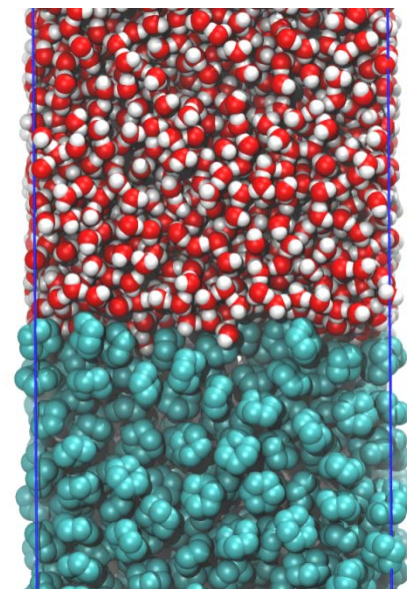
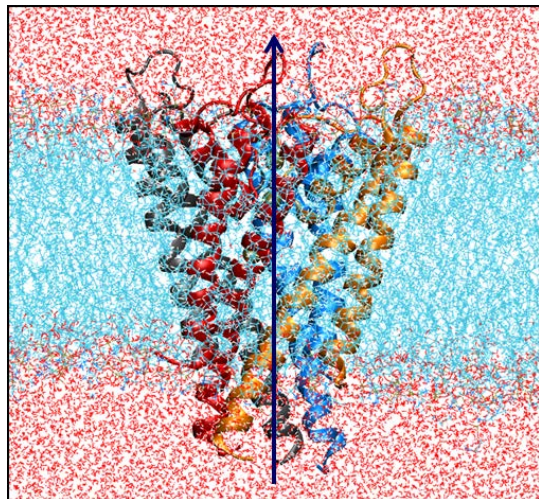


# Virtual Chemistry: Building labs inside computers



**Suman Chakrabarty**  
**Physical and Materials Chemistry Division**  
**CSIR-NCL, Pune**

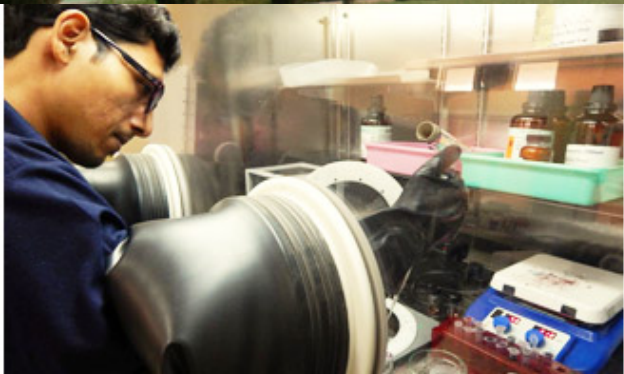
**Email: [s.chakrabarty@ncl.res.in](mailto:s.chakrabarty@ncl.res.in)**

**Web: [www.nambsite.com](http://www.nambsite.com)**



Council of Scientific and Industrial Research  
National Chemical Laboratory

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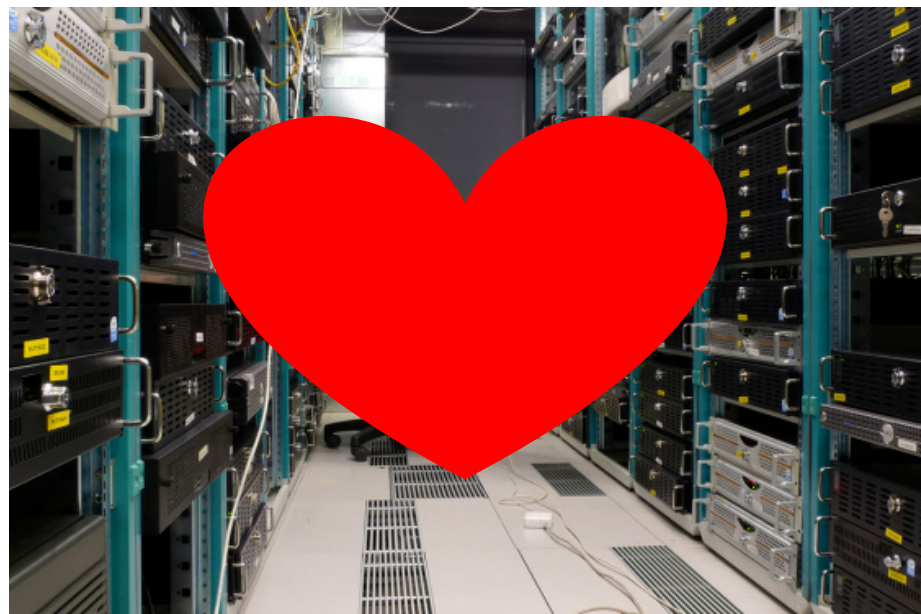
# ➤ Why “virtual chemistry”?!



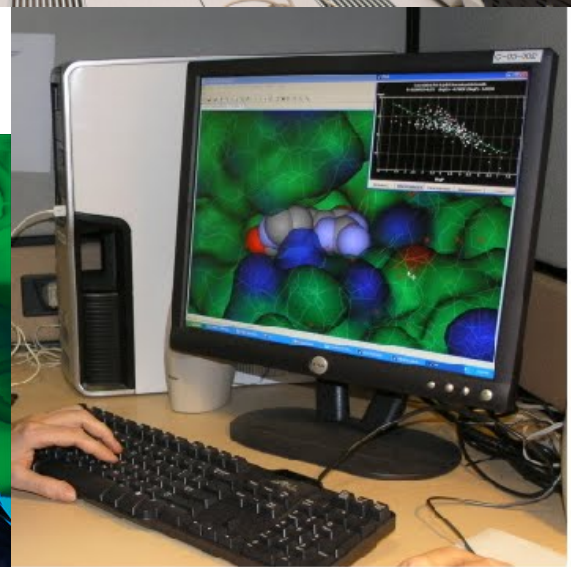
# ➤ Why “virtual chemistry”?!



