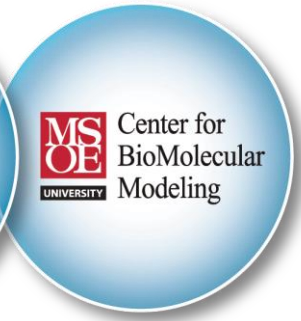
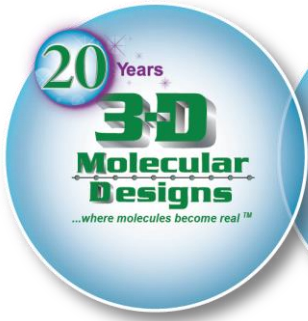




Celebrate World Water Day!

Aquaporin Channels



Modeling Resources

From the MSOE Center for BioMolecular Modeling

The digital resources below complement our physical models as well as teach students and teachers how to create their own 3D printed molecular models and interactive web pages.

The screenshot shows the homepage of the MSOE Center for BioMolecular Modeling. The browser address bar displays <https://cbm.msoe.edu>. The website features a navigation bar with three main categories: **STUDENT PROGRAMS**, **TEACHER PROGRAMS**, and **LEARNING RESOURCES**. Under **STUDENT PROGRAMS** are MAPS Teams (Modeling a Protein Story), Science Olympiad (Protein Modeling Event), and CREST Teams. Under **TEACHER PROGRAMS** are Summer Professional Development Courses, Regional Workshops, and Lending Library. Under **LEARNING RESOURCES** are Modeling Resources and 3D Molecular Designs. The main content area has a central welcome message: "Welcome to the CBM!" from the MSOE Center for BioMolecular Modeling, followed by the tagline "At the Center for BioMolecular Modeling, **teachers come first.** We work closely with talented science educators from across the US to create innovative instructional materials that make the biosciences understandable." Below this is a section titled "Student Programs" with three circular images: a 3D molecular model, two students working with a model, and two women standing together. On the right, a "What's New From the CBM?" section features social media icons and a video titled "The AeroNab Story" by Tim Herman, PhD - CBM Director. Below the video is a section for "A New Antibody MAPS Module" posted 1-6-2021, which focuses on antibodies and their role in the immune system, mentioning the current focus on a coronavirus vaccine.

MSOE Center for BioMolecular Modeling

STUDENT PROGRAMS

- MAPS Teams
Modeling a Protein Story
- Science Olympiad
Protein Modeling Event
- CREST Teams

TEACHER PROGRAMS

- Summer Professional Development Courses
- Regional Workshops
- Lending Library

LEARNING RESOURCES

- Modeling Resources
- 3D Molecular Designs

Student Programs

Teacher Programs

Learning Resources

Welcome to the CBM!
MSOE Center for BioMolecular Modeling

*At the Center for BioMolecular Modeling, **teachers come first.**
We work closely with talented science educators from across the US to
create innovative instructional materials that make the biosciences
understandable.*

What's New From the CBM?

The AeroNab Story
Tim Herman, PhD - CBM Director

A New Antibody MAPS Module
Posted 1-6-2021

This new MAPS Module will focus on **antibodies and their role in our immune system.** With everyone's current focus on a coronavirus vaccine, we

Certificate of Participation



Name

Participated in

Celebrate World Water Day!

Monday, March 22, 2021, 6:00 – 7:30 PM Central

Tim Herman

Tim Herman, Ph.D.
Center for BioMolecular Modeling



Center for
BioMolecular
Modeling

Diane Herman

Diane Herman
3D Molecular Designs



MSOE Center for BioMolecular Modeling
<https://cbm.msoe.edu>

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Celebrate World Water Day Webinar Resources
Monday, March 22, 2021

The video will be posted a day or two after the webinar.

Alice Scheele, Patrick Henry High School
Tim Herman, PhD, MSOE Center for BioMolecular Modeling

Session Resources

- Mentimeter

Aquaporin Links

- Peter Agre's biography on the 2003 Nobel Prize Site
- 1992 Agre paper on the exploding frog egg experiment
- Structure, Function and Dynamics of Aquaporin, Theoretical and Computational Biophysics Group
- Water moving through the aquaporin channel, Theoretical and Computational Biophysics Group
- 2000 Murta paper describing the structure of aquaporin

Center for BioMolecular Modeling Resources

- Aquaporin MAPS Module
- Loading Library

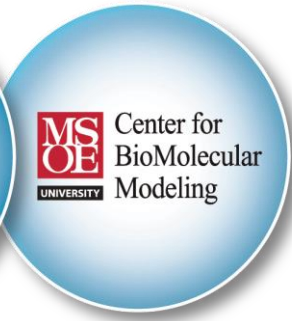
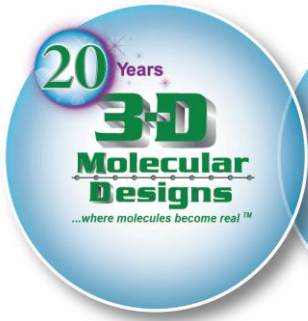


Alice Scheele
Patrick Henry High School
Ashland, VA

Biology teacher for 13 years
(AP, IB, Dual Enrollment and Intro)

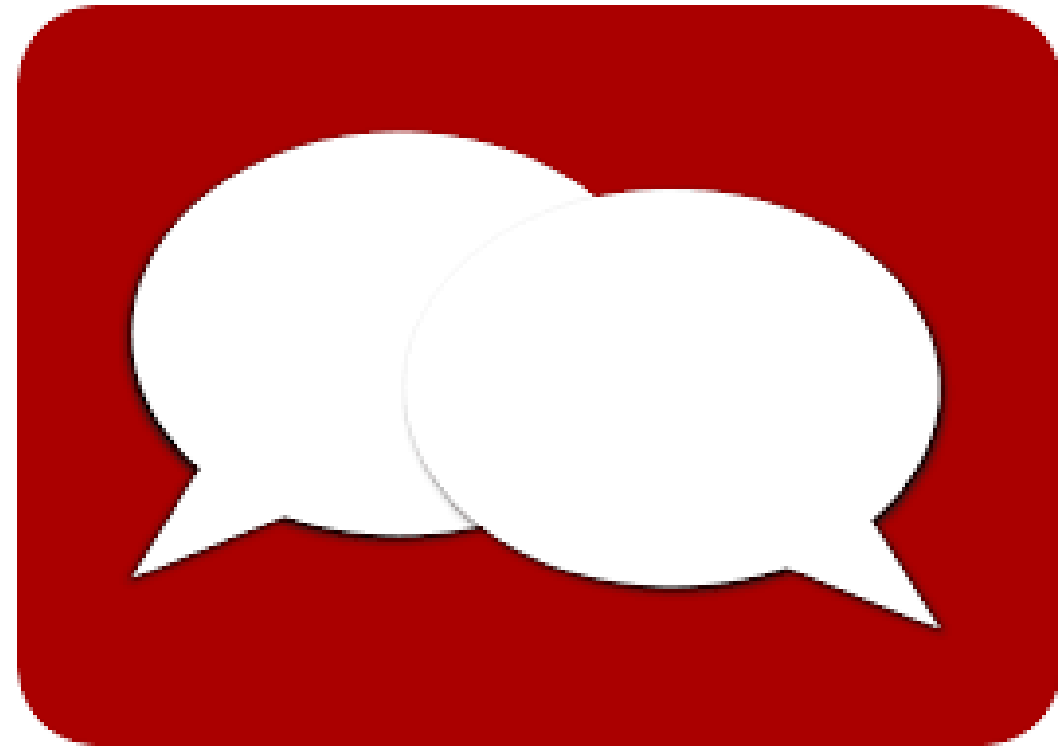
Contact Information:
ascheele@hcps.us





Using the chat box, Introduce yourself!

