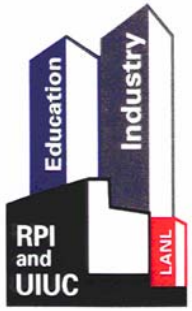


Molecular Modeling and Simulation: Opportunities for Research, Education, and Outreach

Shekhar Garde, Linda S. Schadler,

and Richard W. Siegel

Chemical & Biological Engineering & Materials Science & Engg.

Nanoscale Science and Engineering Center for Directed Assembly of Nanostructures

Rensselaer Polytechnic Institute.

2nd US-Korea Forum

on Nanotechnology, Los Angeles, CA.

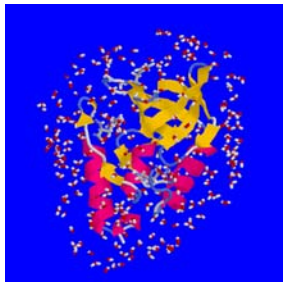
February, 17-18, 2005

Biological Systems

- Protein Folding/stability
- Peptide Folding/structure
- Bioinformatics
- Biomaterials (enzymes in novel media)
- Mechanistic Studies (intein splicing)

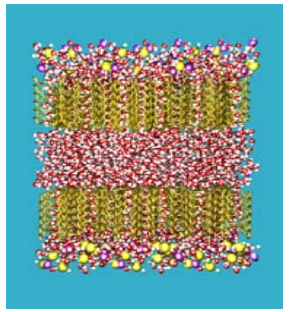
Water & aqueous solutions

- Liquid state theory
- Water structure near stuff
- Water-mediated interactions



Statistical Mechanics
Molecular Simulations
Experiments (collaboration)

Garde Group@ RPI



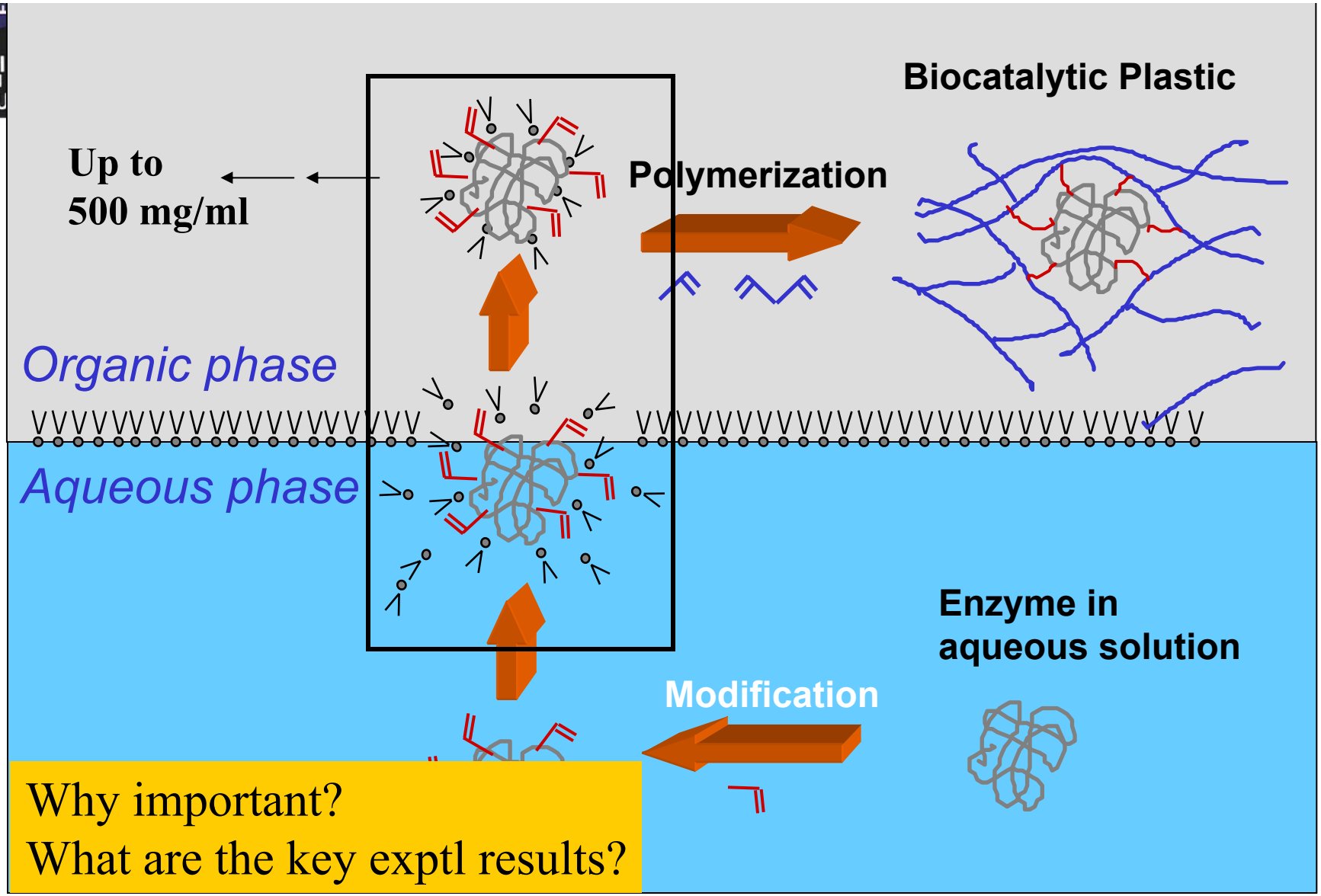
Polymers

- Coarse-graining strategies
- Phase behavior

Nanosystems

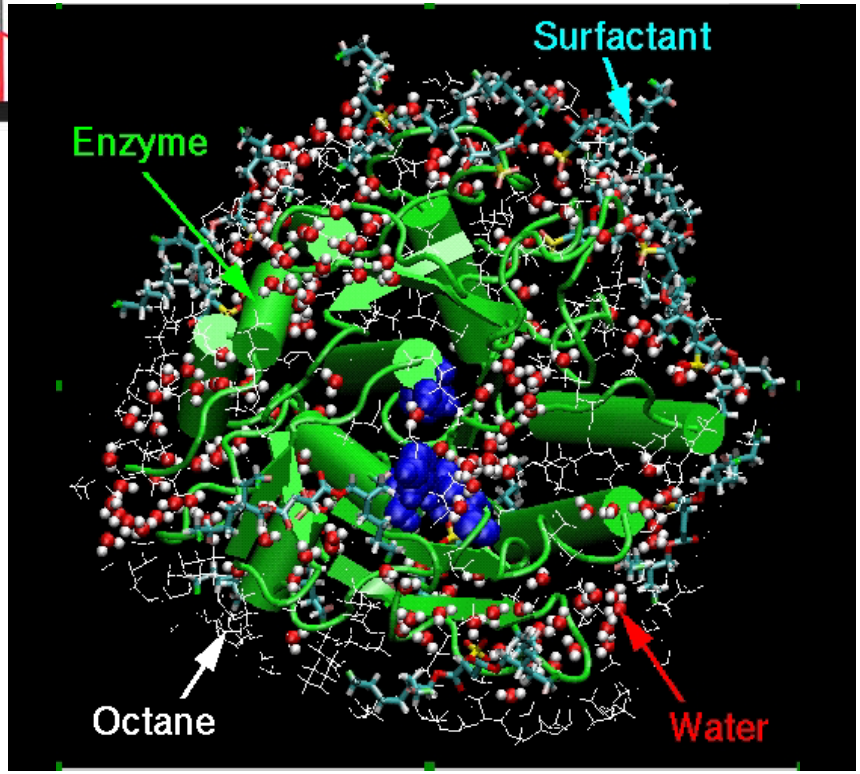
- Water flow through CNTs
- Selective partitioning into CNTs
- Friction at the nanoscale

Synthesis of Biocatalytic Plastic Materials



Why important?
What are the key exptl results?