OR

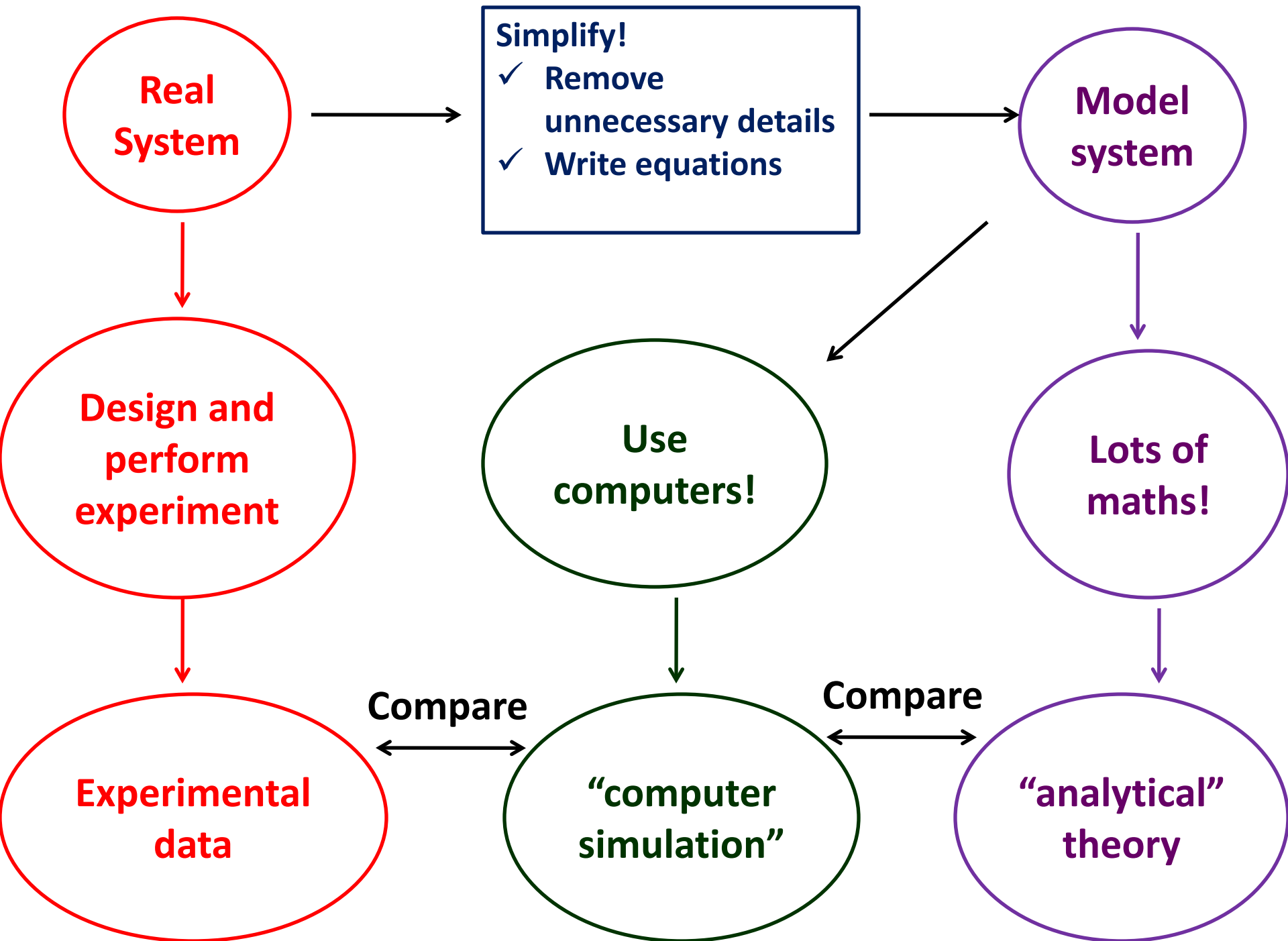


- ✓ Cleaner
- ✓ Cheaper
- ✓ Easier (?)
- ✓ Cooler! ;)