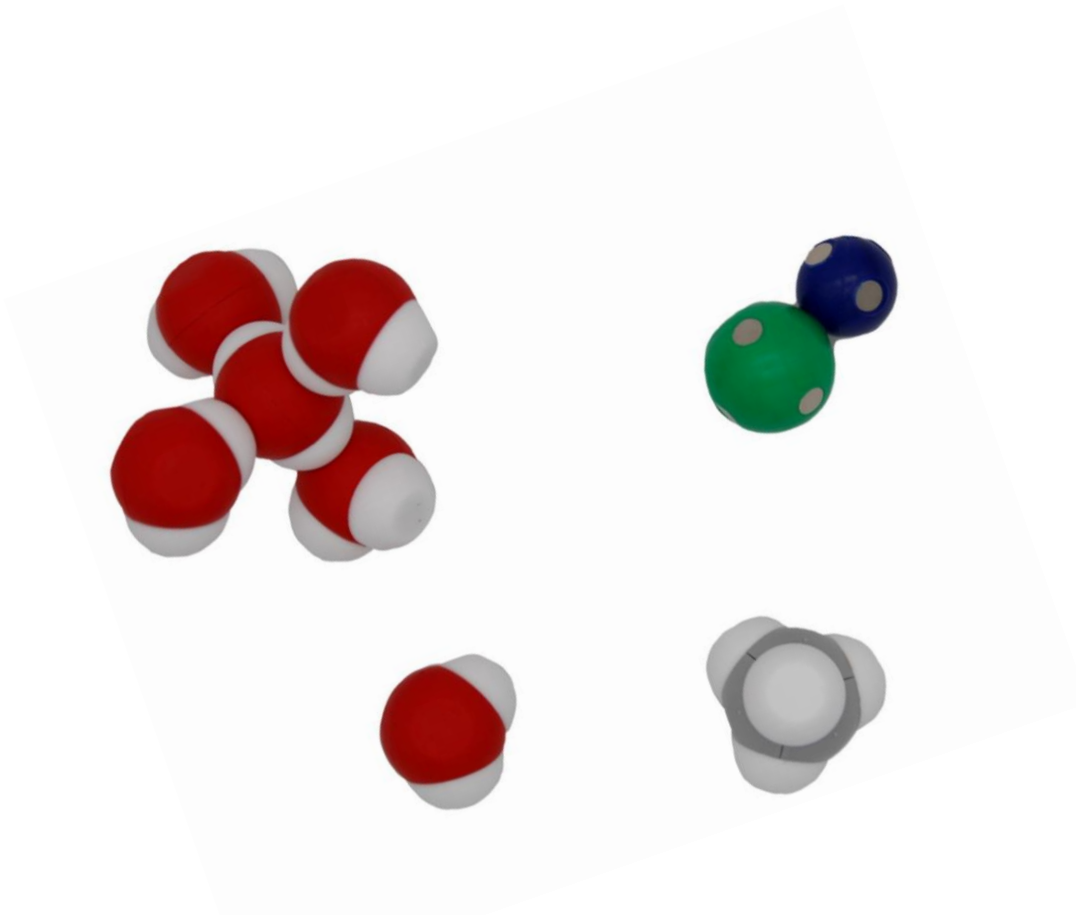
- Where are you from?
- What do you teach?
- Have you used models in your classroom?





Workshop Learning Goals:

1. To use models to facilitate questions with my students
2. To explore the structure of water molecules
3. To examine the properties of water



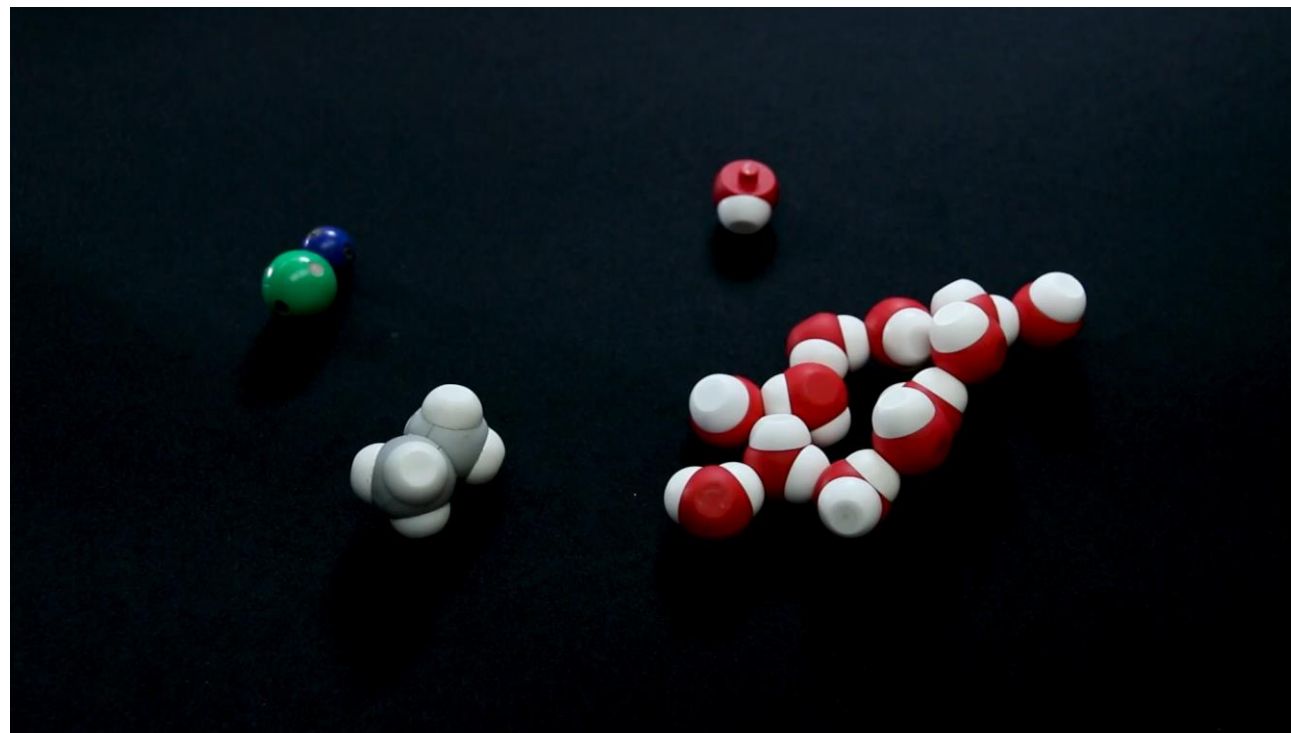
Water Student
Modeling pack



Water 1-cup Kit



What do you notice? What questions do you have?



