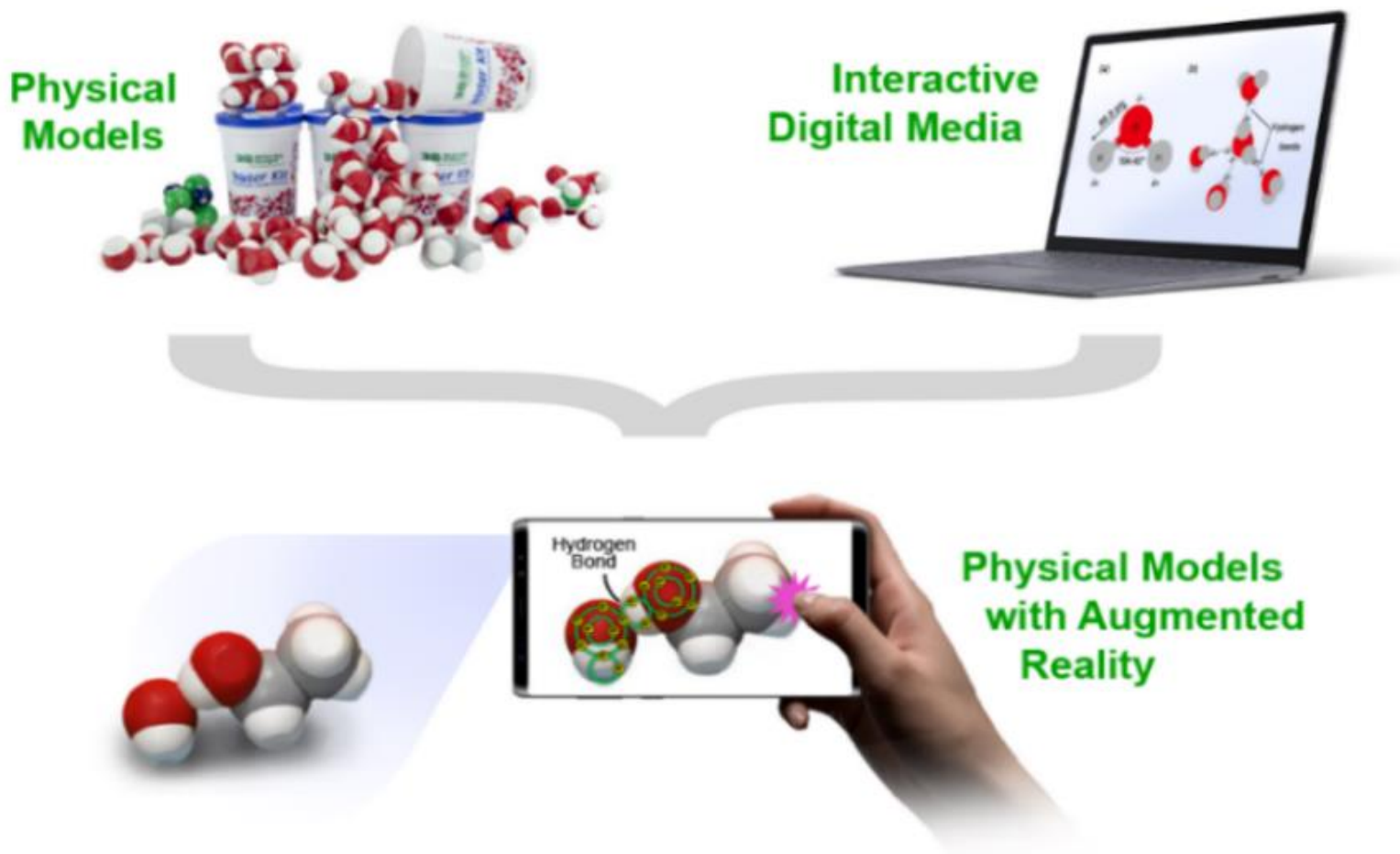
- easy to increase quantity or scale
- easy to animate or change
- easy to annotate

Limitations:

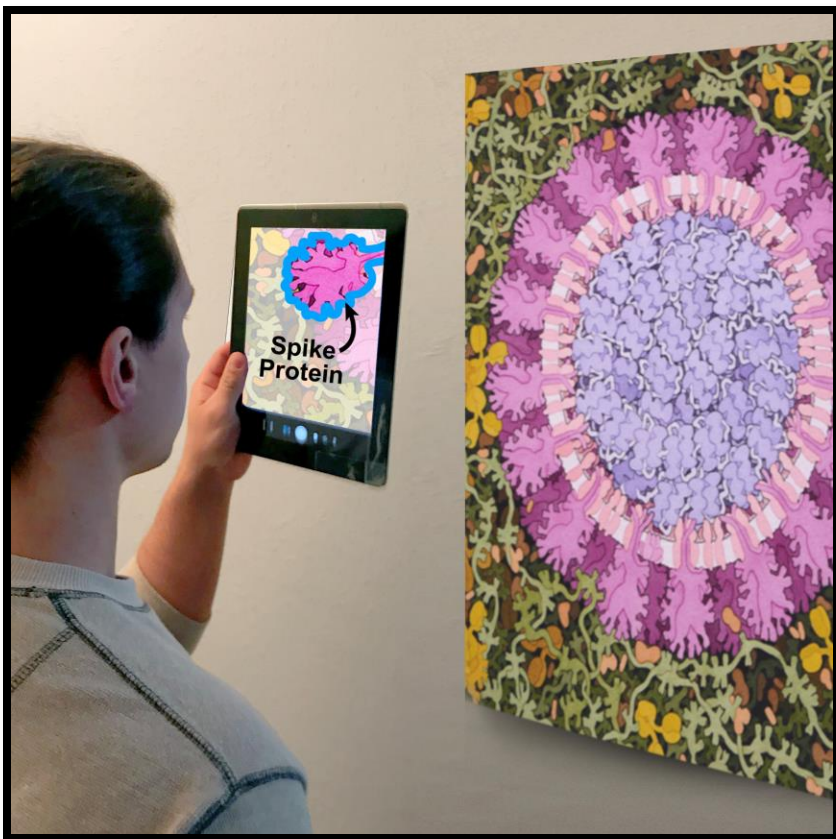
- Disconnected from the physical models
- not always tangible or easy to manipulate