Molecular Dynamics Simulations



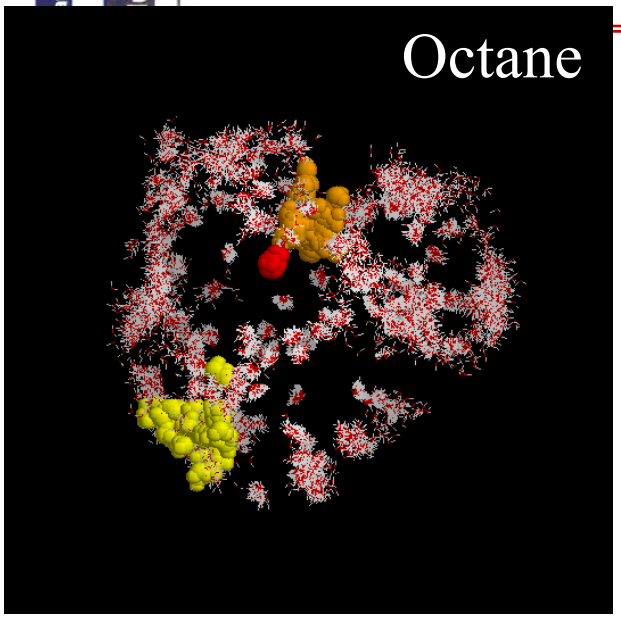
A snapshot from MD simulation in octane: subtilisin, water molecules, AOT, sodium ions, and octane molecules are shown.
Active site is shown in magenta

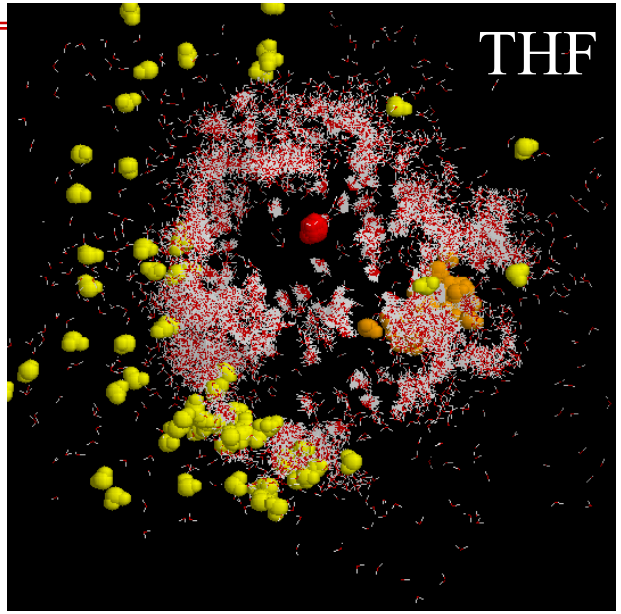
- **AMBER6.0**
- **Periodic Boundary Conditions**
- **Particle Mesh Ewald**
- **Equilibration 0.5 ns**
- **Production 5-8 ns**

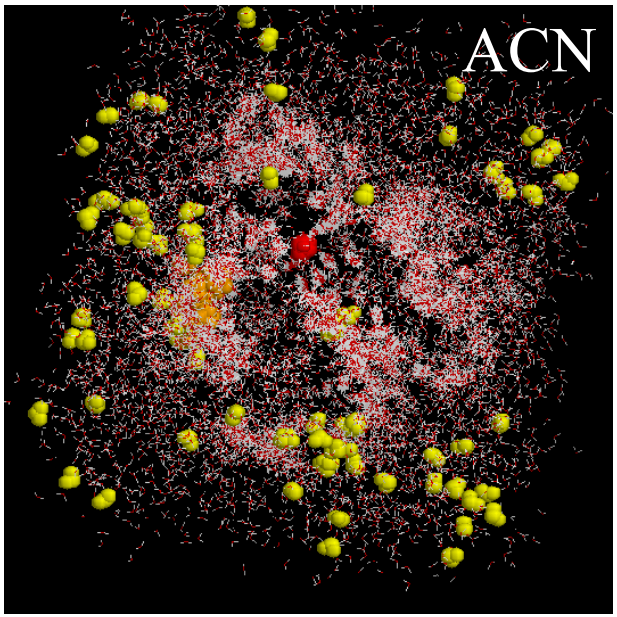
Systems	
Subtilisin	1
Water	186
Na+	11
AOT	13
Solvent	
Octane	949
THF	2074
Water	9580

Total ~33000 atoms

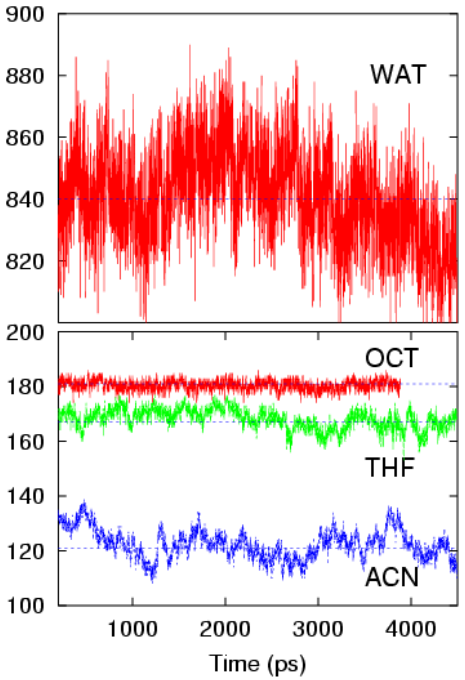
Water stripping from protein in different solvents







# of hydration waters



What is being shown?