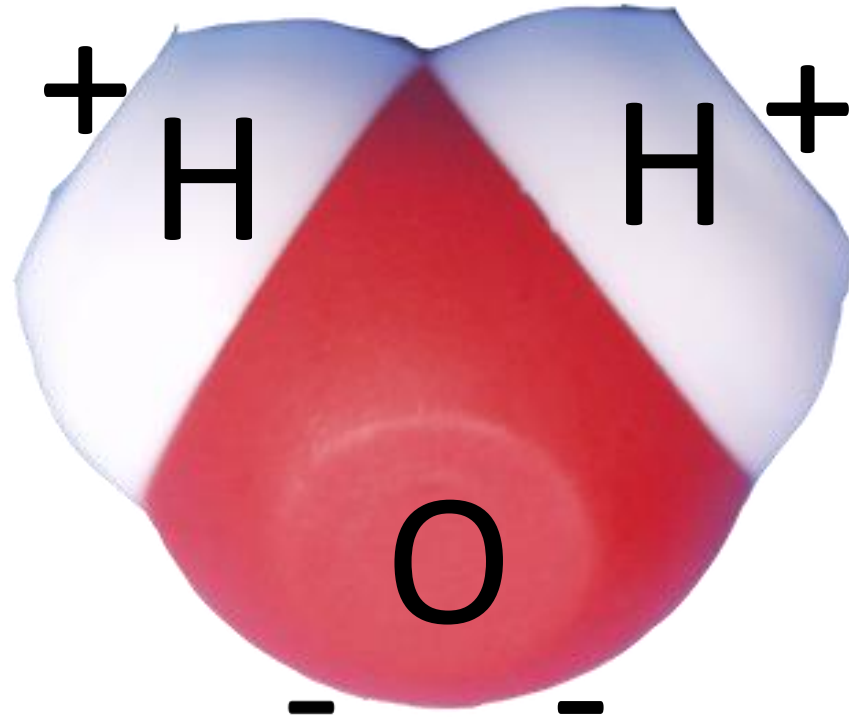
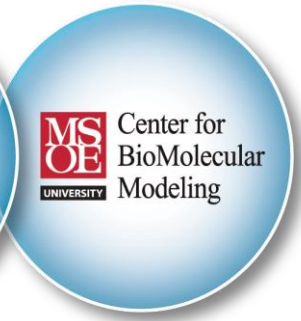
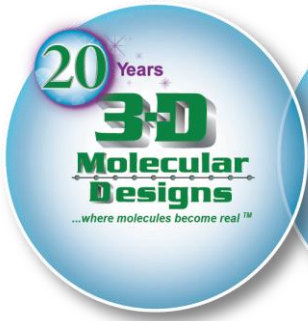


What questions do you have about this model?

is it a molecule

what is it

what is the white
do they represent h₂o
what is the red
why does it fit so good
why is it red and white
why is it magnetic
r the colors significant
why does white go on red
how does it know
why cant red touch red
why are there flat spots
why magnetic
why do opposites attract
why do they connect
are the molecules water
what are the flat spots
why is it so small
why is it so magnetic
what does it represent
is it a water molecule



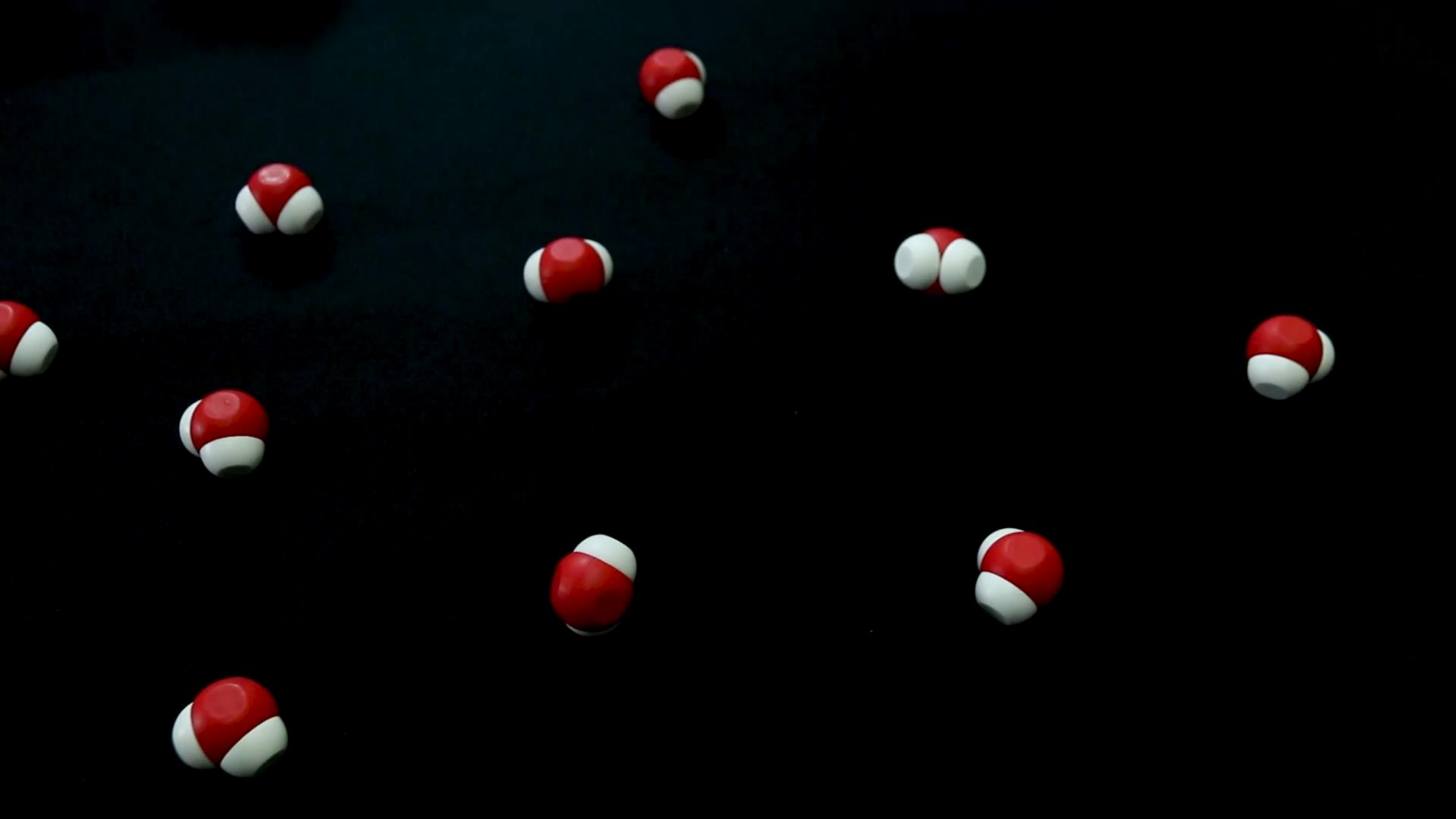






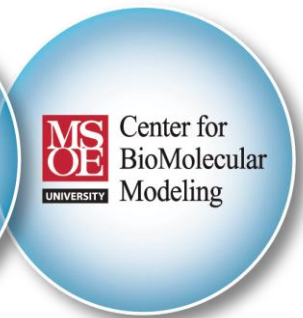
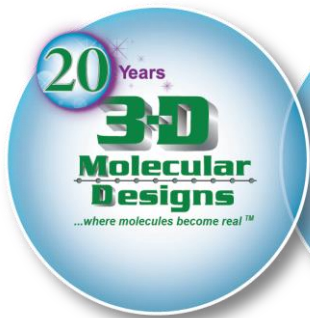
BRAINSTORM











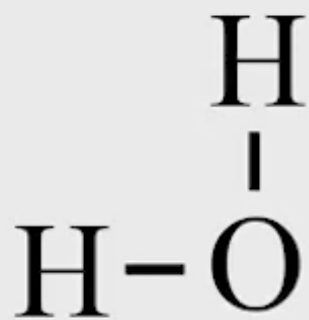




Building a Water Molecule

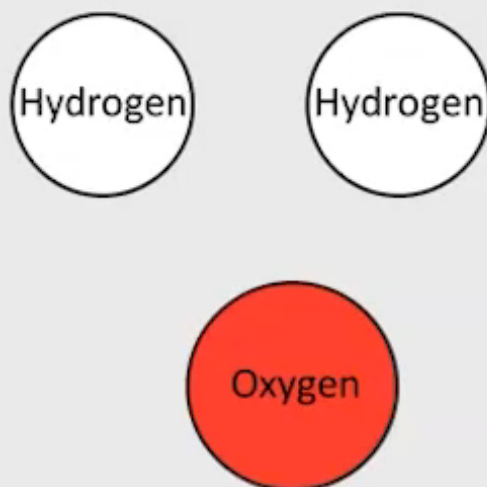
A single **water molecule** contains **one oxygen atom** and **two hydrogen atoms** that are **covalently bonded** together, meaning that they share electrons.