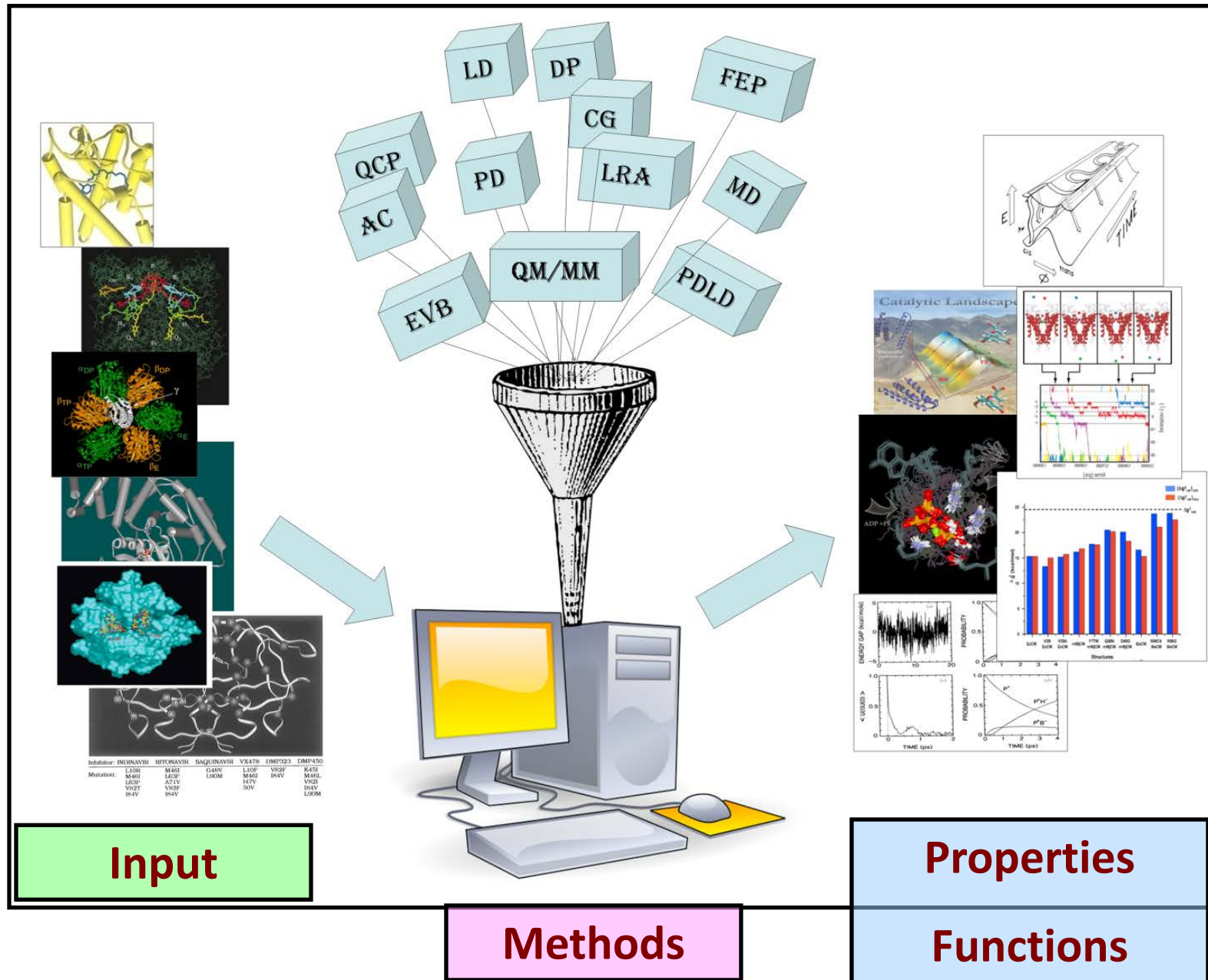


Molecule Modeling

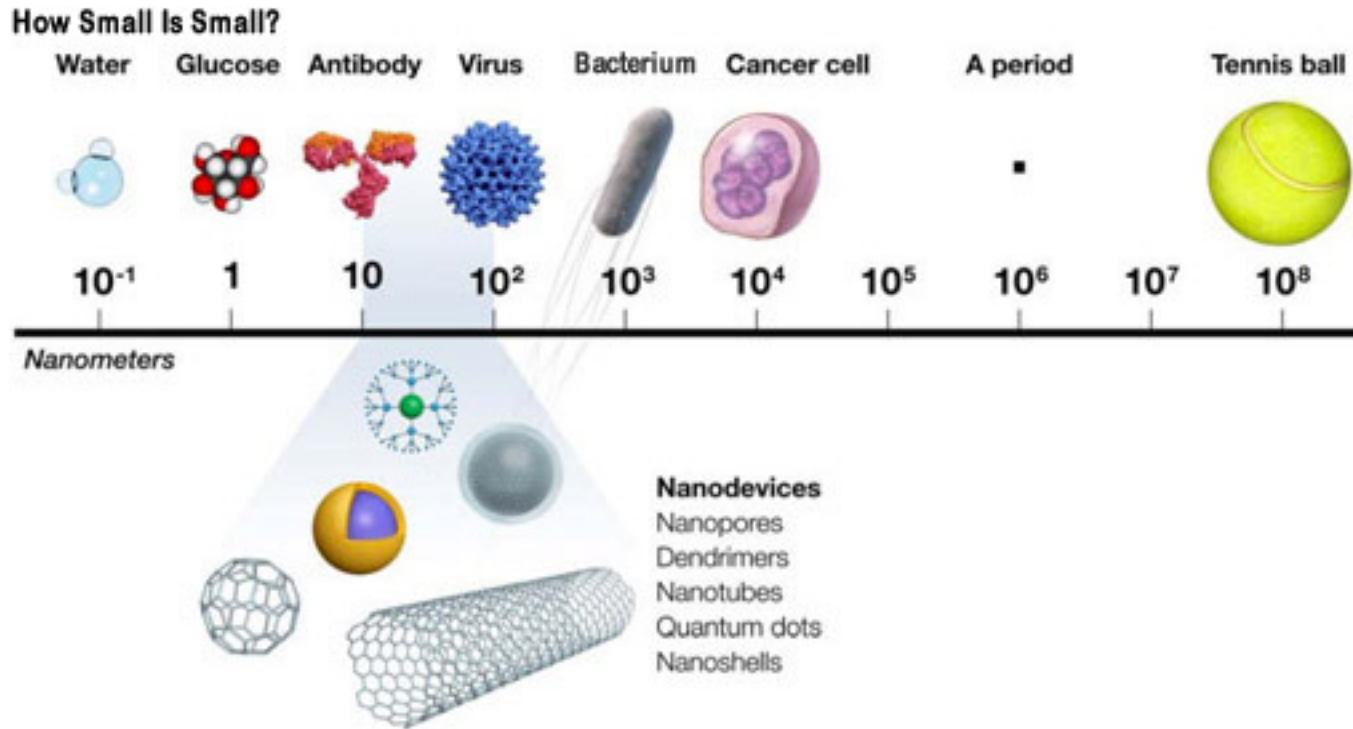




# Virtual Chemistry Lab (Ideally)



# How big/small we are?



**Video Clip:** <https://www.youtube.com/watch?v=EMLPJqeW78Q>

(The Smallest to the Biggest thing in the Universe!)

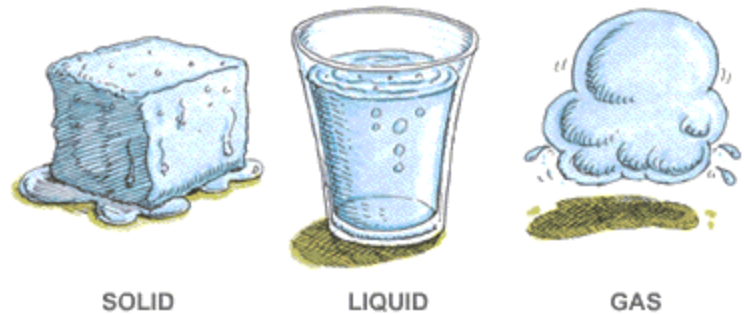
(Find the Ted-Ed videos in Youtube:

<https://www.youtube.com/user/TEDEducation>)

# Why ice floats on water?



... and why some things are solid or liquid or gas?

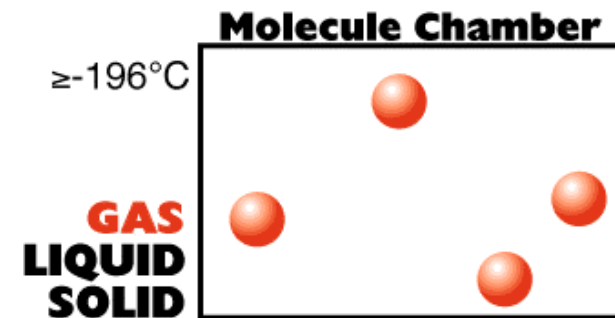
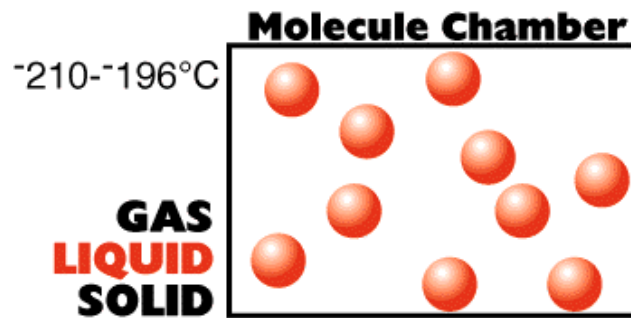
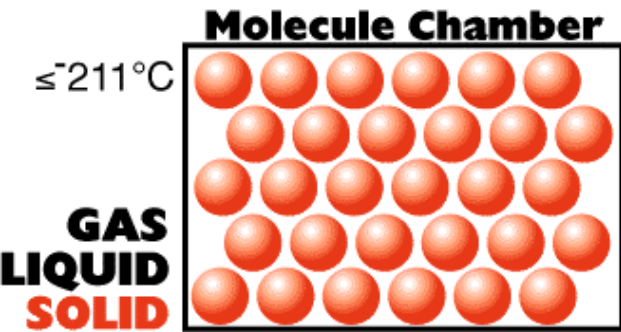
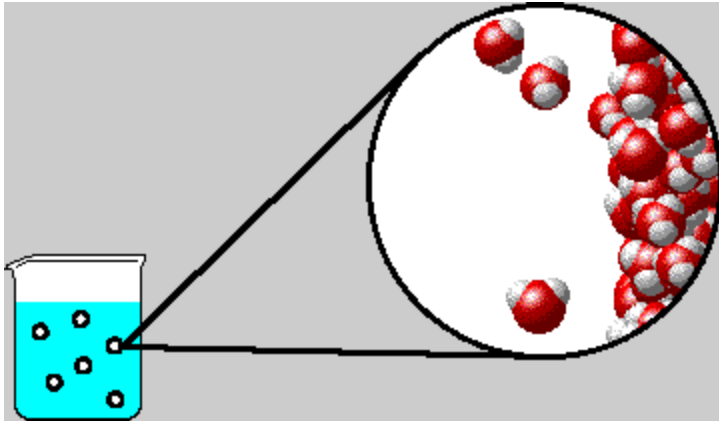


Watch at home (TED-ED):

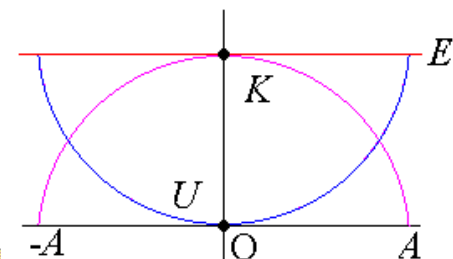
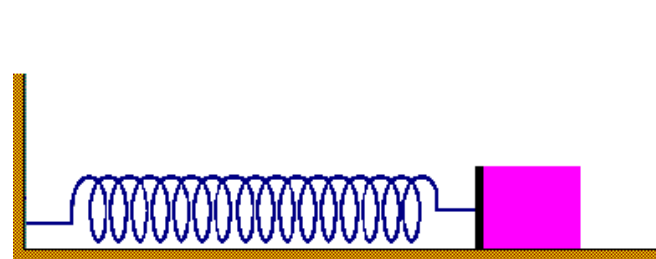
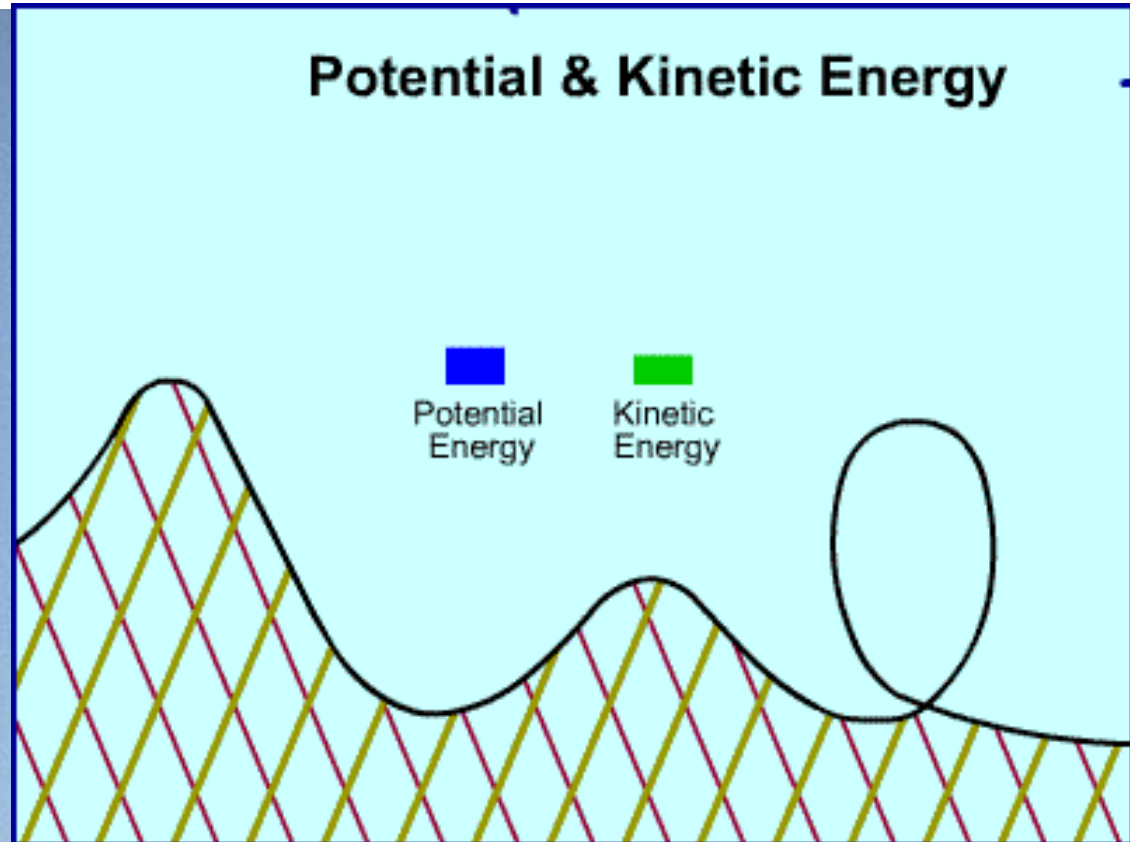
<https://www.youtube.com/watch?v=UukRgqzk-KE>