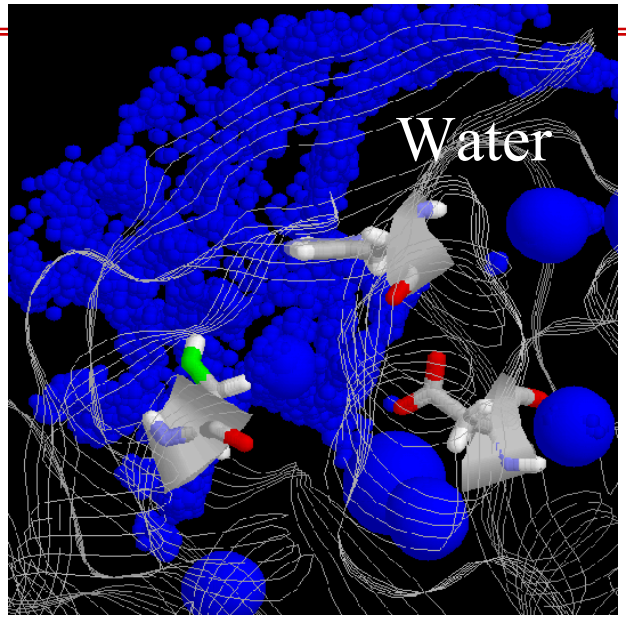
- **186 waters in every picture**
- **90 pictures are superimposed**

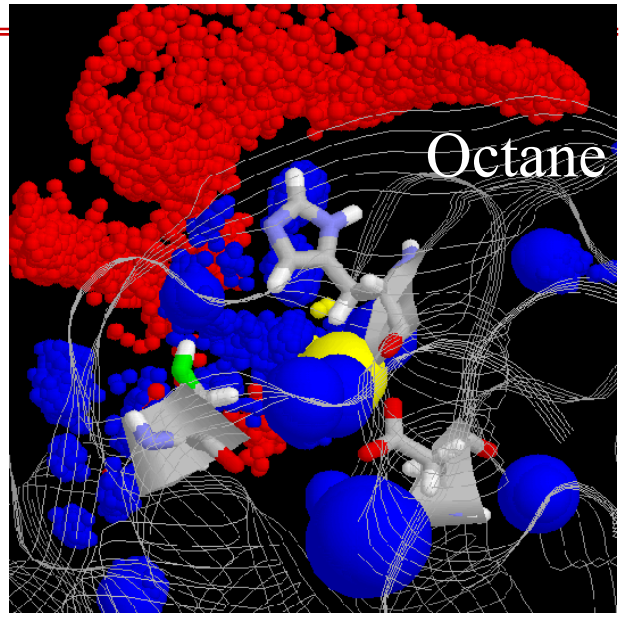
tightly bound | weakly bound | mobile

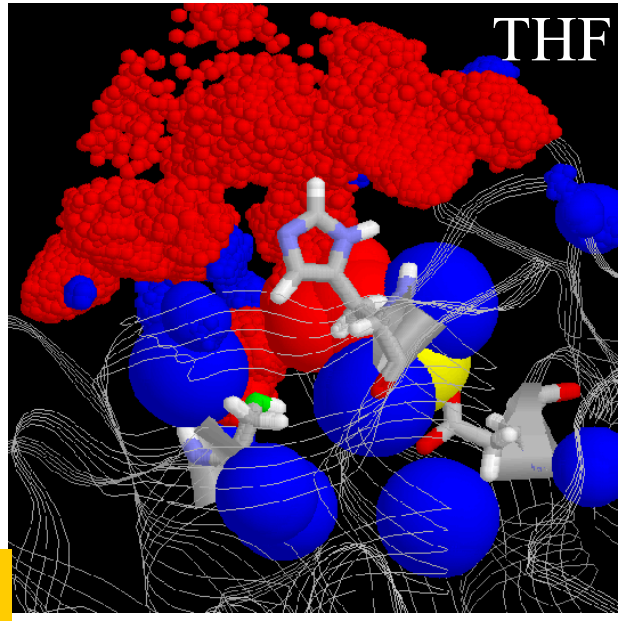
A closer look at the active site hydration

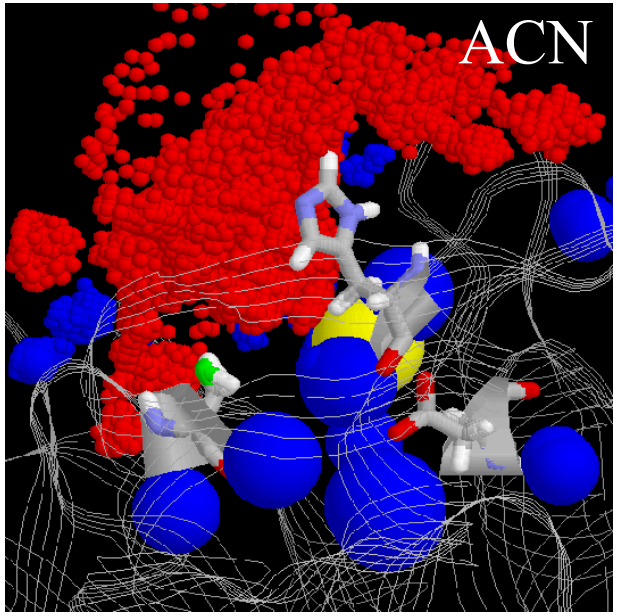
The well-hydrated active site in water and octane contains both mobile and tightly bound waters

THF and ACN penetrate the active site. Very little mobile water is observed









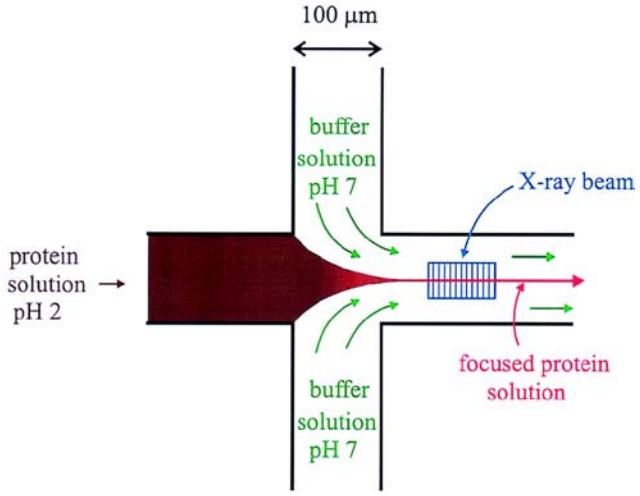
Biophys J. Aug, 2004.

Hydration of the active site of the enzyme by dynamic layer(s) of waters appears to be essential for its biological function.

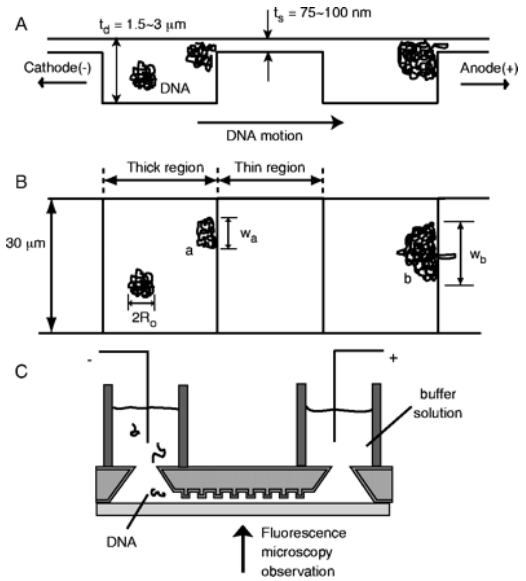
Motivation for studies of nanotubes and nanopores

- Mechanical and electrical properties
- Components in nanoscale devices
- Nanochannels for separations
- Confinement and protection of species or delivery
- Biomolecular nanopores as valves for selective transport