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

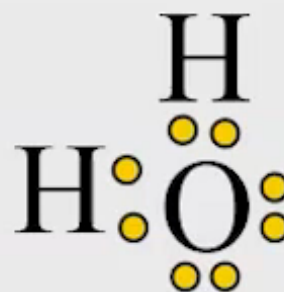


Chemical Structure
Representation

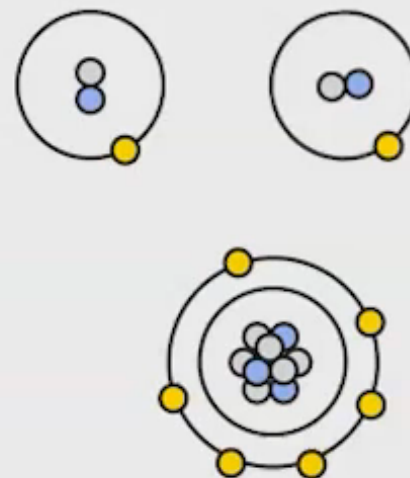
Atom Spacefill
Representation



Lewis Structure
Representation



Bohr Model
Representation



What is the bond called that joins a hydrogen to an oxygen in a water molecule?

Life Science	Biology	Chemistry
Water cycle Osmosis Eutrophication	Water chemistry Cell membrane structure Aquaporin Story! ~Tim Time Structure of protein channels Bonding ~DNA structure ~Replication ~Protein Synthesis	Phase of water Hydrogen bonding Dissolving/ionic salts Crystal structures