# Molecules talk to each other

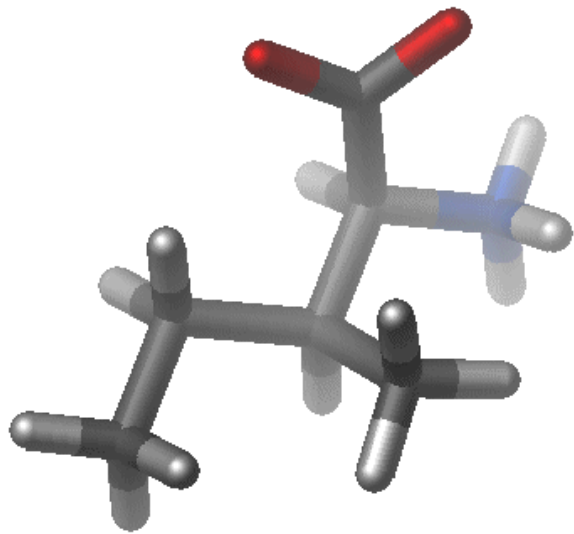


# Motion: potential energy vs. kinetic energy





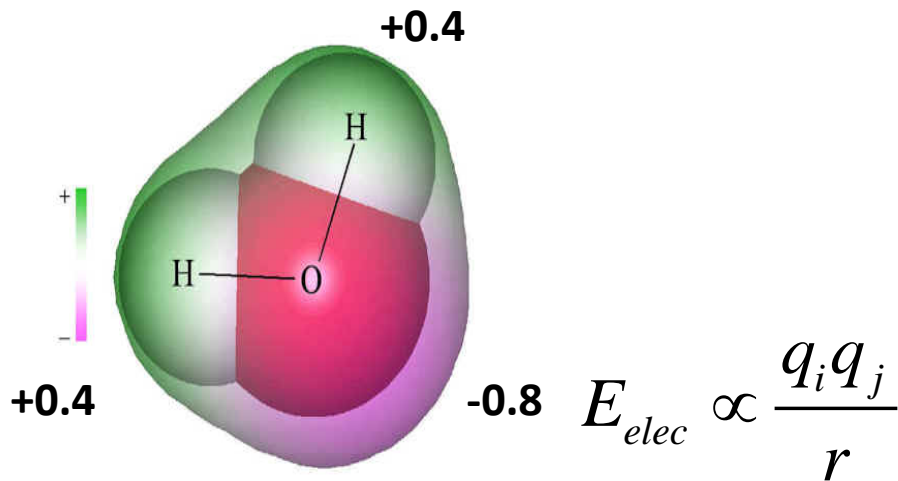
# Molecule: many balls and springs



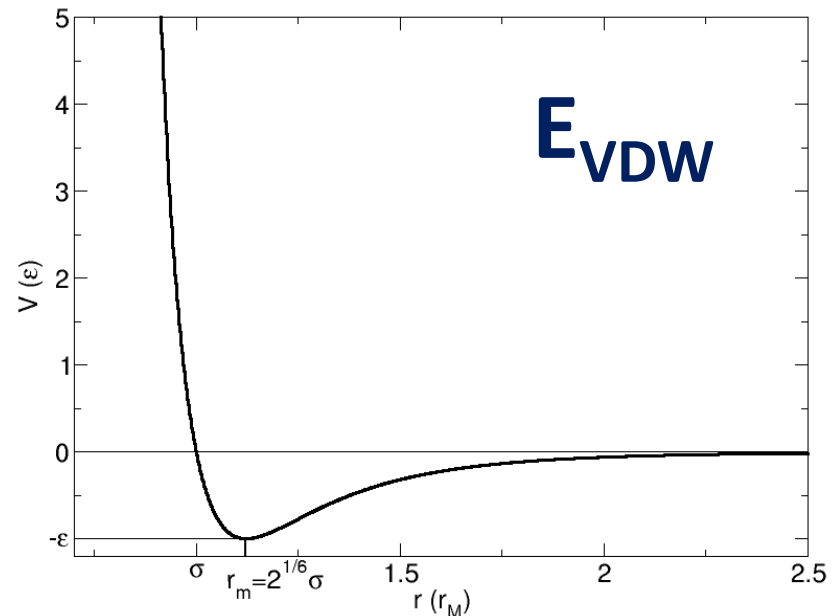
$$E_{\text{total}} = E_{\text{bonded}} + E_{\text{non-bonded}}$$

$$E_{\text{bonded}} = E_{\text{bond}} + E_{\text{angle}} + \dots \text{ etc.}$$

$$E_{\text{non-bonded}} = E_{\text{VDW}} + E_{\text{electrostatic}}$$



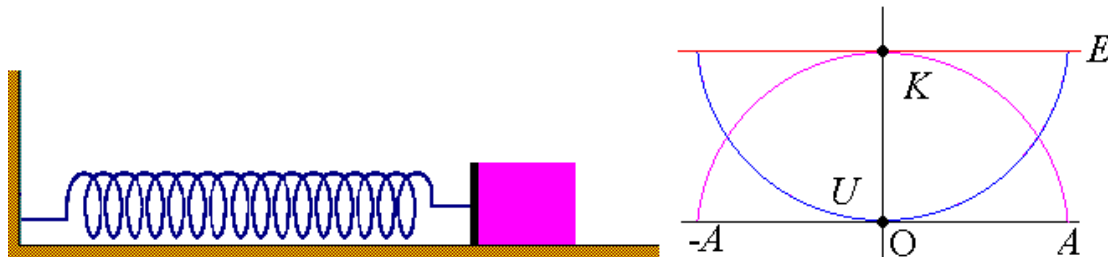
Opposite charges like each other



# Molecular Dynamics == Newton's Equation of Motion

(i) Rate of change of (potential) energy == Force

$$\mathbf{F} = -\frac{\Delta V}{\Delta x}$$

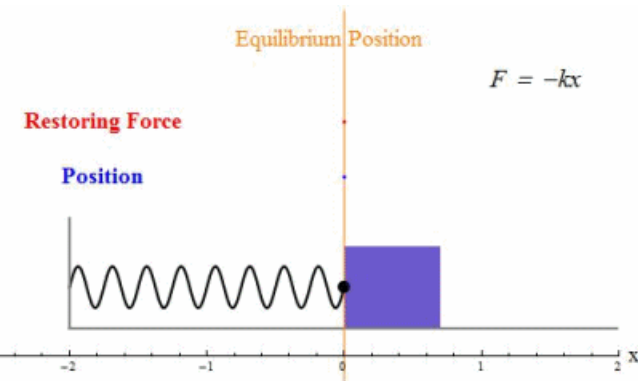


Equilibrium Position

$$F = -kx$$

Force = mass X (rate of change in velocity)