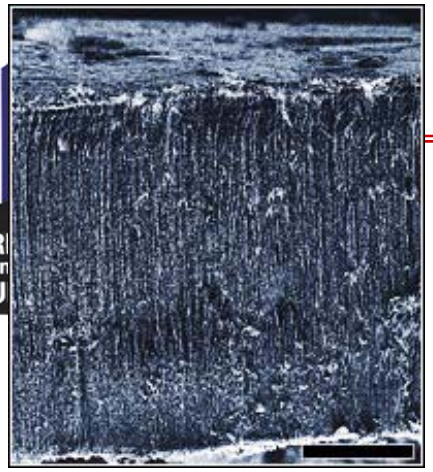
Micro / Nanofluidic devices



Austin and coworkers, PNAS (1999)



Han and Craighead, Science (2000)



http://www.rpi.edu/

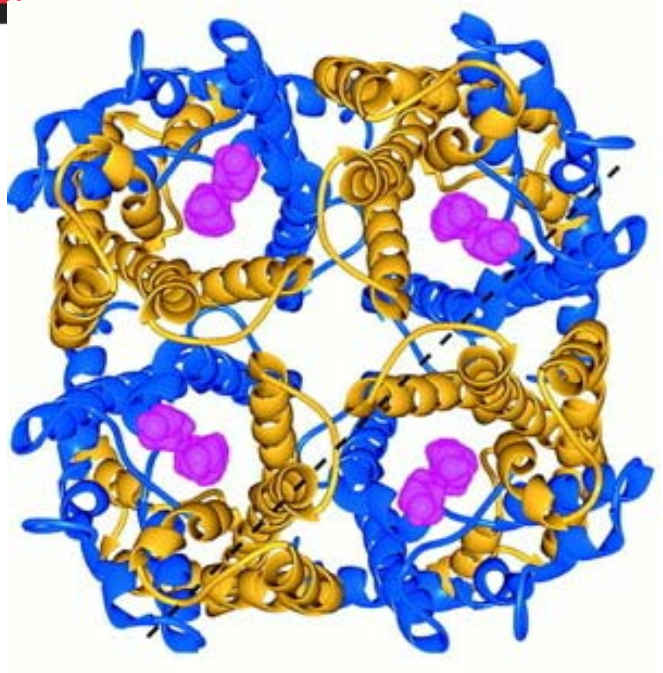
Efficient Filters Produced From Carbon Nanotubes Through Rensselaer Polytechnic Institute-Banaras Hindu University Collaborative Research

Filters remove nano-scale germs from water, heavy hydrocarbons from petroleum

TROY, N.Y. — Researchers at Rensselaer Polytechnic Institute and Banaras Hindu University (India) have devised a simple method to produce carbon nanotube filters that efficiently remove micro- to nano-scale contaminants from water and heavy hydrocarbons from petroleum. Made entirely of carbon nanotubes, the filters are easily manufactured using a novel method for controlling the cylindrical geometry of the structure.

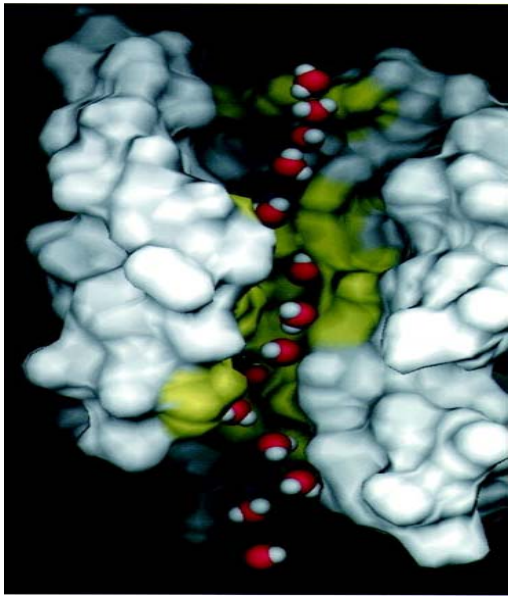
Membrane channel proteins: selectivity filters

Biological nanopores



Escherichia coli glycerol facilitator (GlpF)

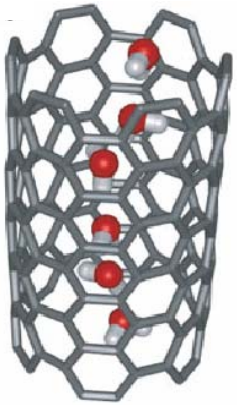
Fu et al., Science (2000)



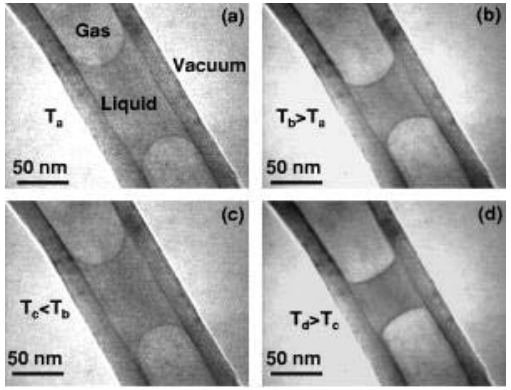
Water permeation across Aquaporin (AQP1)

de Groot and Grubmüller, Science (2001)

Carbon nanotubes as fluid channels?



Water inside nanotubes



Water conduction through a hydrophobic channel of a nanotube

Hummer et al., Nature (2001)

In situ multiphase fluid experiments in hydrothermal carbon nanotubes

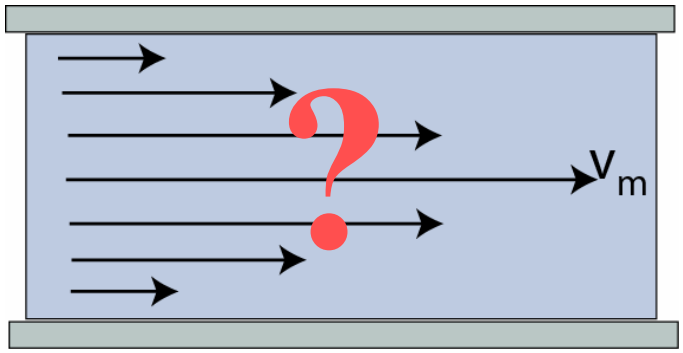
Gogotsi et al., APL (2001)

Fundamental questions

Transport

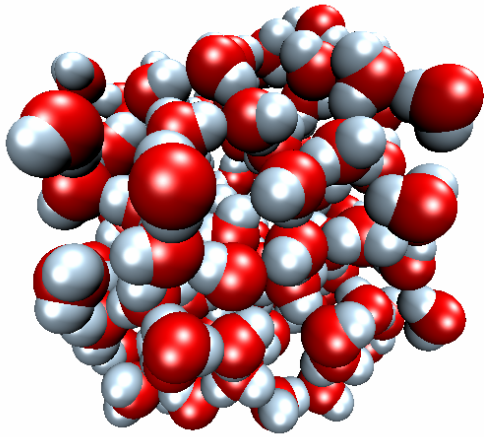
-- Can water flow through open ended CNTs?