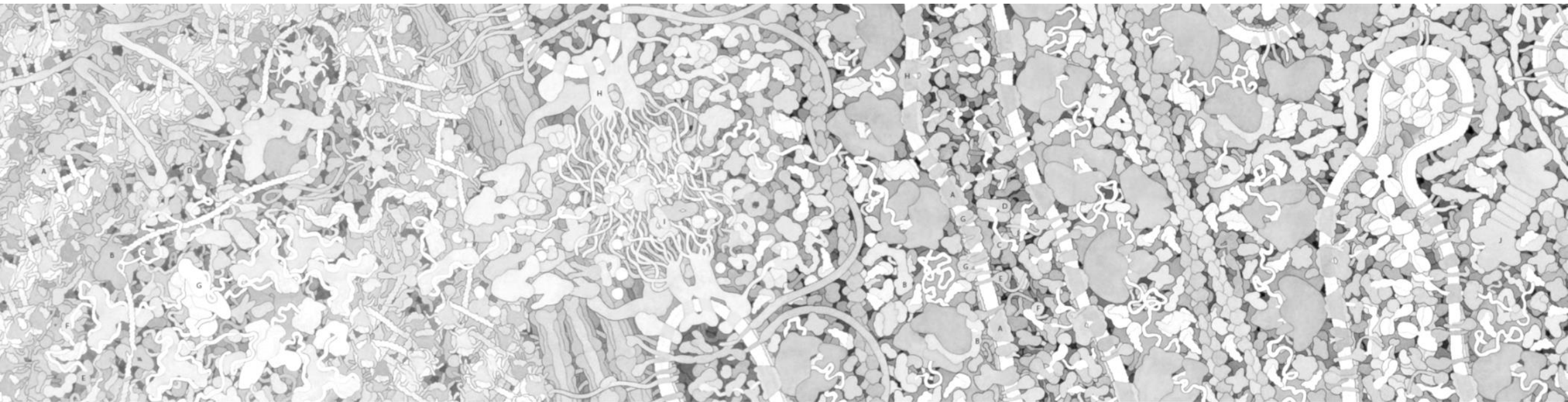


Augmented Reality (AR) can combine the best of both mediums



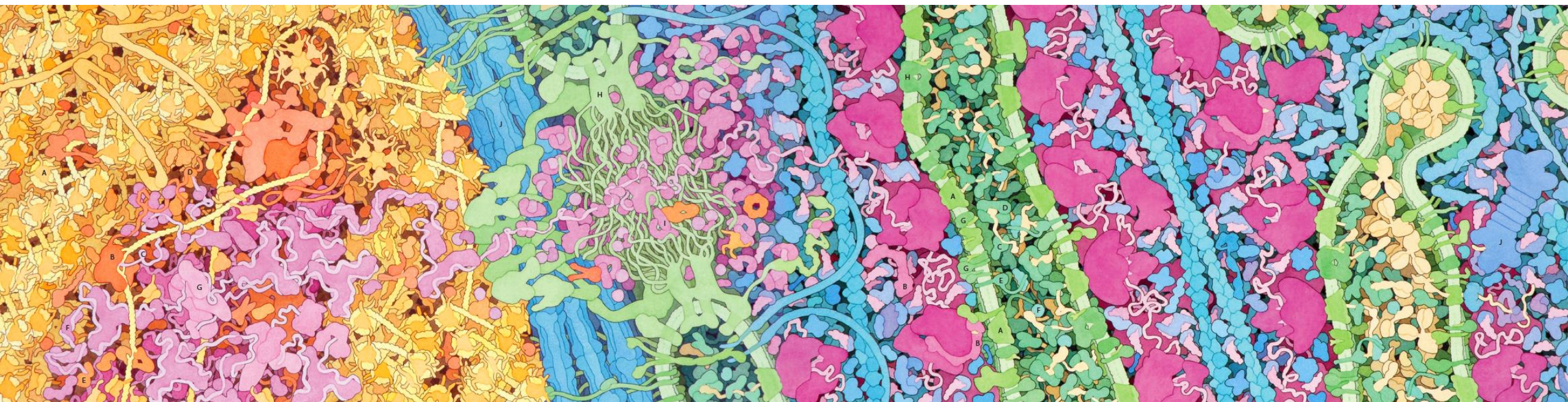
Web-based AR





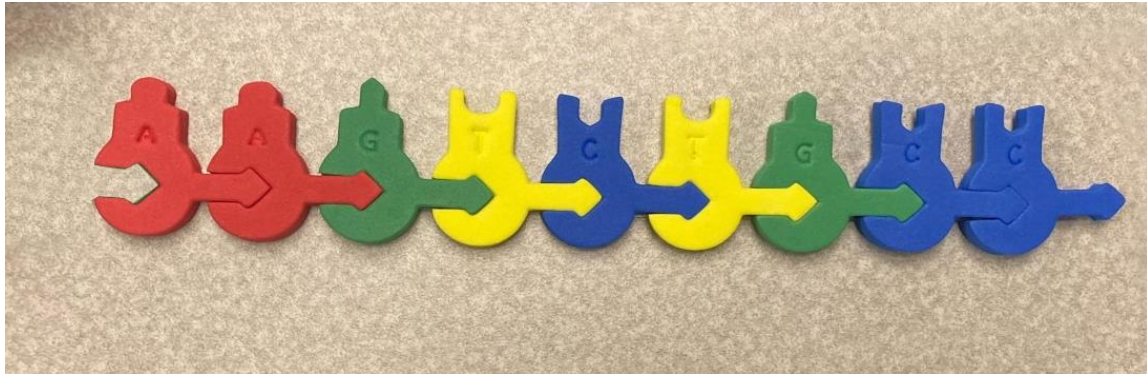
Try it out!