Velocity = rate of change in position



(ii) If we know position (and velocity) of all atoms at all times, we have the **MOLECULAR MOVIE!!!!** 😊



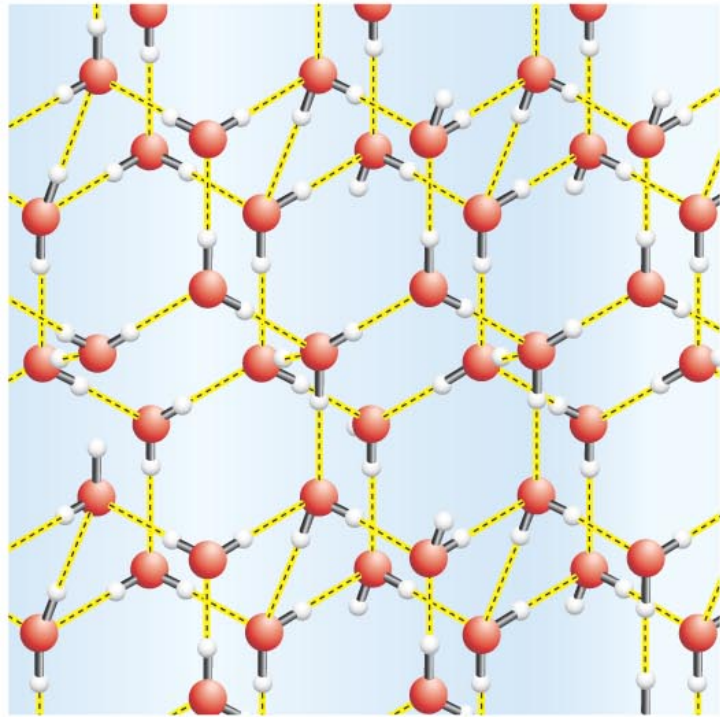
## Some examples:

✓ Gas chamber: hard spheres

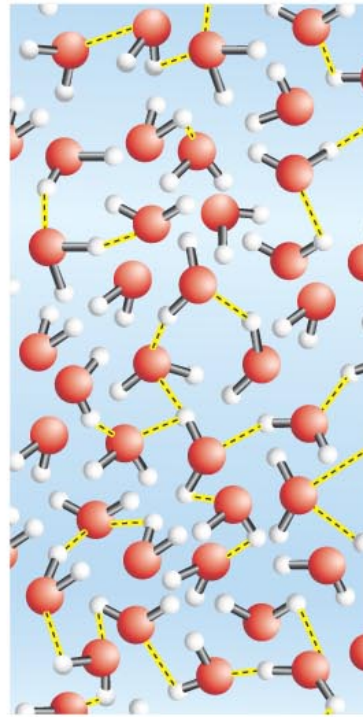
(a movie was shown in the talk)

# Why ice floats on water?

(a) In ice, water molecules form a crystal lattice.



(b) In liquid water, no crystal lattice forms.



(c) Liquid water is denser than ice. As a result, ice floats.



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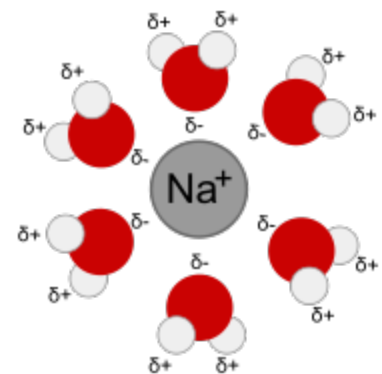
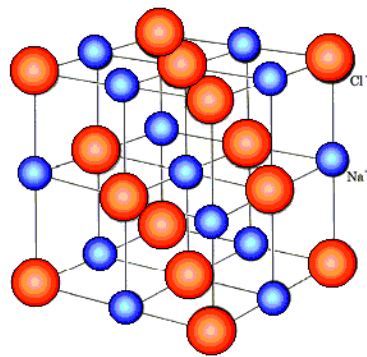
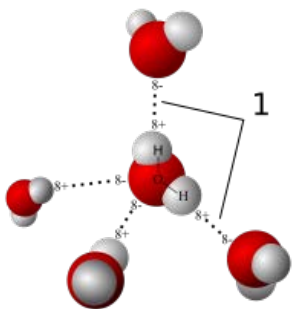
[Movie of water freezing \(Youtube\)](#)



# Why oil and water don't mix?



... and how come salt/sugar dissolves so easily?!



See this: <https://www.youtube.com/watch?v=h5yIJXdltgo>

# Why oil and water don't mix?



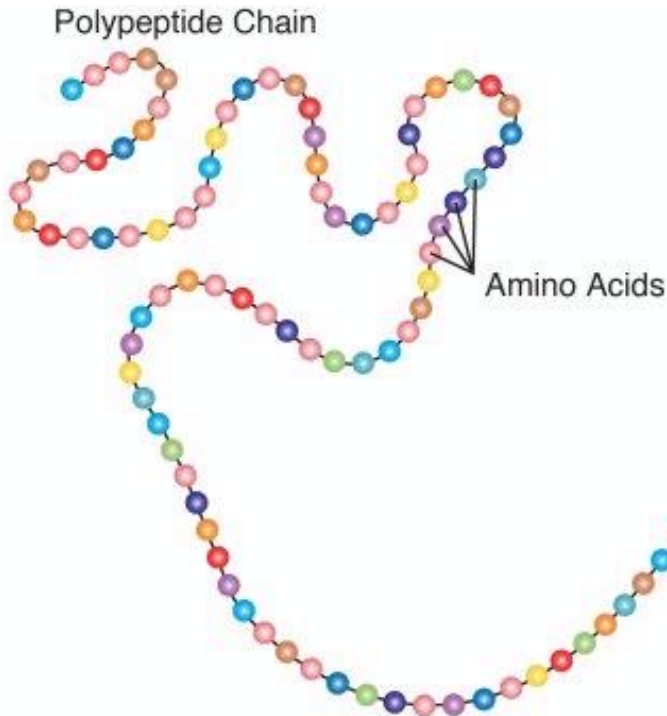
- ✓ First few moments of the life of a Salt (Sodium Chloride) crystal in water (300K) (370K)



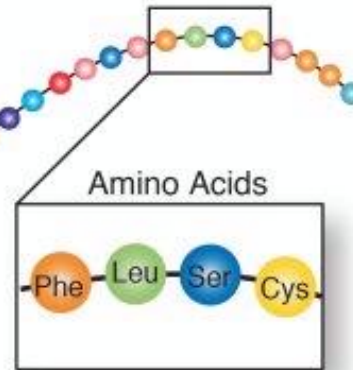
- ✓ Oil and water put together

**(Some movies were shown in the actual talk)**

# ➤ Proteins: The workhorses of life



**Amino acids: The 20 building blocks of life**



## Amino Acids

Ala: Alanine  
Arg: Arginine  
Asn: Asparagine  
Asp: Aspartic acid  
Cys: Cysteine