-- How can we describe the flow?

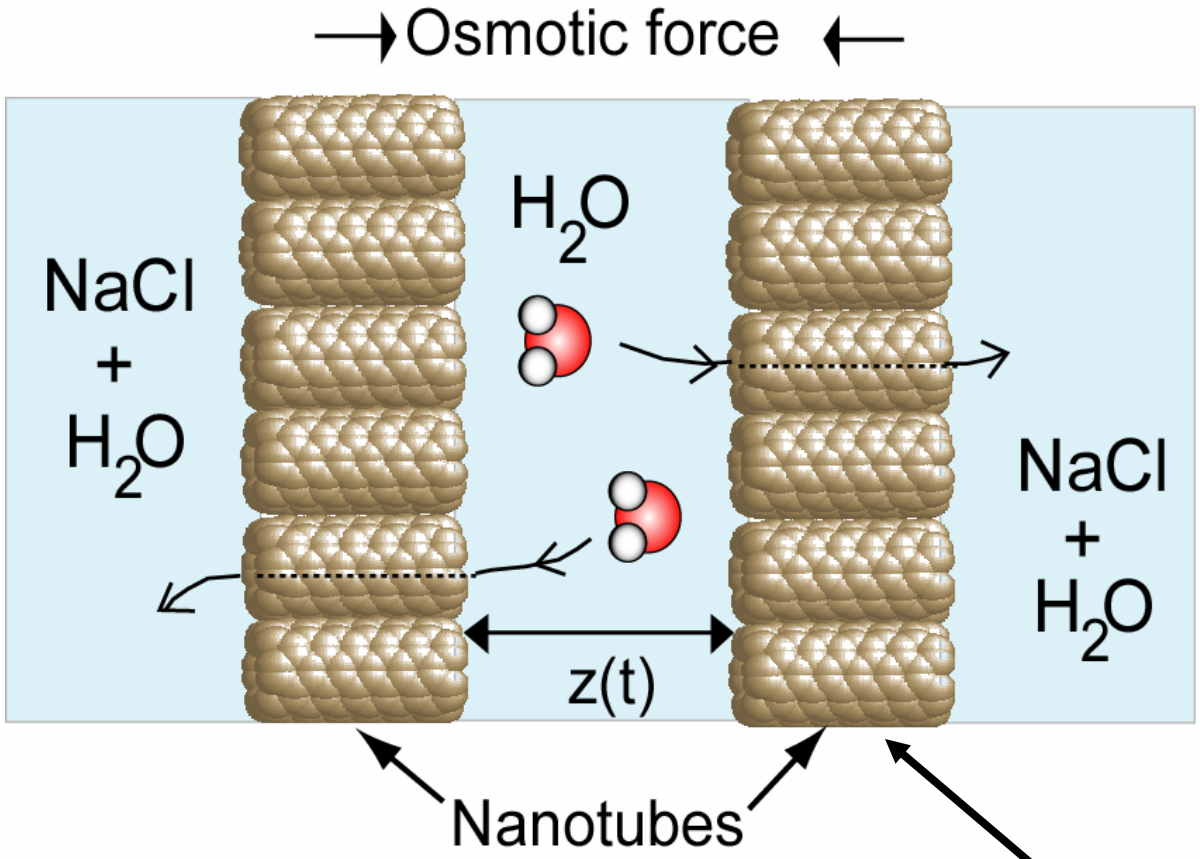


Structure/dynamics

-- What is the effect of confinement on molecular structure and dynamics of water ?