<https://www.centerforbiomolecularmodeling.org/markMyweb/tempNsta/>

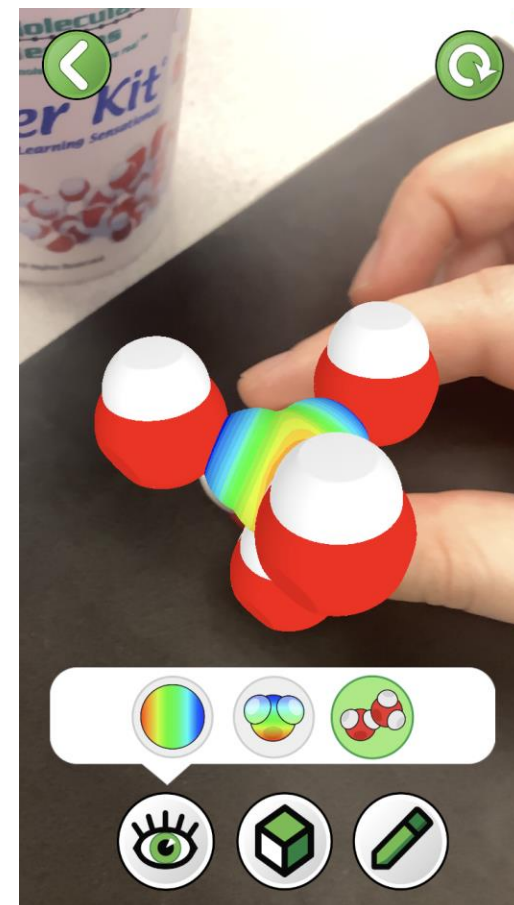
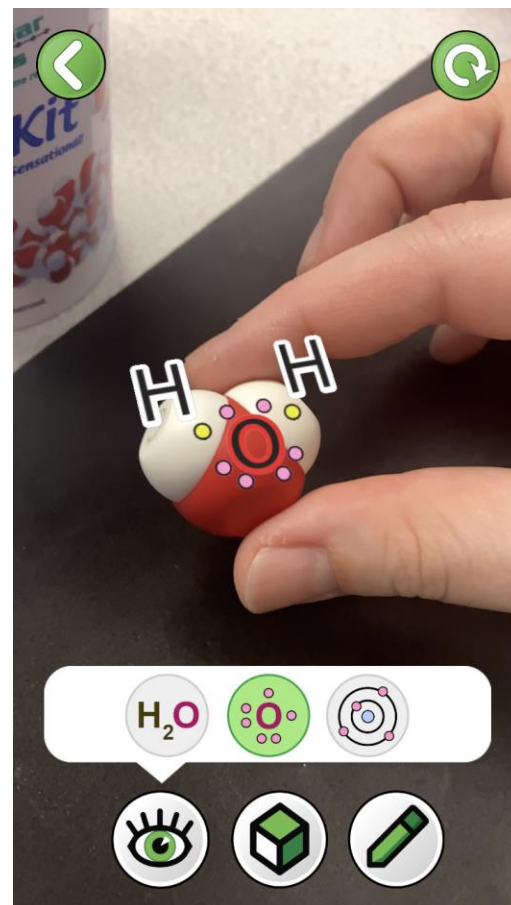


Try it out!

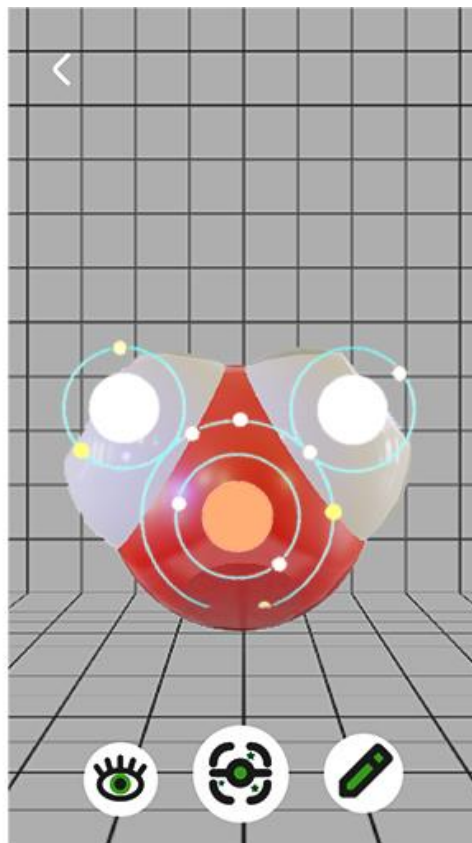
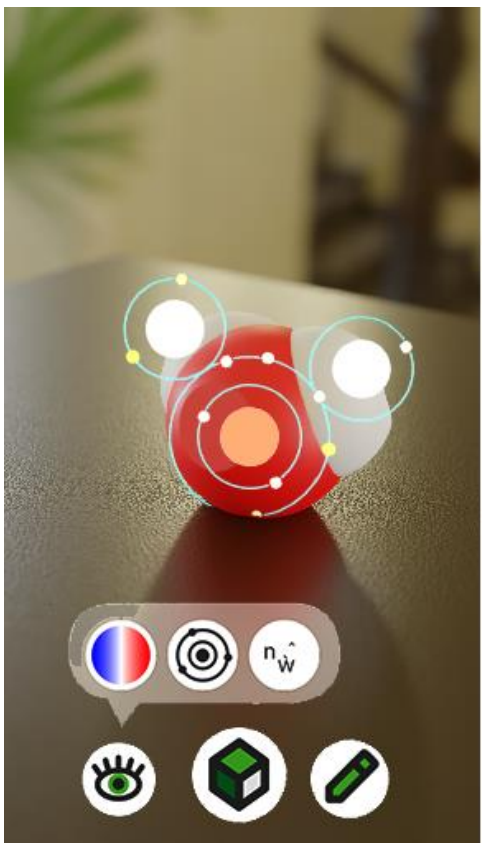
<https://www.centerforbiomolecularmodeling.org/markMyweb/tempNsta/>