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

A

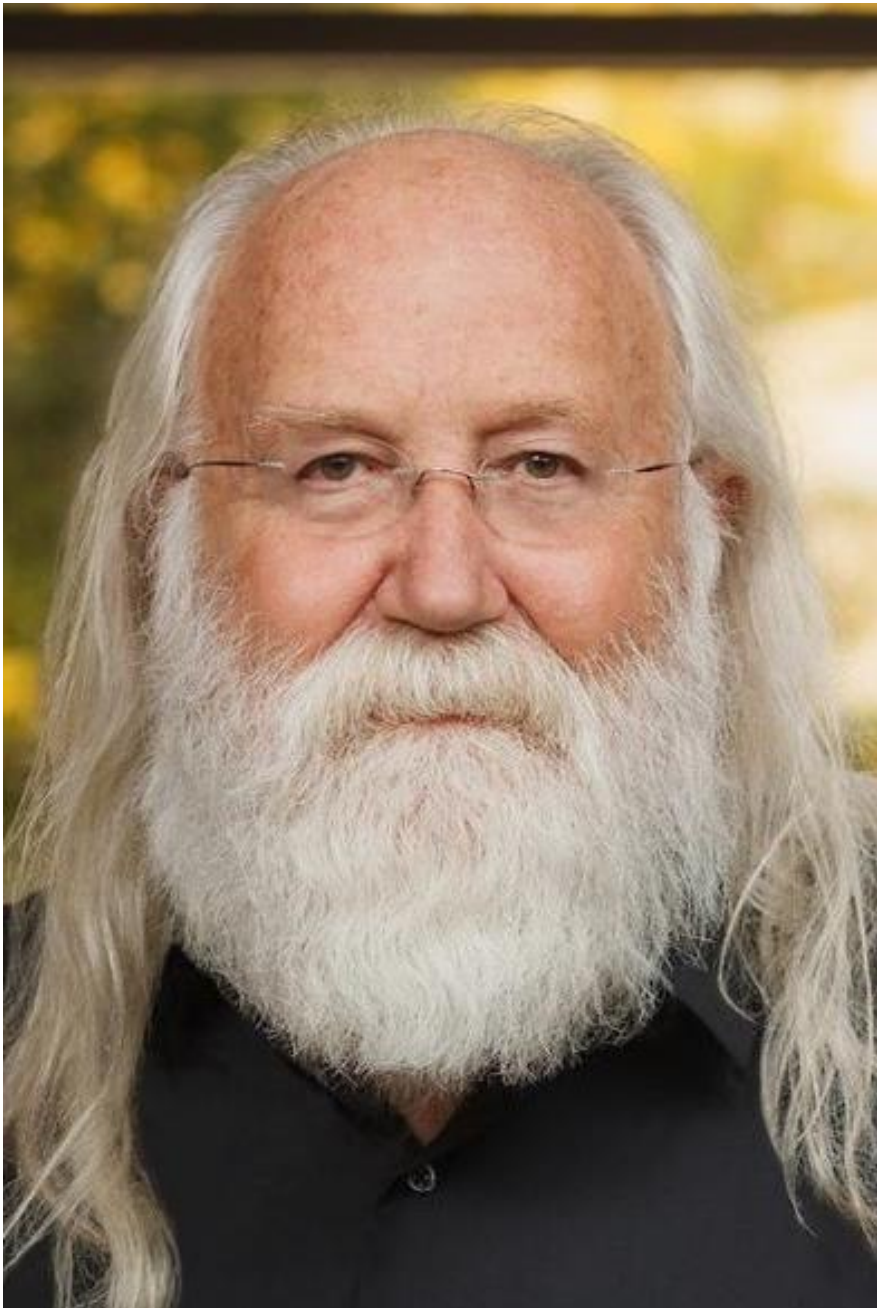
B

F

E

G

H

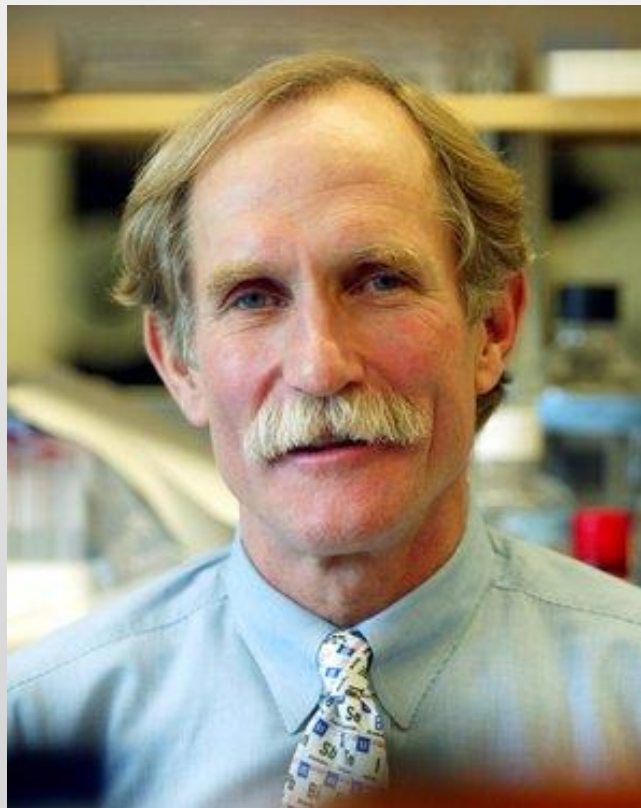


Aquaporin Channels

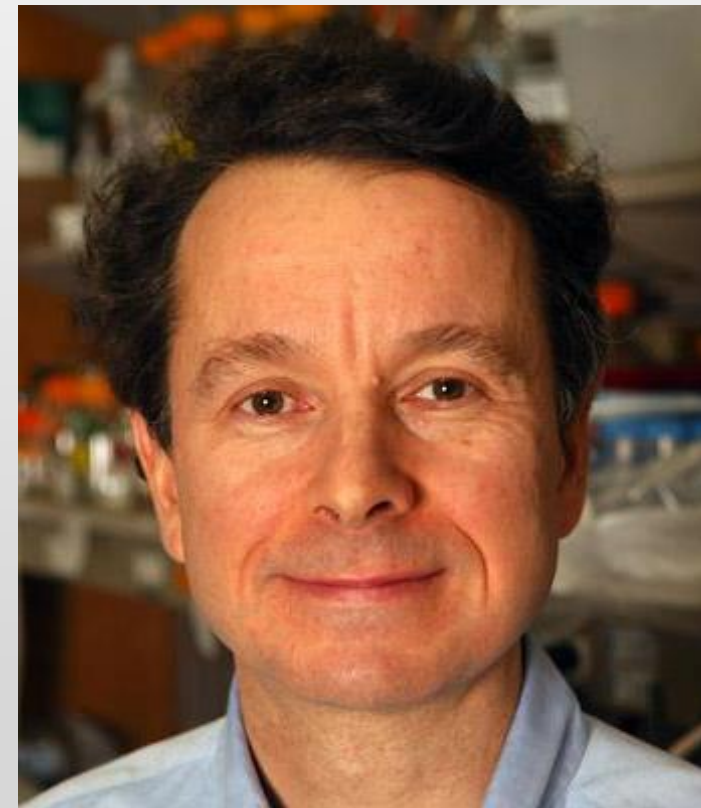


2003 Nobel Prize in Chemistry

The Nobel Prize in Chemistry 2003 was awarded "for discoveries concerning channels in cell membranes" jointly with one half to Peter Agre "for the discovery of water channels" and with one half to Roderick MacKinnon "for structural and mechanistic studies of ion channels."



Peter Agre



Roderick MacKinnon

Appearance of Water Channels in *Xenopus* Oocytes Expressing Red Cell CHIP28 Protein

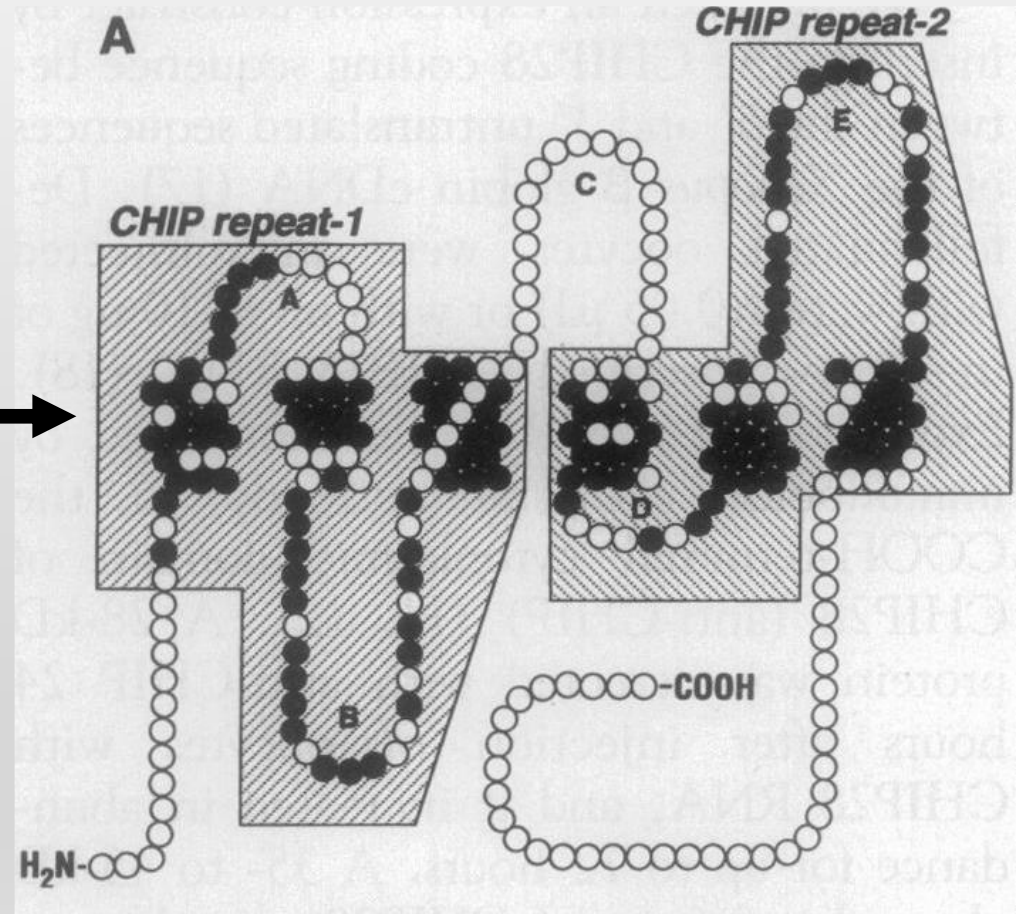
**Gregory M. Preston, Tiziana Piazza Carroll,
William B. Guggino, Peter Agre***

Water rapidly crosses the plasma membrane of red blood cells (RBCs) and renal tubules through specialized channels. Although selective for water, the molecular structure of these channels is unknown. The CHIP28 protein is an abundant integral membrane protein in mammalian RBCs and renal proximal tubules and belongs to a family of membrane proteins with unknown functions. Oocytes from *Xenopus laevis* microinjected with in vitro-transcribed CHIP28 RNA exhibited increased osmotic water permeability; this was reversibly inhibited by mercuric chloride, a known inhibitor of water channels. Therefore it is likely that CHIP28 is a functional unit of membrane water channels.