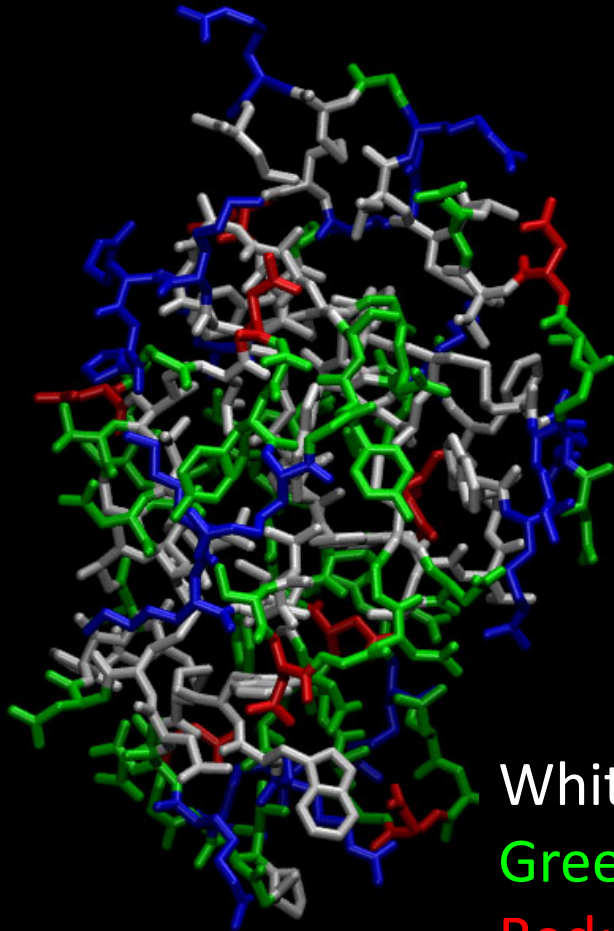
Gln: Glutamine  
Glu: Glutamic acid  
Gly: Glycine  
His: Histidine  
Ile: Isoleucine

Leu: Leucine  
Lys: Lysine  
Met: Methionine  
Phe: Phenylalanine  
Pro: Proline

Ser: Serine  
Thr: Threonine  
Trp: Tryptophane  
Tyr: Tyrosine  
Val: Valine



# What about LARGE molecules with both salt-like and oil-like parts?



White: non-polar: "oily"

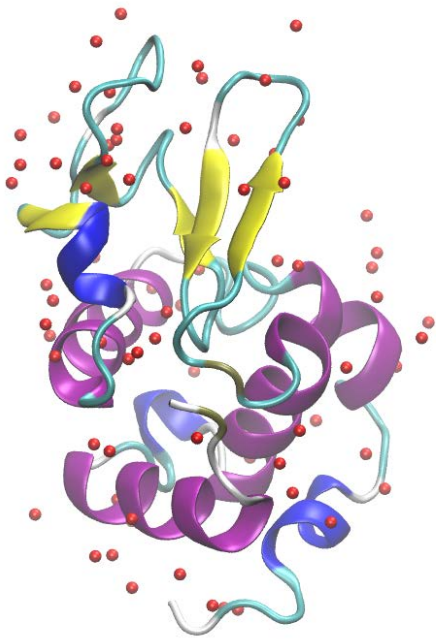
Green: polar: "watery"

Red: negative charge: "salty"

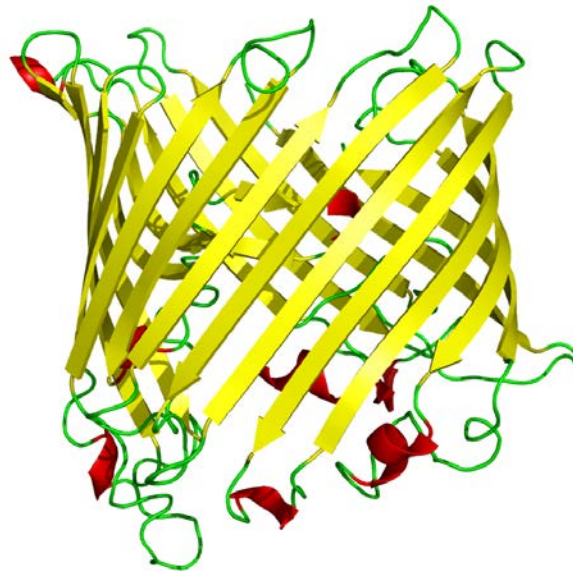
Blue: Positive charge: "salty"

# Challenge: Protein Folding Problem

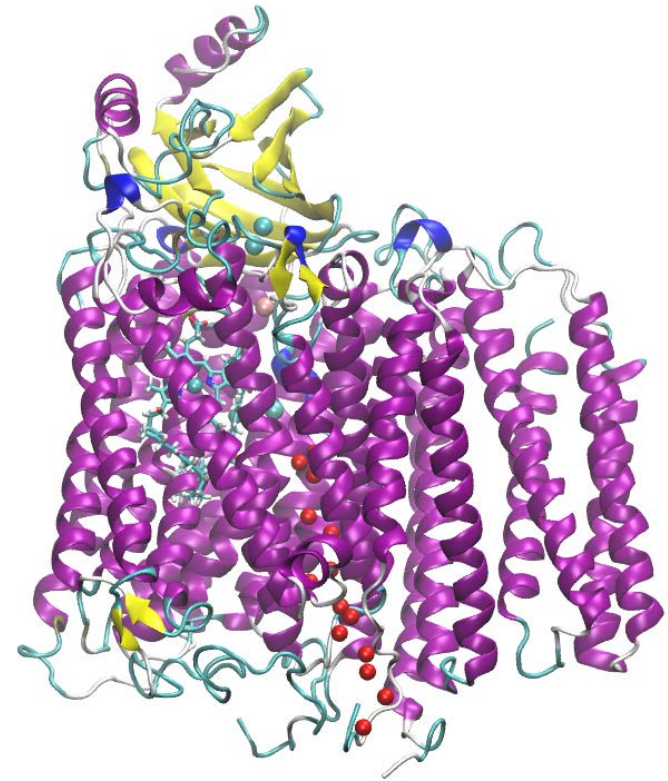
Given the amino acid sequence, can you predict the natural folded structure?



**Lysozyme**



**Porin**



**Cytochrome c Oxidase**

Video clip: Protein folding

<https://www.youtube.com/watch?v=gFcp2Xpd29I>

# Designing new molecules: for better materials, better medicines

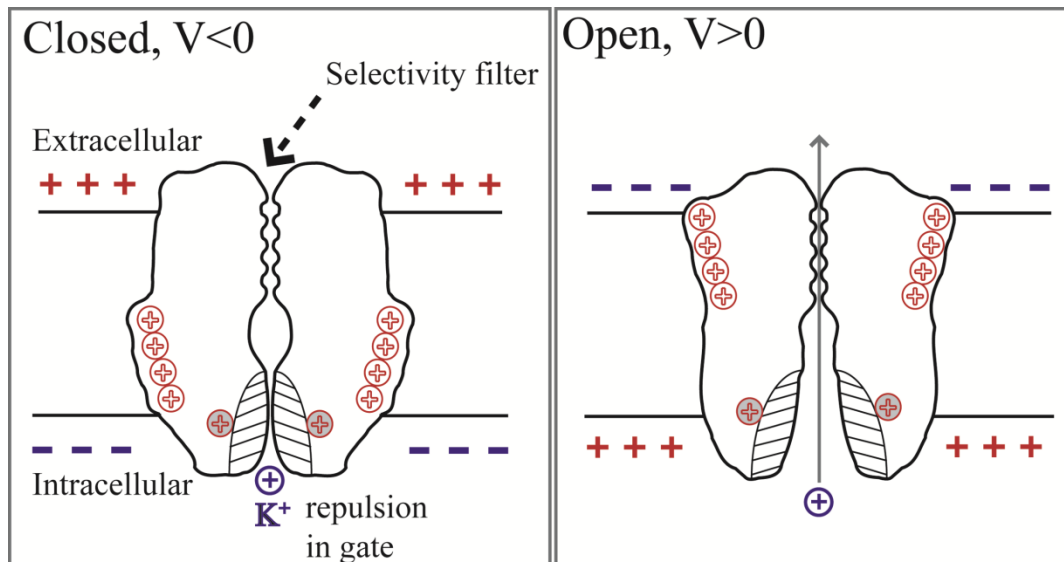
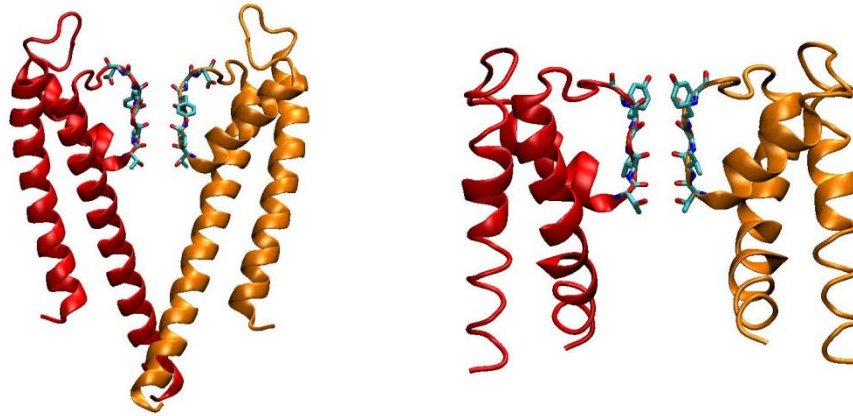
How does your medicines (drug!) work? Let's look into the "moleculoscope": MD movie