App-based AR



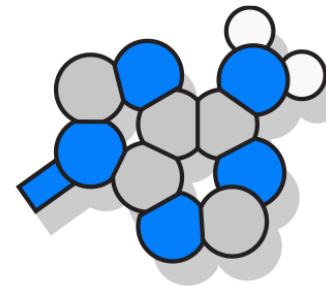
App-based AR



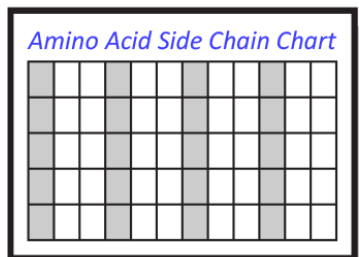
Demo "Training Activity"



Water Molecule



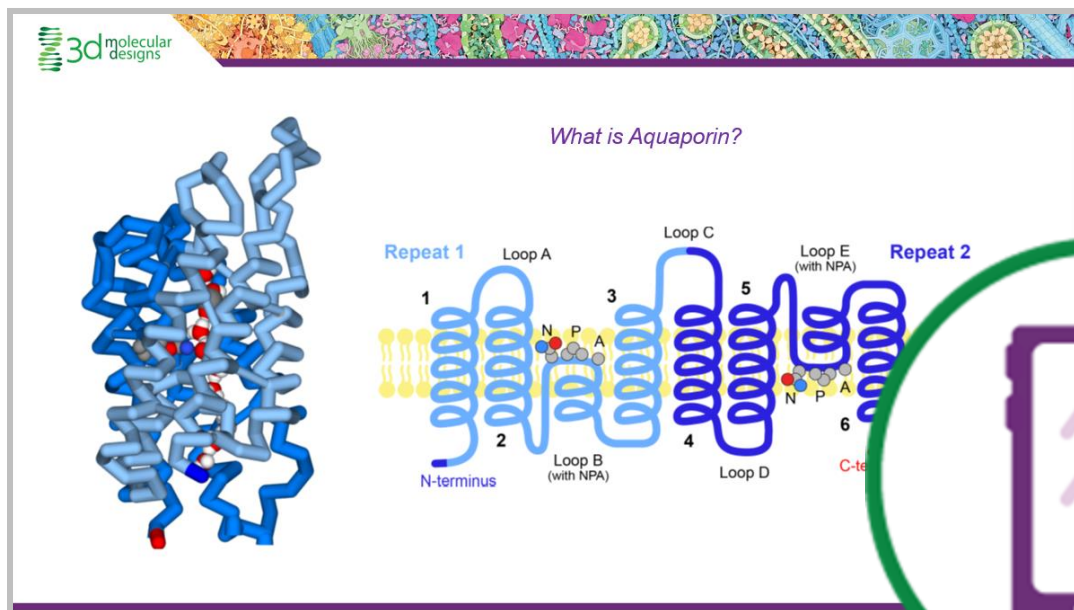
Adenine (A)



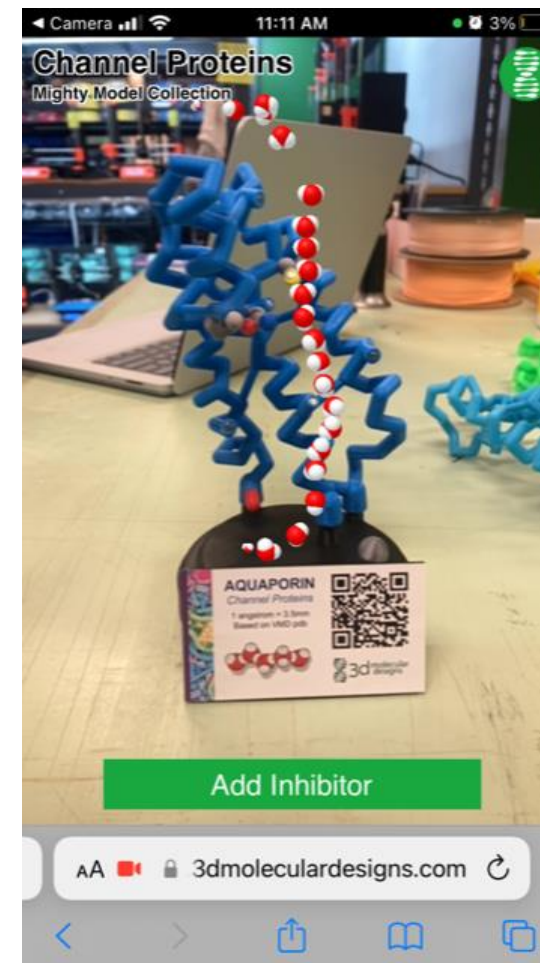
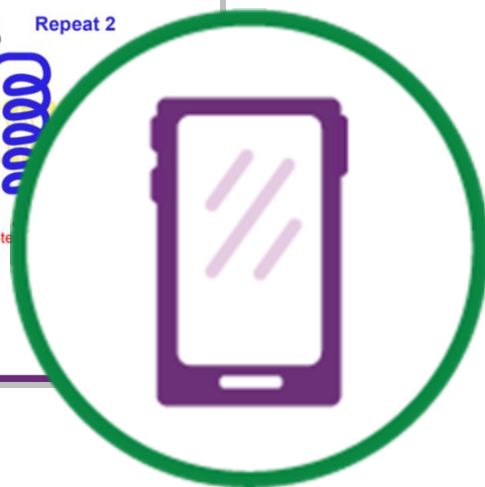
Amino Acid Sidechain Chart



Foam
Nucleotides
(AGTC)