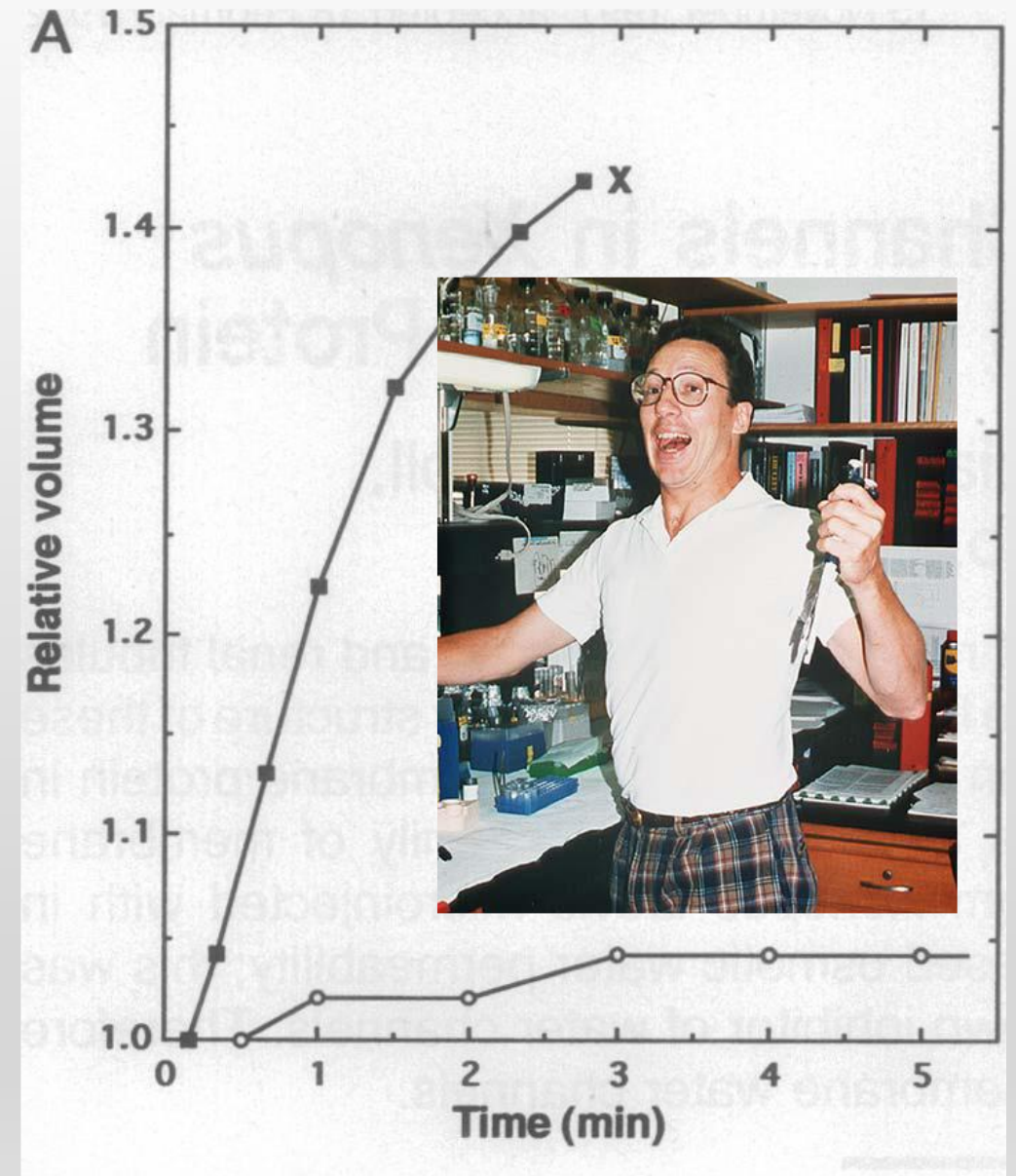
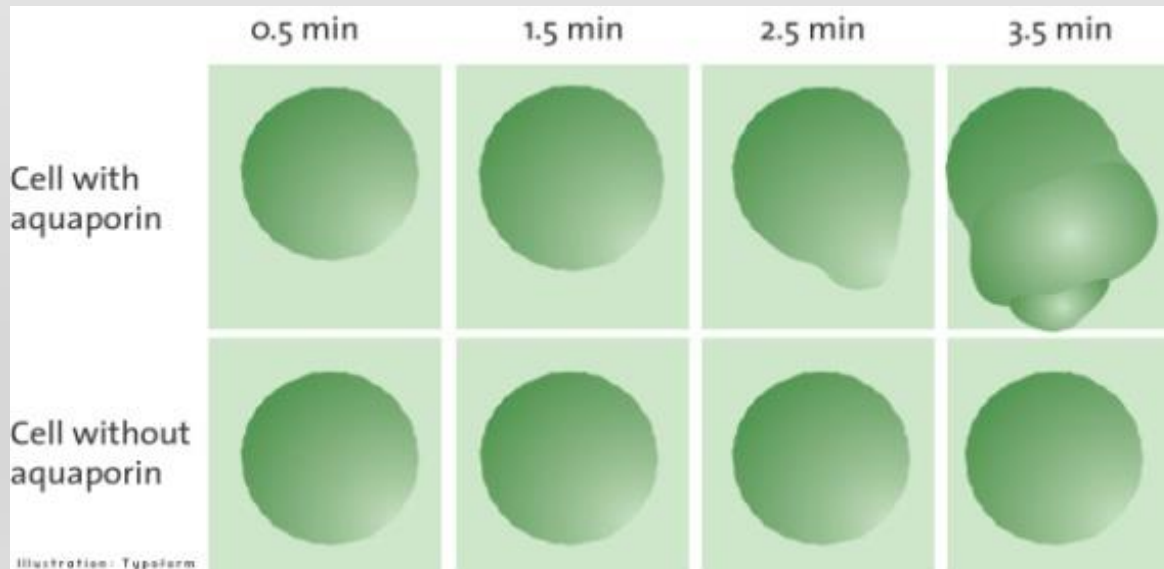
Science 256, 365-387 (1992)

1992 “Model” of Aquaporin

- Based on its Amino Acid Sequence
- 6 Transmembrane Helices
- 2-Fold Symmetry



Micro-injection of aquaporin (CHIP28) mRNA into frog oocytes



Structural determinants of water permeation through aquaporin-1

Kazuyoshi Murata^{*†}, Kaoru Mitsuoka^{†‡}, Teruhisa Hirai^{†‡}, Thomas Walz[§], Peter Agre^{||}, J. Bernard Heymann[¶], Andreas Engel[¶] & Yoshinori Fujiyoshi[‡]

^{*} National Institute for Physiological Sciences, Okazaki 444-8585, Japan

[‡] Department of Biophysics, Faculty of Science, Kyoto University, Kitashirakawa, Sakyo-ku, Kyoto, 606-8502, Japan

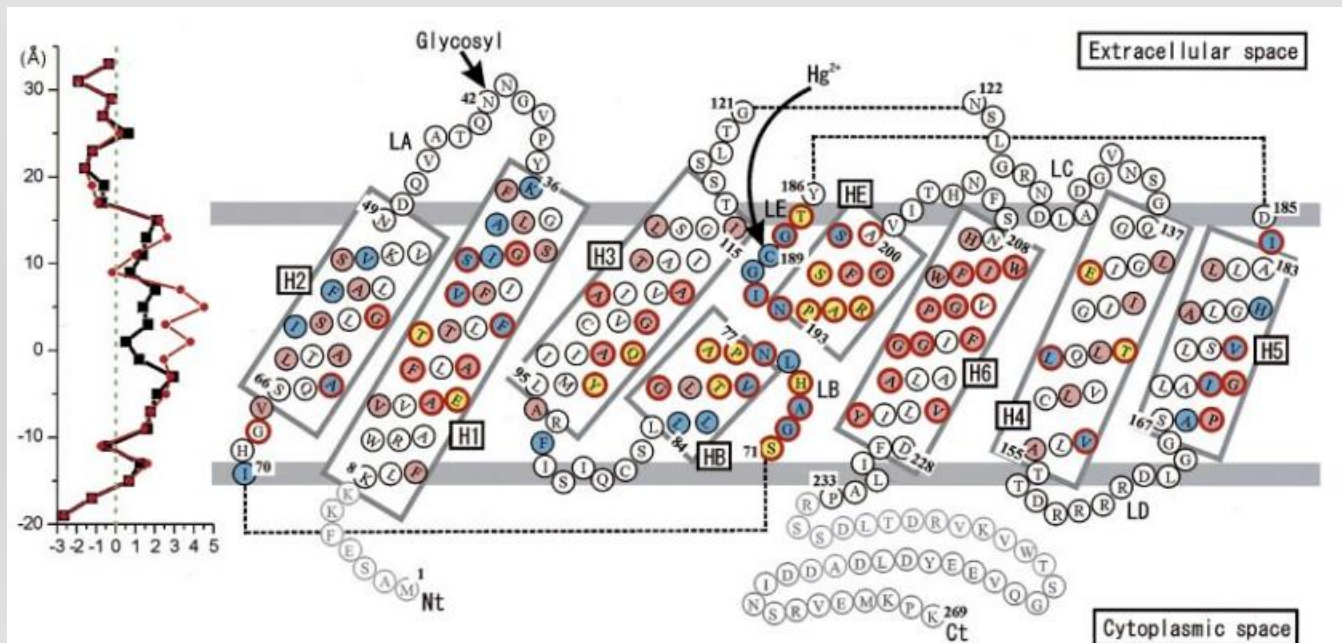
[§] Department of Cell Biology, Harvard Medical School, 240 Longwood Avenue, Boston, Massachusetts, 02115-5730, USA

^{||} Departments of Biological Chemistry and Medicine, Johns Hopkins University School of Medicine, Baltimore, Maryland 21205-2185, USA