Molecular dynamics simulations

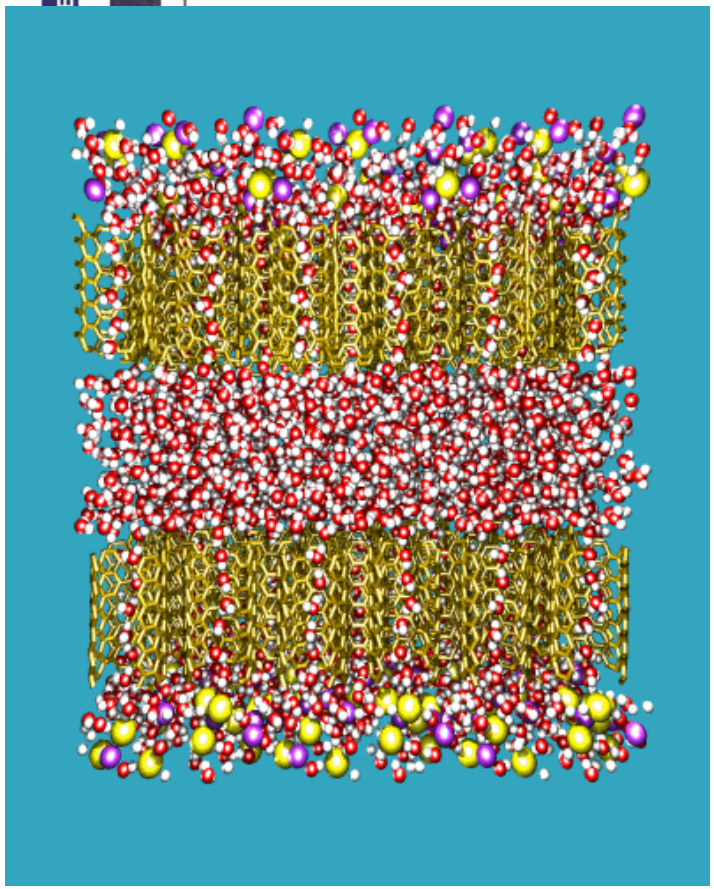


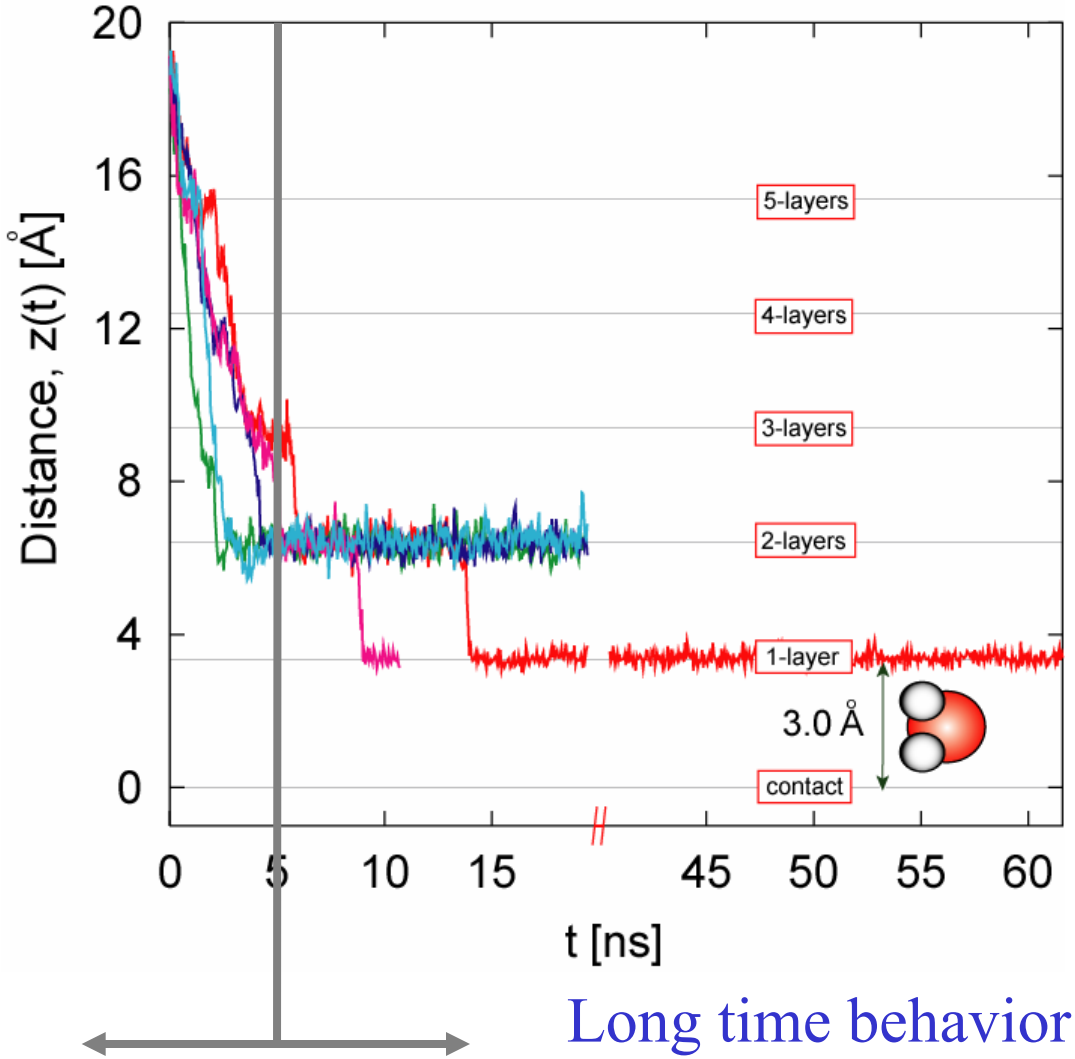
Osmotic pressure difference between pure water and aqueous salt chambers drives water flow

CNT (6,6)
Length = 13.4 Å
Diameter = 8.1 Å

Kalra et al. PNAS 2003.

Water flow through CNT membranes

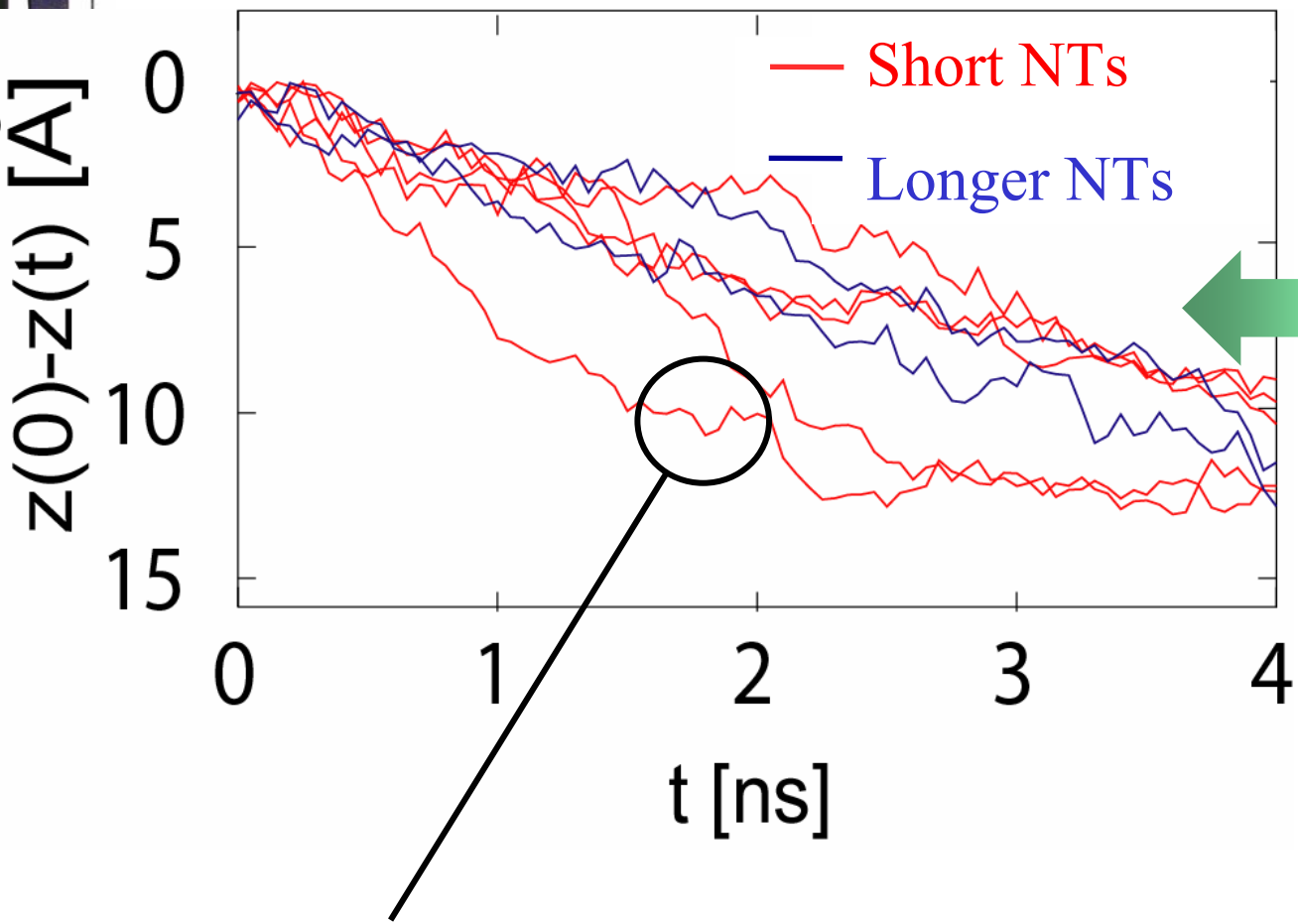




Short time behavior
(water flow can be monitored)

Long time behavior
(interrupted flow)
Study effects of confinement

Signatures of water flow through "small" short pipes



Flow = 5-8 #/ns

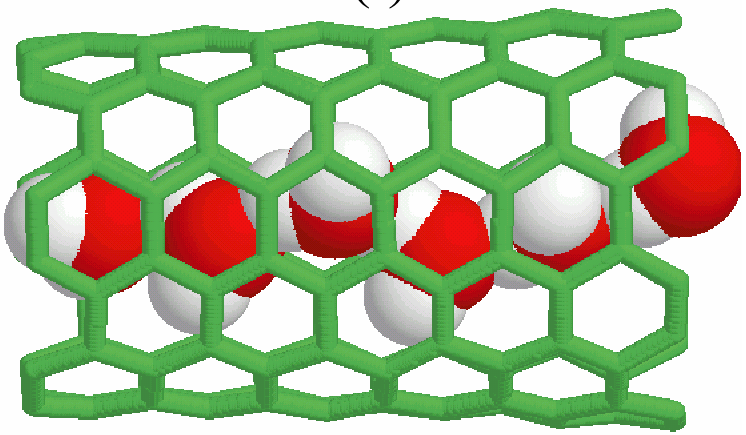
Thermal fluctuations lead to frequent back flow against the driving force