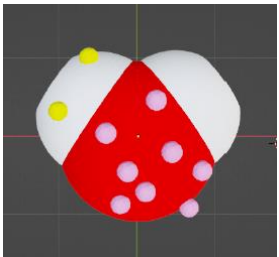


Slide Deck



Activity 2: States of Matter

- *States of Matter*
- *Impact of temperature*
- *Density*






Discovering Polarity

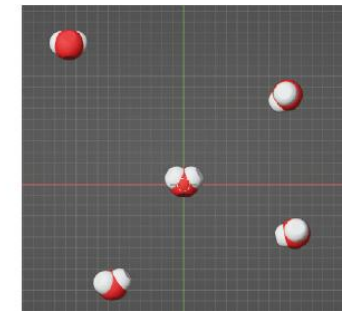
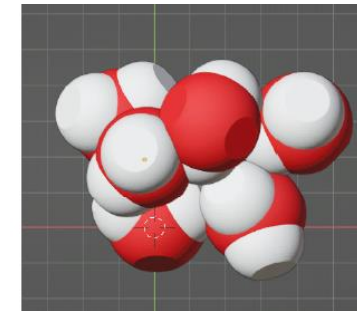
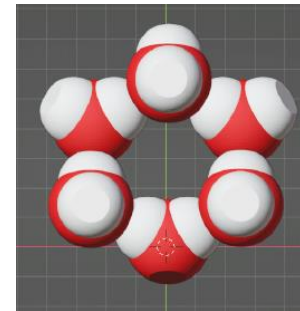
Water Kill A/R Activity

Lorem ipsum et voluolatum accusantium dolorumque leorantium, tellus non aperiam, eaque ipsa quae ab illo inventore veritatis et quasi architecto beatae vitae dicta sunt explicabo. Nemo enim ipsam voluptatem quia voluptasem ipsam quia dolor et amet, consectetur, adipisci velit,

	Hydrogen 1	Hydrogen 2	Oxygen
Expected Average Electron Distribution:	1.0	1.0	8.0

Test 1:	0	0	10
Test 2:	1	0	9
Test 3:	0	1	9
Test 4:	2	1	7
Test 5:	2	0	8
Test 6:	0	0	10
Test 7:	0	2	8
Test 8:	0	0	10
Test 9:	1	1	8
Test 10:	1	2	7

	Hydrogen 1	Hydrogen 2	Oxygen
Actual Average Electron Distribution:	0.7	0.7	8.6

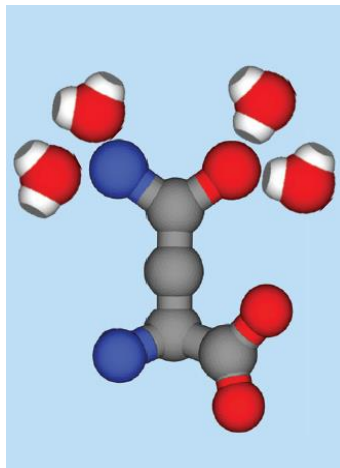
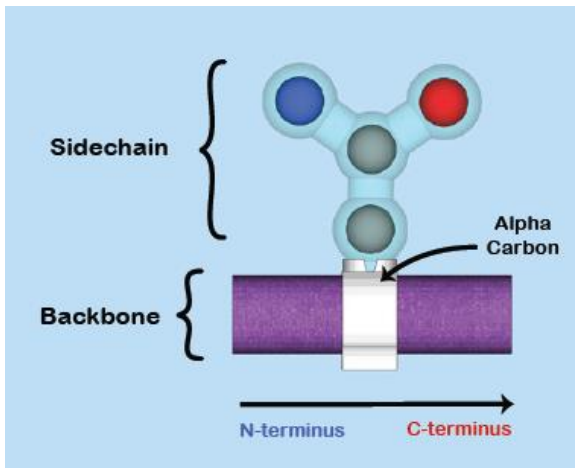


100° C



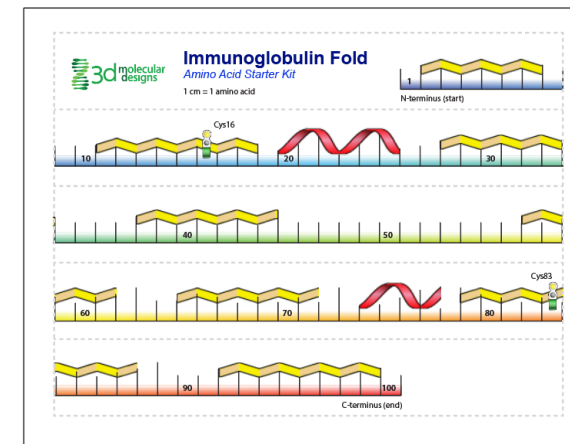
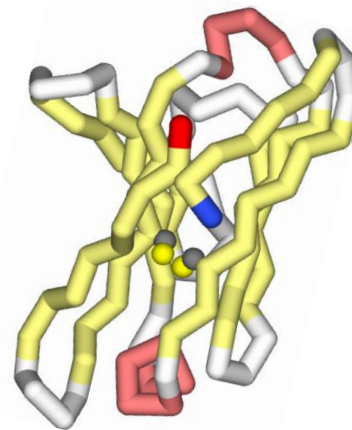
Activity 3: Sorting Sidechains

- Amino Acid Structure
- Amino Acid Chemical Properties
- Principles that Drive Protein Folding



Activity 4: Folding Real Proteins

- Protein Structure/Function
- Principles that Drive Protein Folding
- Secondary Structures

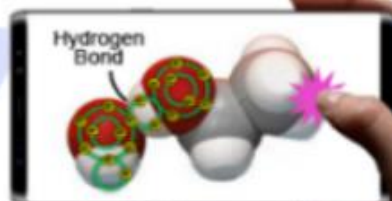


Do not replace the models. . . enhance them!