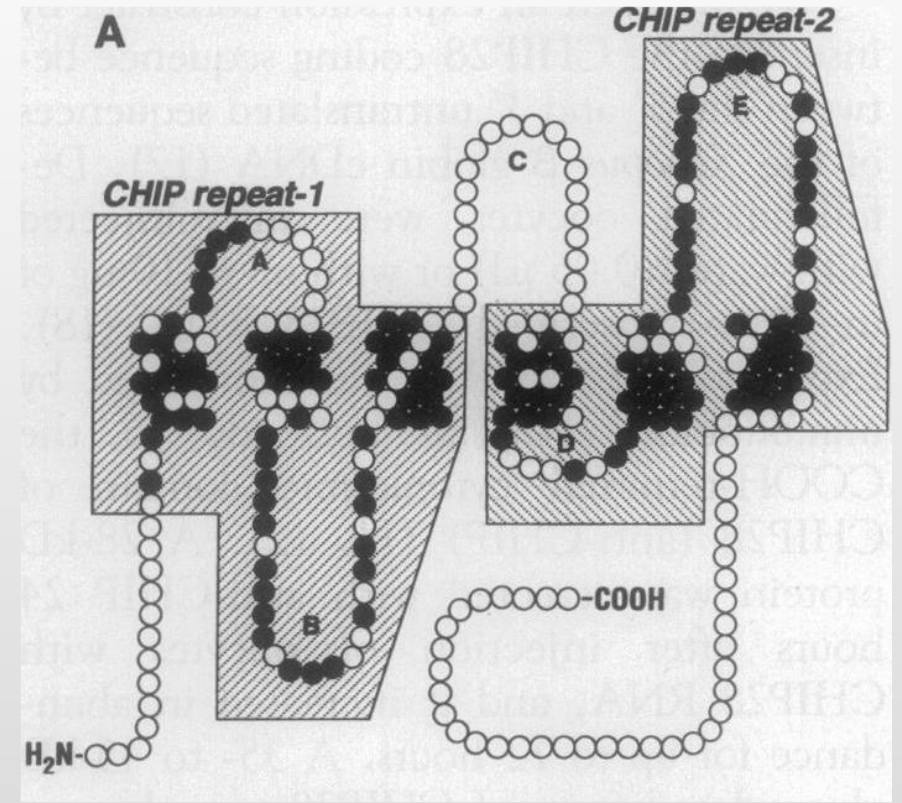
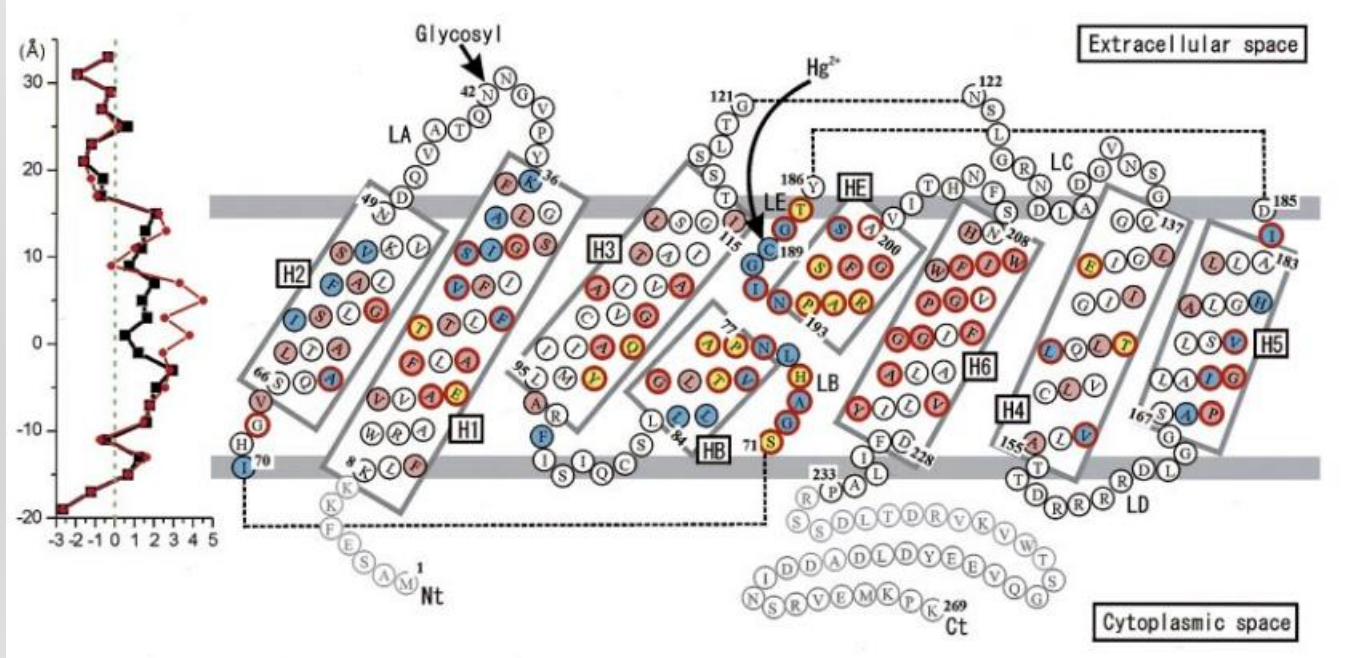
[¶] M. E. Müller-Institute for Microscopy at the Biozentrum, University of Basel, Basel CH-4056, Switzerland

[†] These authors contributed equally to this work.

NATURE | VOL 407
5 OCTOBER 2000. pp599



Agre “model”, 1992 →



← Murata model,...
based on x-ray
diffraction, 2000

Let's look at some models.....

Alpha Helix

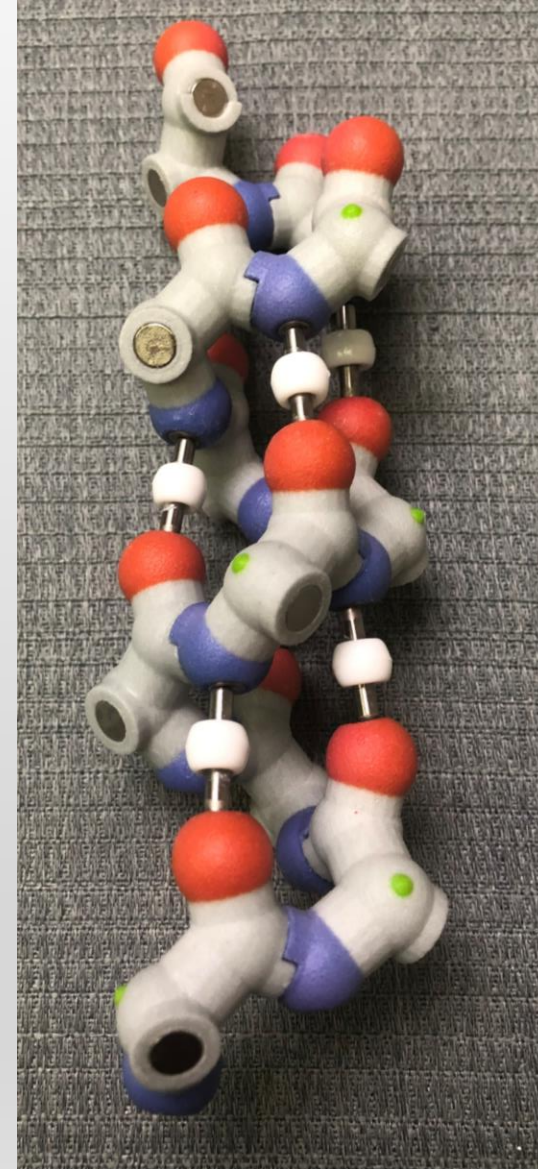
what's so special about 7-helix bundles?