**Watch at home:** A basic introduction to drugs, drug targets, and molecular interactions

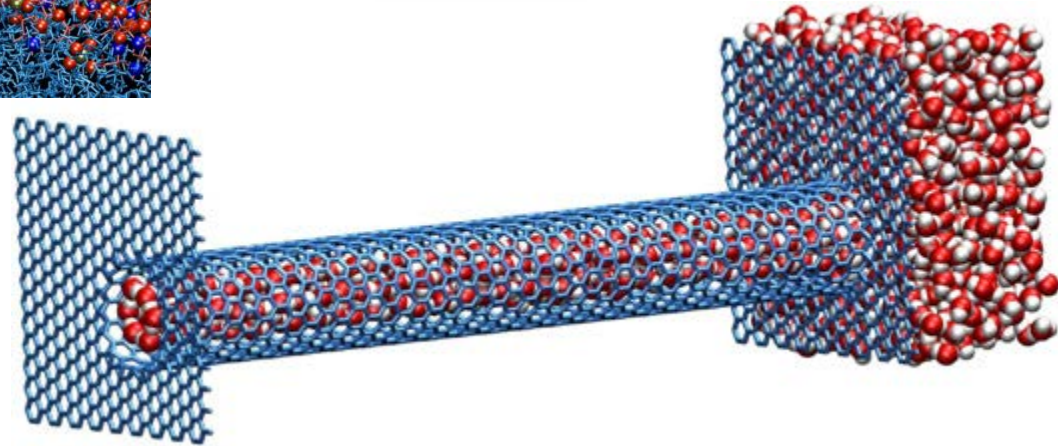
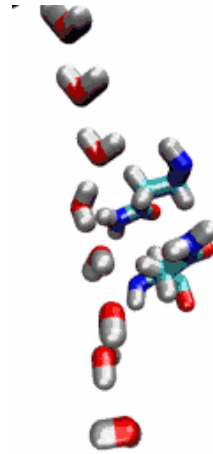
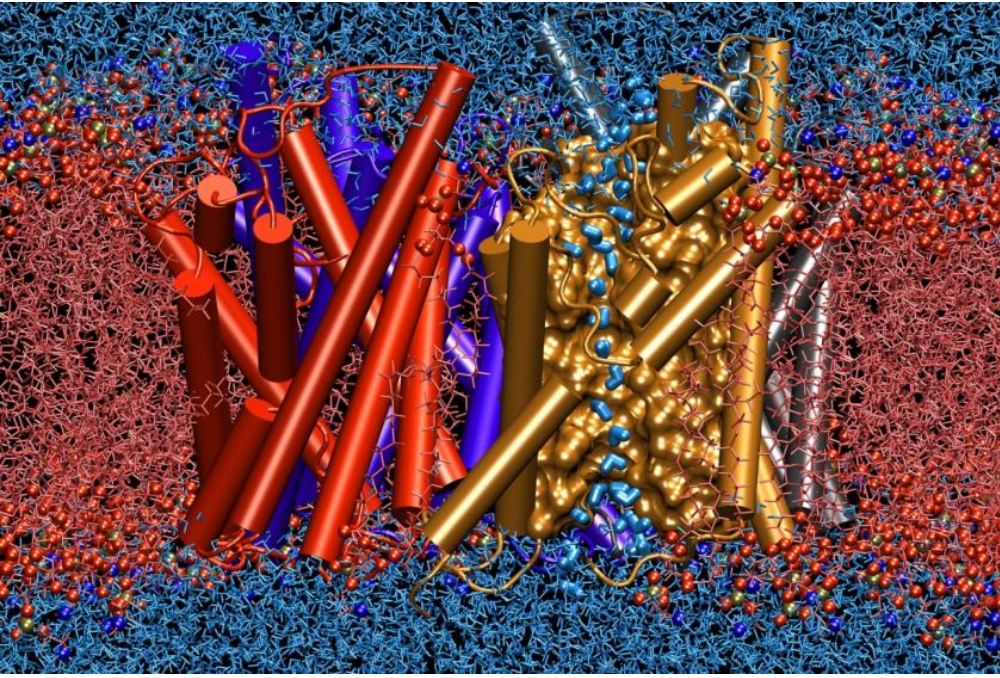
<https://www.youtube.com/watch?v=u49k72rUdyc>