**Physical
Models**



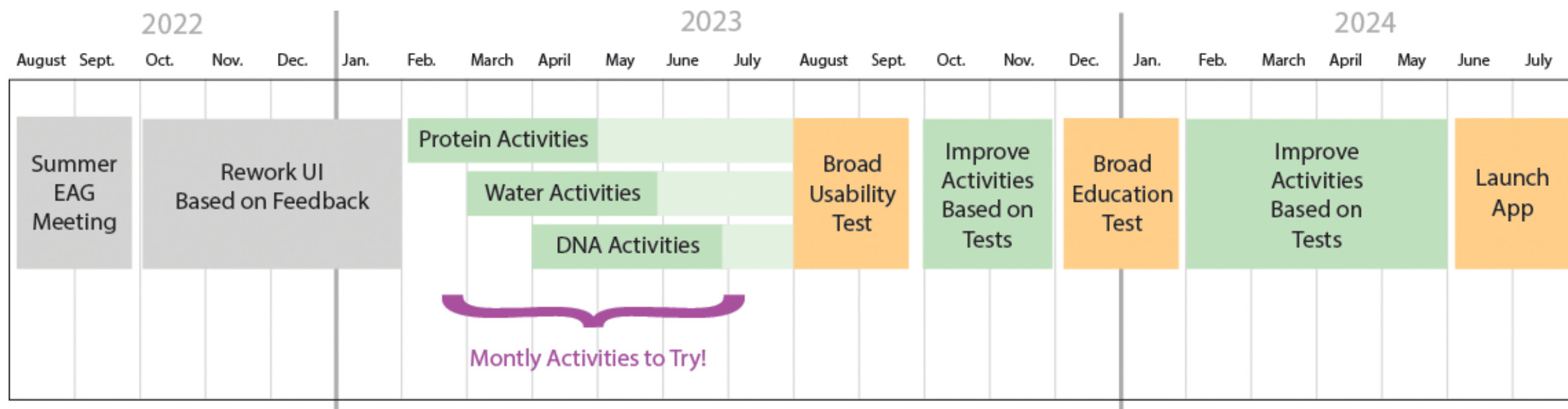
**Interactive
Digital Media**



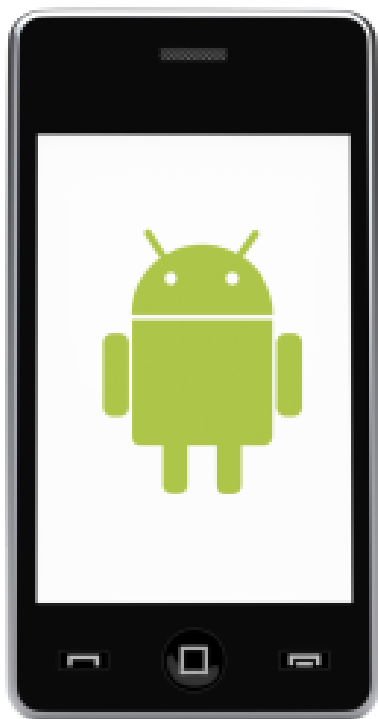
**Physical Models
with Augmented
Reality**



Where is this work going? What is next?



Making this work in the classroom



Accessories sold separately.



Beyond AR: Articulate Storyline

3d Molecular Designs

Building a Water Molecule

A single water molecule contains one oxygen atom and two hydrogen atoms that are covalently bonded together, meaning that they share electrons.

- Study the chemical structure shown below.
- Drag and connect the pieces on the right to build your own single water molecules in three common molecule representations.
- Answer the question below and move to the next slide.

Atom Spacefill Representation

Lewis Structure Representation

Bohr Model Representation

Chemical Structure Representation

$$\begin{array}{c} \text{H} \\ | \\ \text{H}-\text{O} \end{array}$$

Question Needed
Answer needed

3d Molecular Designs

The Three States of Matter

Matter can exist in three states, solid, liquid and gas.

Water as a Gas
(above 100°C)

Water as a Liquid
(between 0°C and 100°C)

Water as a Solid
(below 0°C)

As a gas (above 100°C), water molecules barely form hydrogen bonds with each other, and are very spread out.

As a liquid (between 0°C and 100°C), water molecules are very close to each other and form and break hydrogen bonds quickly.

As a solid (below 0°C), water molecules form permanent hydrogen bonds that crystallize into a hexagonal lattice structure.

- Study the various chemical drawings shown above and to the right.
- Drag and rotate the water molecule shown to the right to create three illustrations of the three states of matter.
- Answer the question to the right and move to the next slide.

Question Needed
Answer needed

3d Molecular Designs

The Polar Nature of Water

The shared electrons in a water molecule spend more time near the oxygen atom and less near the two hydrogen atoms, resulting in a **slightly positive** and **slightly negative** regions.

This impacts how they interact with other molecules, forming **hydrogen bonds** when they get close to an opposite charge.

- Study how two water molecules interact using the image shown below.
- Drag the water molecule shown to the right to demonstrate how water molecules might interact with the other common molecules.

Glucose

Chloride Ion

Sodium Ion

Fatty Acid

3d Molecular Designs

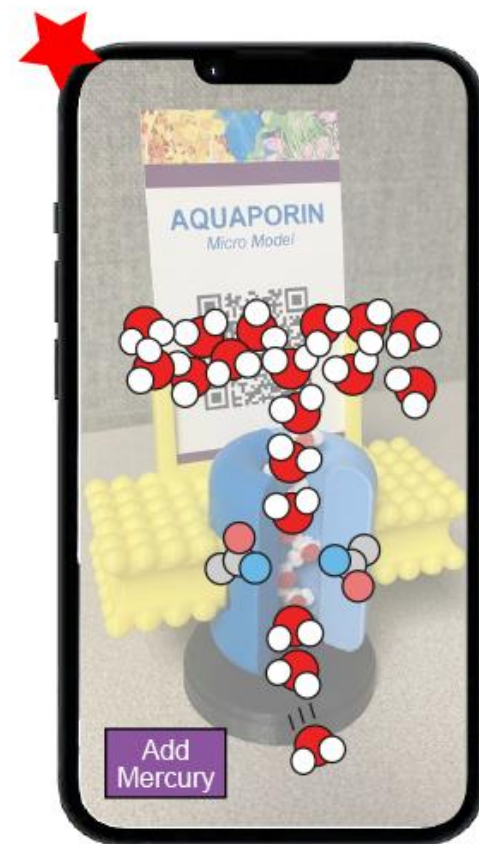
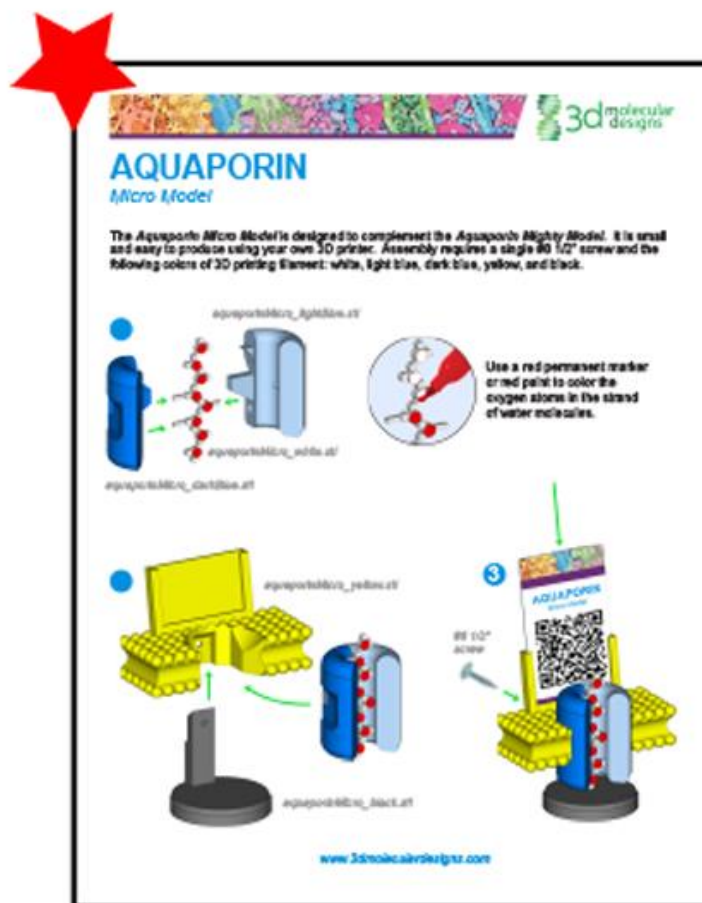
The Three States of Matter