Flow rates are independent of the length of the NTs (13.4Å – 45Å)

Modeling stochastic nature of water flow

Net flow

$\Delta N(t)$



NaCl + H_2O

H_2O

k - hopping frequency (# of hops per unit time)

Average net flow

$\overline{\Delta N(t)} = k\,t\,(p-q)$

Variance

$\sigma\,(\Delta N(t)) = kt$

- Water chain remains intact
- Flow occurs by hopping forward/backward

p q

Continuous time random walk model

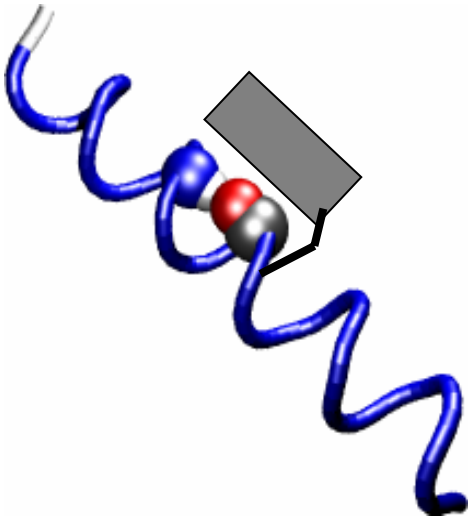
$P[\Delta N(t) = n] = \exp(-kt)(p/q)^{n/2}\, I_n(2kt\, p^{1/2}\, q^{1/2})$

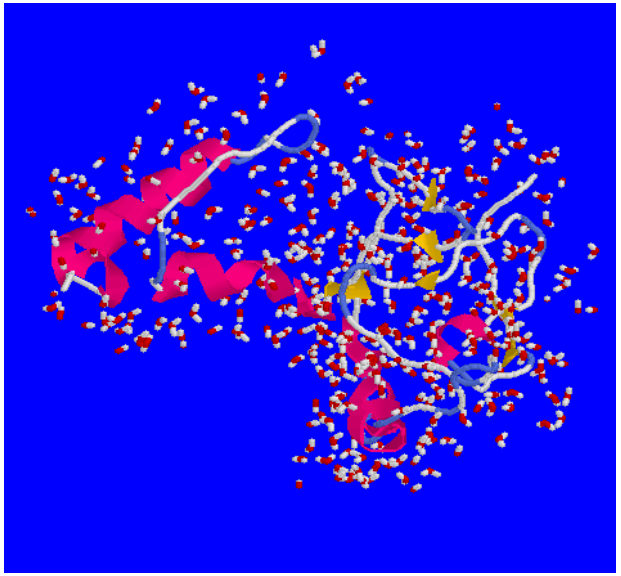
Summary (water flow through NTs)

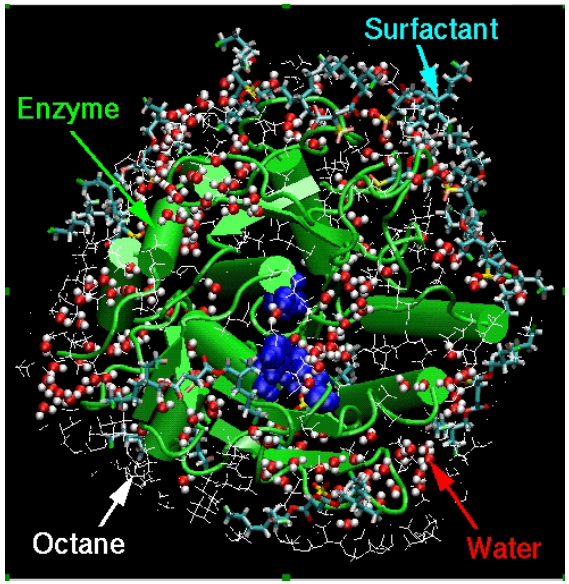
- Water flows through arrays of open-ended nanotubes with negligible friction
- Water transport is influenced by microscopic fluctuations and can be described by a one-dimensional continuous time random walk.
- The observed flow rates are comparable to those measured for biological water channels (aquaporin)*.
- Water can form remarkably (meta)stable one- and two-water thick sheets sandwiched between the membranes
- Carbon nanotubes can be used as channels for partitioning of molecular species

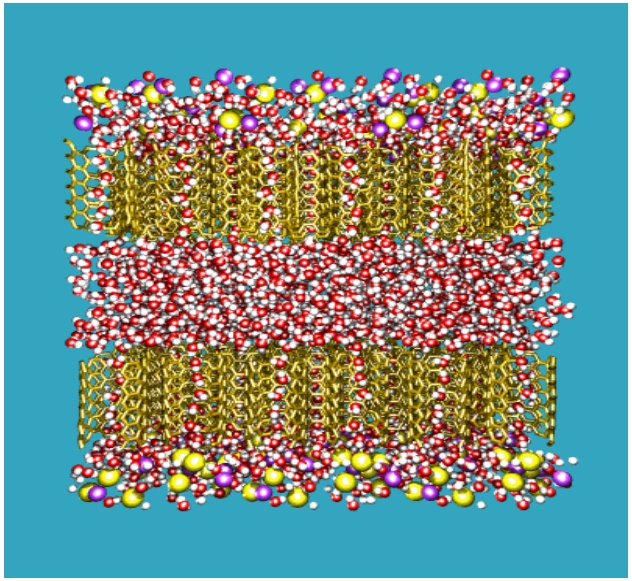
PNAS, 2003; JPCB, 2004.

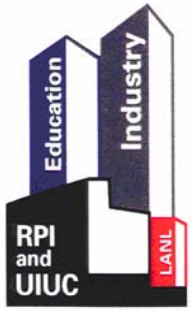
* Zeidel et al., *Biochemistry* **31**, 7436 (1992)






Surfactant
Enzyme
Octane
Water





- Molecular simulations provide fundamental understanding (as well as beautiful visuals!)

- Could we use them in a creative way to educate and excite children about Science and Engineering?

- Science awareness, education of the broader public is a critical need
  - -- science and technology is fast evolving
  - -- modern paradigm in science
    atoms, molecules → properties of materials

How do we reach children effectively?