# Voltage gated ion channels: How these things work?



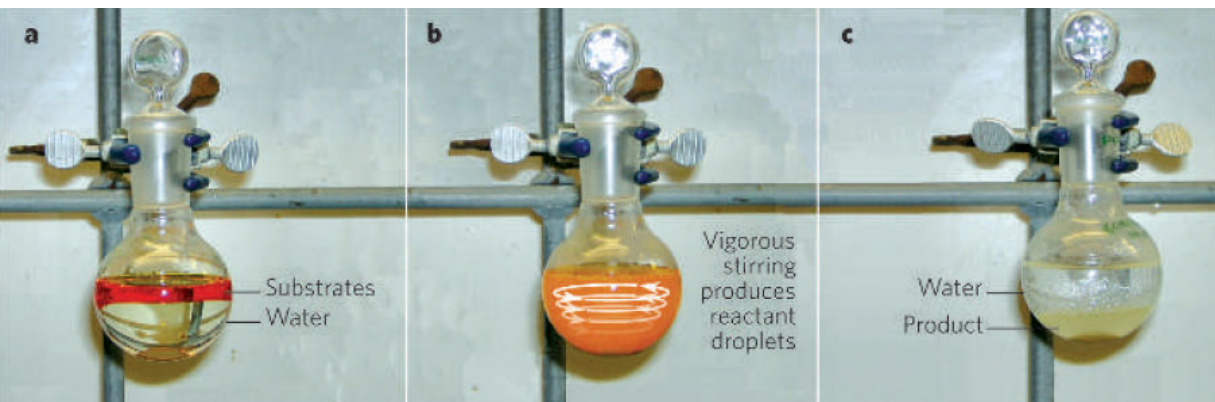
# Aquaporin: A molecular sieve



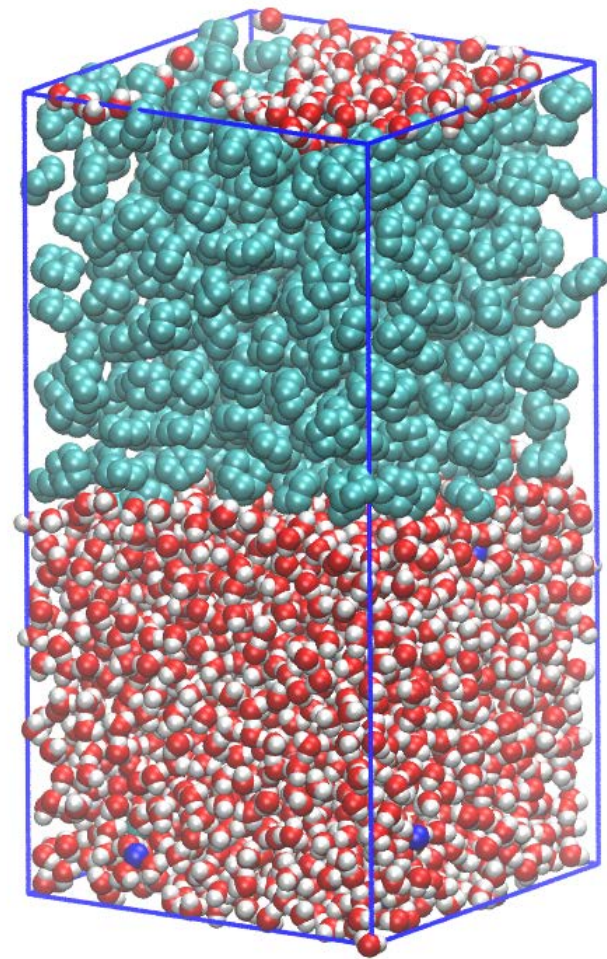
➤ Can we learn from aquaporins: The ultimate water purifier?



# “on water” reactions



Certain reactions happen many times faster at the oil-water surface!





# ❑ Advantages of computer simulation:

- ✓ “Moleculoscope”: Molecular microscope to see their real-time motion
- ✓ Molecular view of nature connected to properties/functions
- ✓ Full control over molecular interactions and how they affect properties
- ✓ Setting up (or even execution) of “computer experiments” is easier and faster compared to labwork!
- ✓ Acceleration of rare events

# ❑ Who can take the challenge?

- ✓ **Jack of all trades:** Chemistry, Physics, Mathematics, Biology, Computer Programming, Visualization ...
- ✓ Love to play with computers (not just for Facebook!)
- ✓ Play with molecules and control them; **Play God!**
- ✓ Don't just follow textbooks, **question/extend them;**  
Don't just follow, **lead/innovate!**

[... a final video clip!](#)



# The Nobel Prize in Chemistry 2013



**Martin Karplus**  
Université de Strasbourg,  
France and Harvard  
University, Cambridge,  
MA, USA



**Michael Levitt**  
Stanford University School of  
Medicine, CA, USA



**Arieh Warshel**  
University of Southern  
California, Los Angeles, CA,  
USA

**“for the development of multi-scale models for complex chemical systems”**

## **Martin Karplus (83)**

U.S. and Austrian citizen. Born 1930 in Vienna, Austria. Ph.D. 1953 from California Institute of Technology, CA, USA. Professor Conventionné, Université de Strasbourg, France and Theodore William Richards Professor of Chemistry, Emeritus, Harvard University, Cambridge, MA, USA.

## **Michael Levitt (66)**

U.S., British and Israeli citizen. Born 1947 in Pretoria, South Africa. Ph.D. 1971 from University of Cambridge, UK. Robert W. and Vivian K. Cahill Professor in Cancer Research, Stanford University School of Medicine, Stanford, CA, USA.

## **Arieh Warshel (73)**

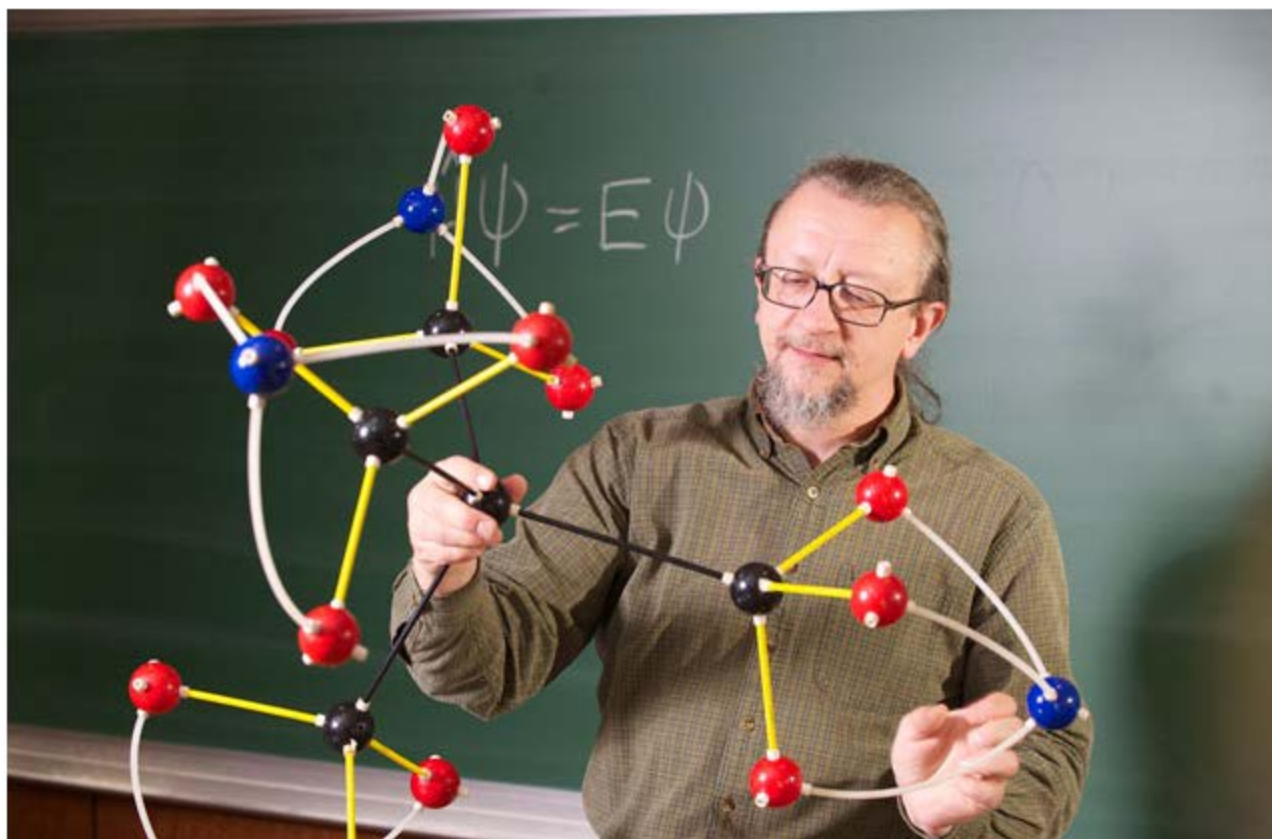
U.S. and Israeli citizen. Born 1940 in Kibbutz Sde-Nahum, Israel. Ph.D. 1969 from Weizmann Institute of Science, Rehovot, Israel. Distinguished Professor, University of Southern California, Los Angeles, CA, USA.

# Professor Publishes 10-year-old's New Molecule

Jan 25, 2012

For Clara Lazen, 10, a classroom assignment turned into a scientific finding. As Chemistry Professor Robert Zoellner confirmed, the fifth-grader's curiosity led to a new molecule, and her first mention in a scientific journal.

When Kenneth Boehr instructed his fifth grade class at Border Star Montessori School in Kansas City, Mo. to build molecules with modeling kits, he didn't expect one of his students to make a scientific discovery.





“Computers are incredibly fast, accurate and stupid. Human beings are incredibly slow, inaccurate and brilliant. Together they are powerful beyond imagination.”

Happy computing! 😊

*Caveat: Garbage in, garbage out!*

# Questions?

**Email: [s.chakrabarty@ncl.res.in](mailto:s.chakrabarty@ncl.res.in)**

**Web: [www.namusite.com](http://www.namusite.com)**