Matter can exist in three states, solid, liquid and gas.

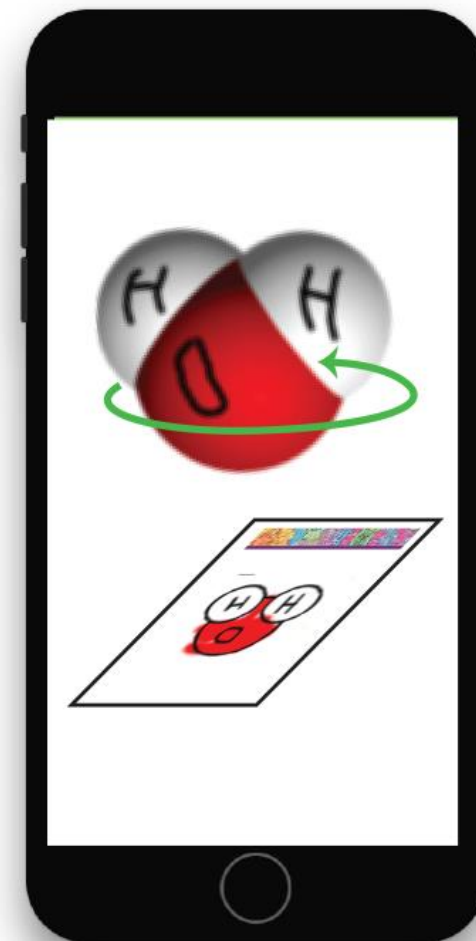
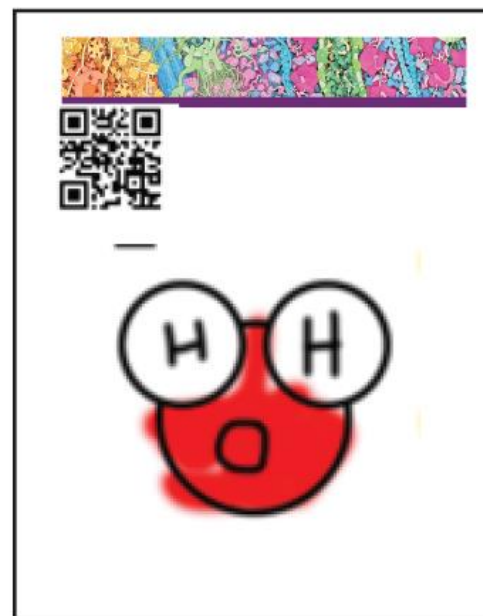
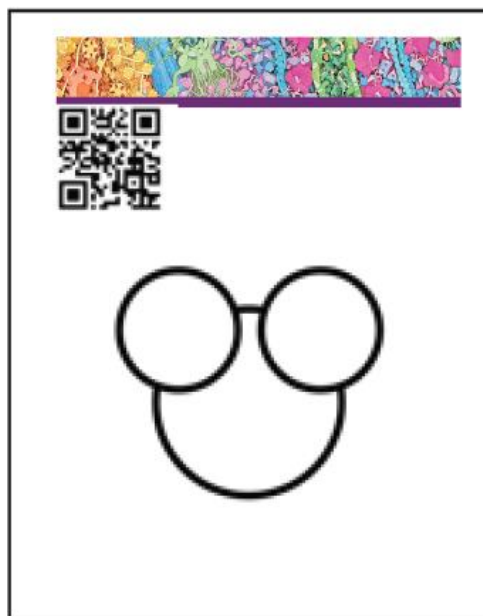
As a gas (above 100°C), water molecules barely form hydrogen bonds with each other, and are very spread out.

As a liquid (between 0°C and 100°C), water molecules are very close to each other and form and break hydrogen bonds quickly.