Aquaporin,... at 3.8 Angstrom resolution

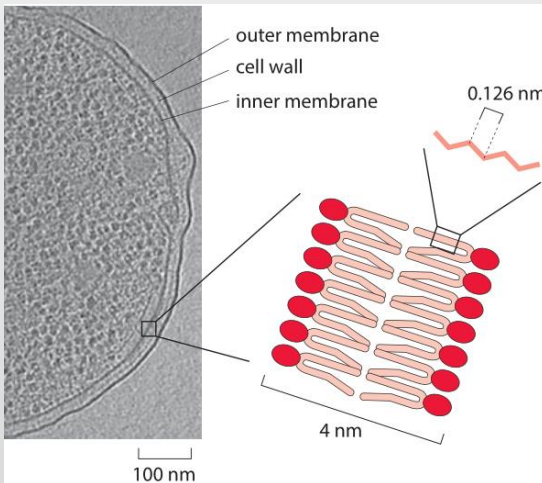
... at 0.9 Angstrom resolution

Molecular Dynamics,... a computational model

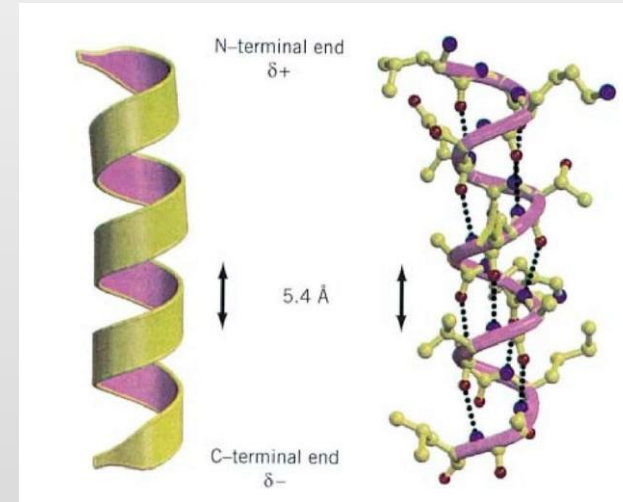
Why are transmembrane proteins often composed of bundles of alpha helices?



How many turns of the helix are required to span a membrane?



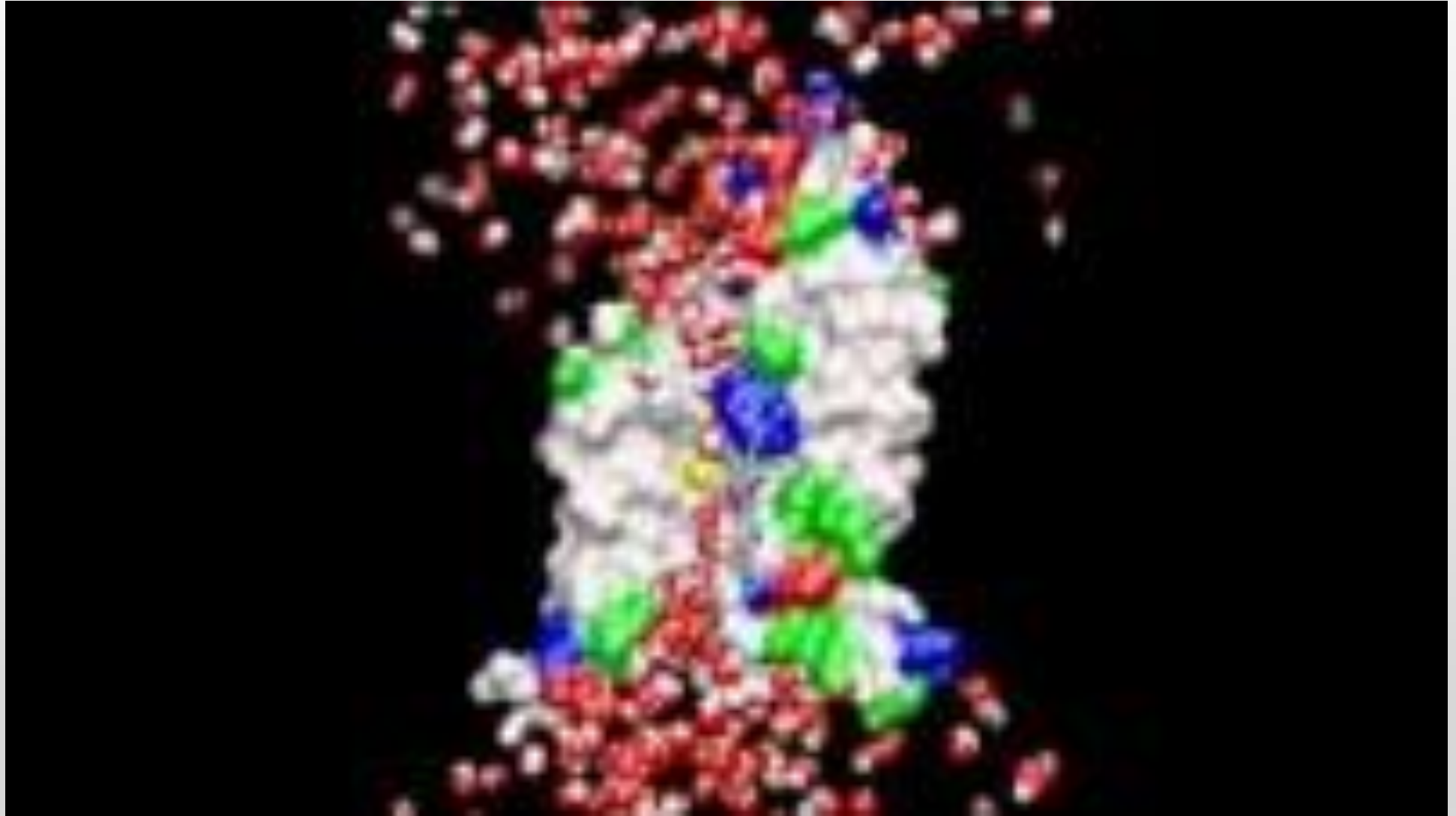
A lipid bilayer
is ~ 3nm thick



An alpha helix makes on
complete turn in 0.54 nm

$3\text{nm} / .54 \text{ nm/turn} = \sim 6 \text{ turns}$ of an alpha helix to span a membrane.
(22 amino acids)

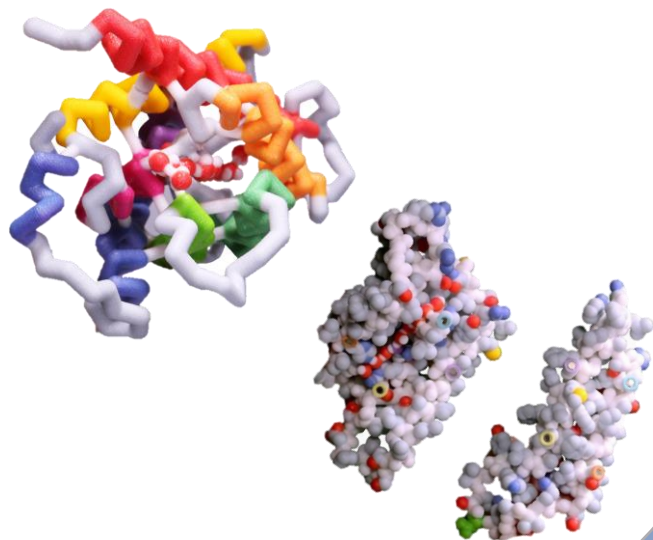
**A molecular
dynamics
simulation
from the
Klaus Shulten
group at
UIUC**





Peter Agre with Aquaporin Model





Thank you for attending!

For a Certificate of Participation

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3dmolecular designs.com.

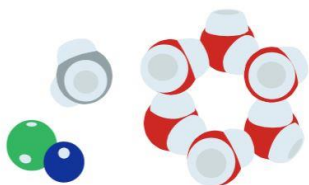
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Exploring the Wonderful World of Cell Membranes: Proteins, Lipids, and Ions, Oh My!

Wednesday, April 14, 2021 at 6:00 PM Central



DNA Structure & Function

Inspiring Student Questions with a TWIST in DNA Modeling

Wednesday, April 21, 2021 at 6:00 PM Central



Biotechnology & Coronavirus

The One Kit Wonder: Using Modeling to Teach Biotechnology Concepts

Wednesday, April 28, 2021 at 6:00PM Central

<https://www.3dmoleculardesigns.com/Webinars4.htm>