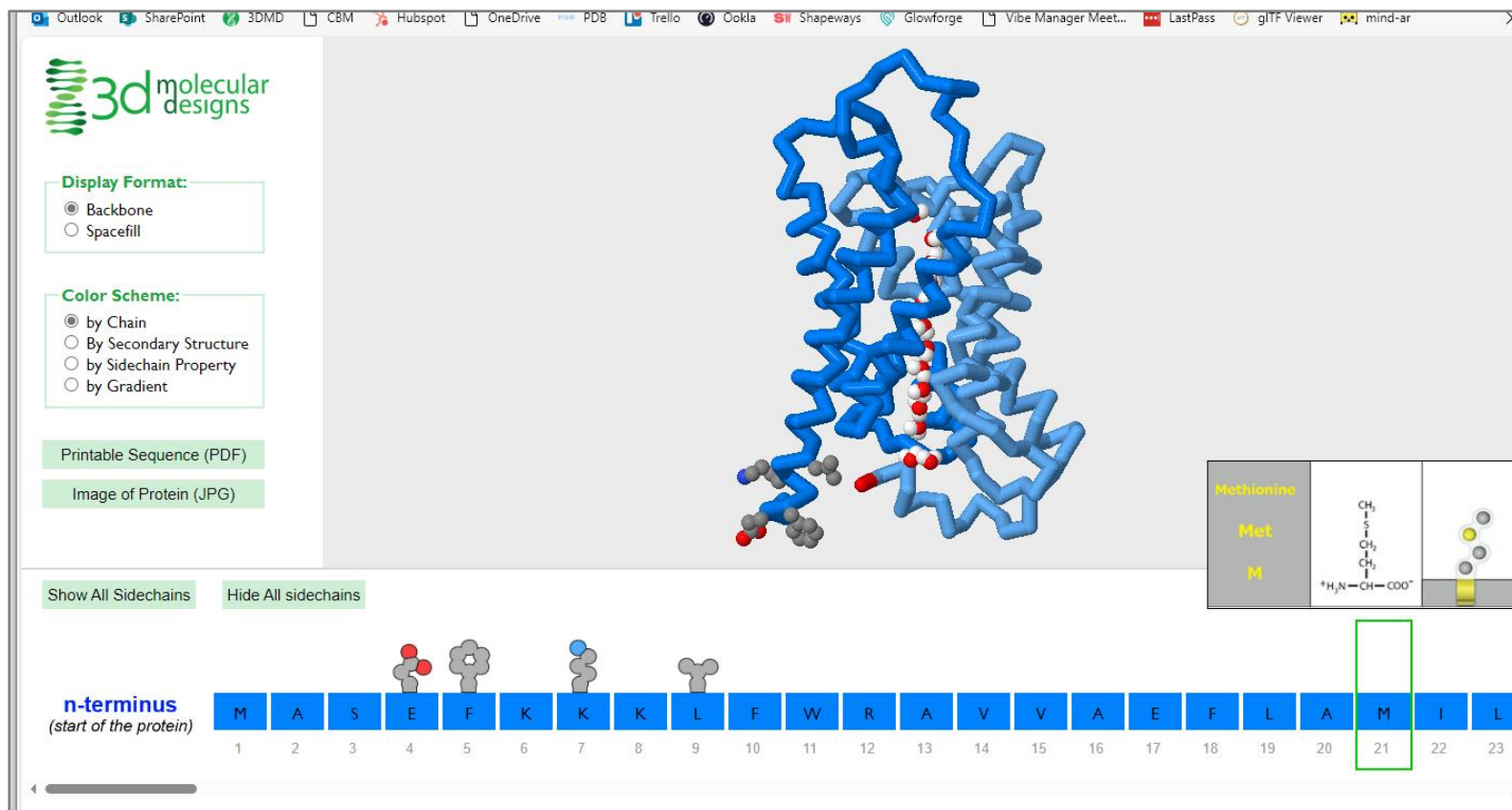
Beyond AR: 3D Print Files



Beyond AR: Coloring Pages



Beyond AR: Protein Exploretorium

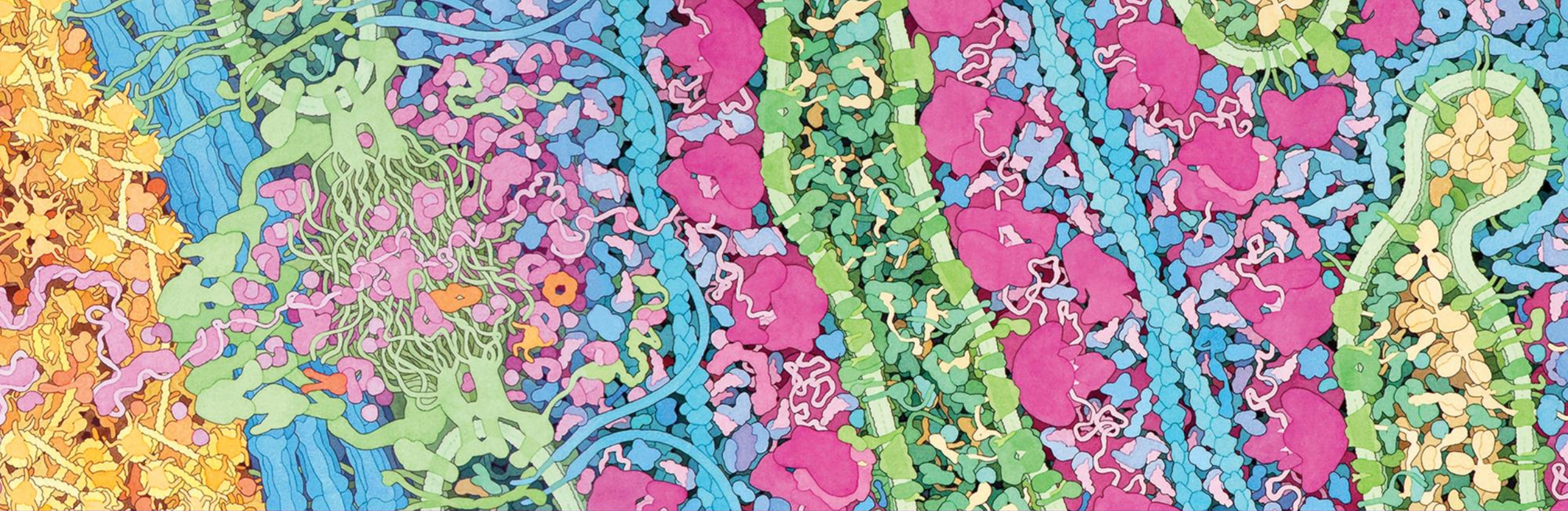


<https://www.centerforbiomolecularmodeling.org/markMyweb/aquaporinMightyModel/>



Scan this QR code and fill out our survey!





3d molecular
designs

Transforming Science Learning