Molecularium…

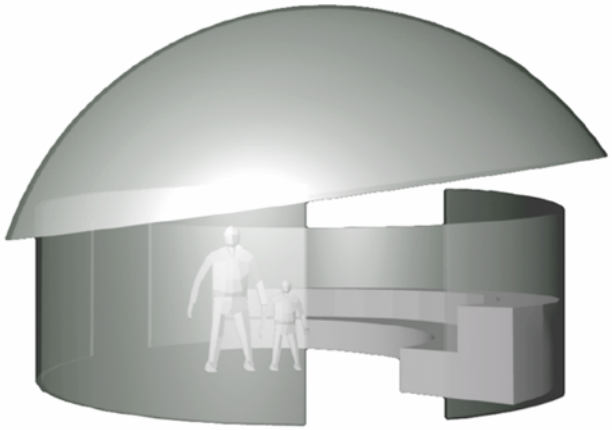
My own challenge

$$E_{total} = \sum_{bonds} K_r (r - r_{eq})^2 + \sum_{angles} K_\theta (\theta - \theta_{eq})^2 + \sum_{dihedrals} \frac{V_n}{2}[1 + \cos(n\phi - \gamma)] + \sum_{i<j} \left[\frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^{6}} + \frac{q_i q_j}{\varepsilon R_{ij}} \right]$$

?

The Molecularium at The Junior Museum of Troy

Goal: To introduce 5-10 year olds to the wonders of the molecular world, much the way that they've been learning about the wonders of the Solar System and Universe.



- Projector installed at Jr. Museum May 31.
- Tektraxadex hired - started Feb 1 part time / May 1 full time.
- Script finalized.
- Production has started.
- Applied to Dreyfuss Foundation to do a Spanish language version.
- IP agreements in place.

From pilot show to a professional show

1st Molecularium animation show

Meet the characters!

Hydro

Oxy

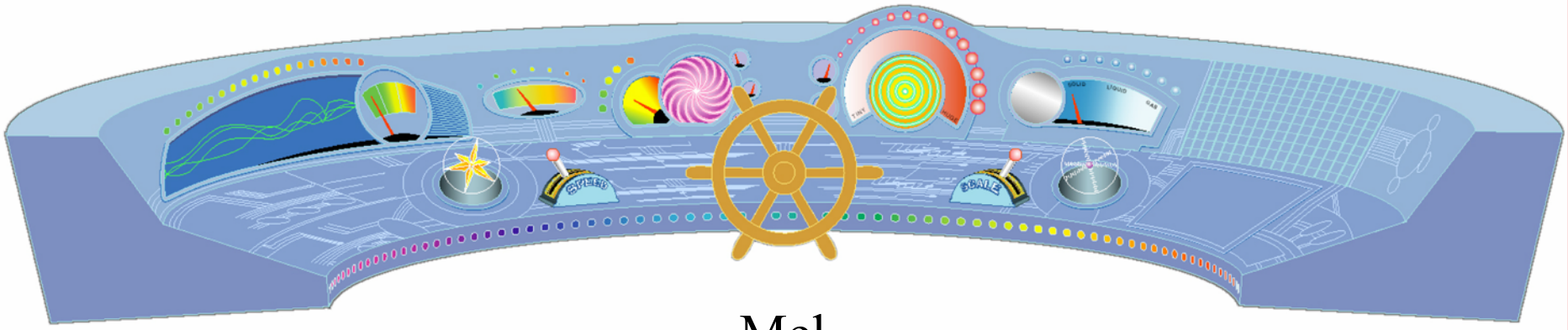
Hydra

Carbone

Trademarked images

The Molecularium - The Ship

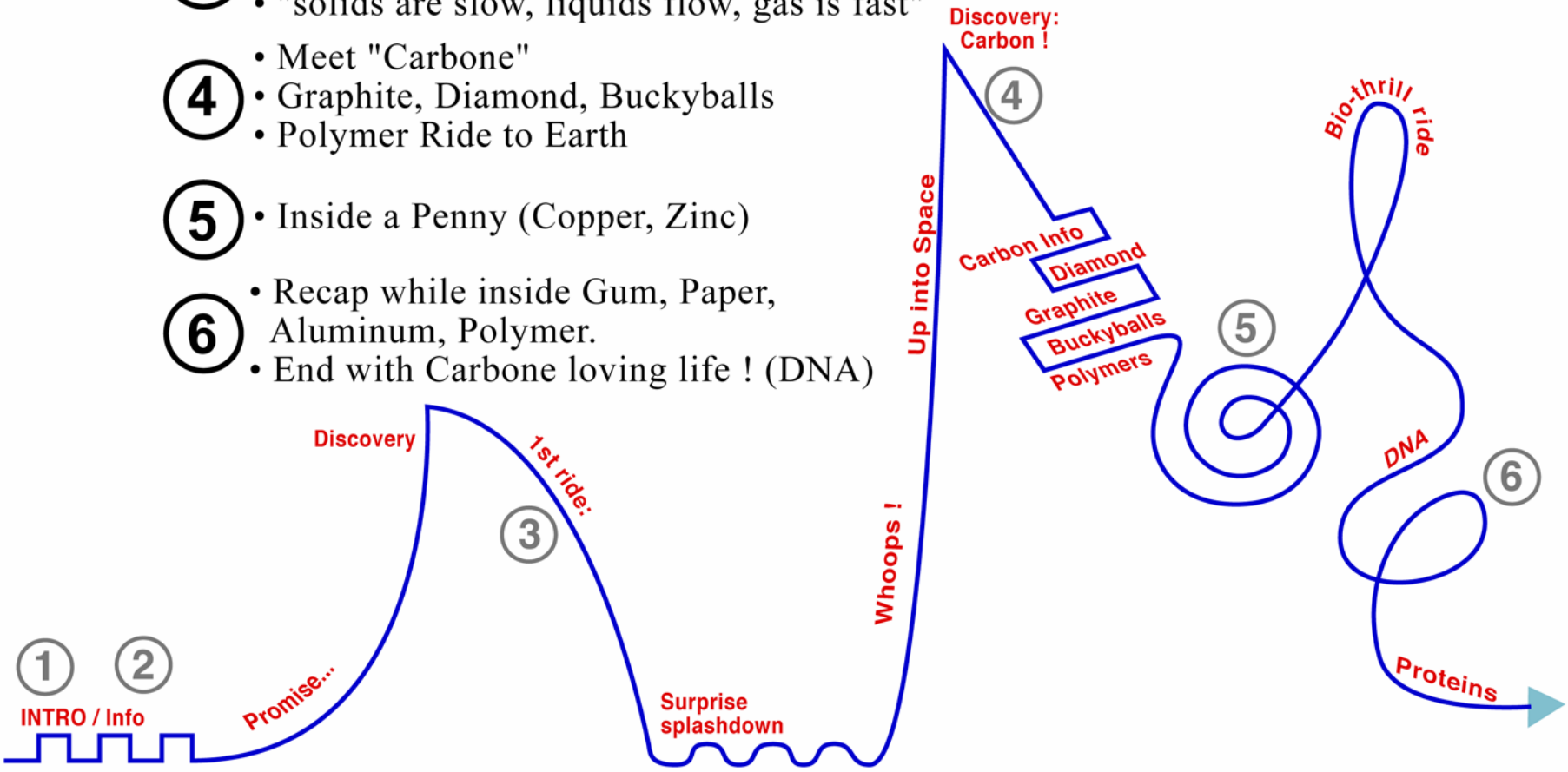
- "Fantastical" ship is a character named MEL.
- Can shrink to see molecules.
- Can change time to see molecular activity.
- Can travel super fast.
- Has multiple view screens to present ideas.



Mel

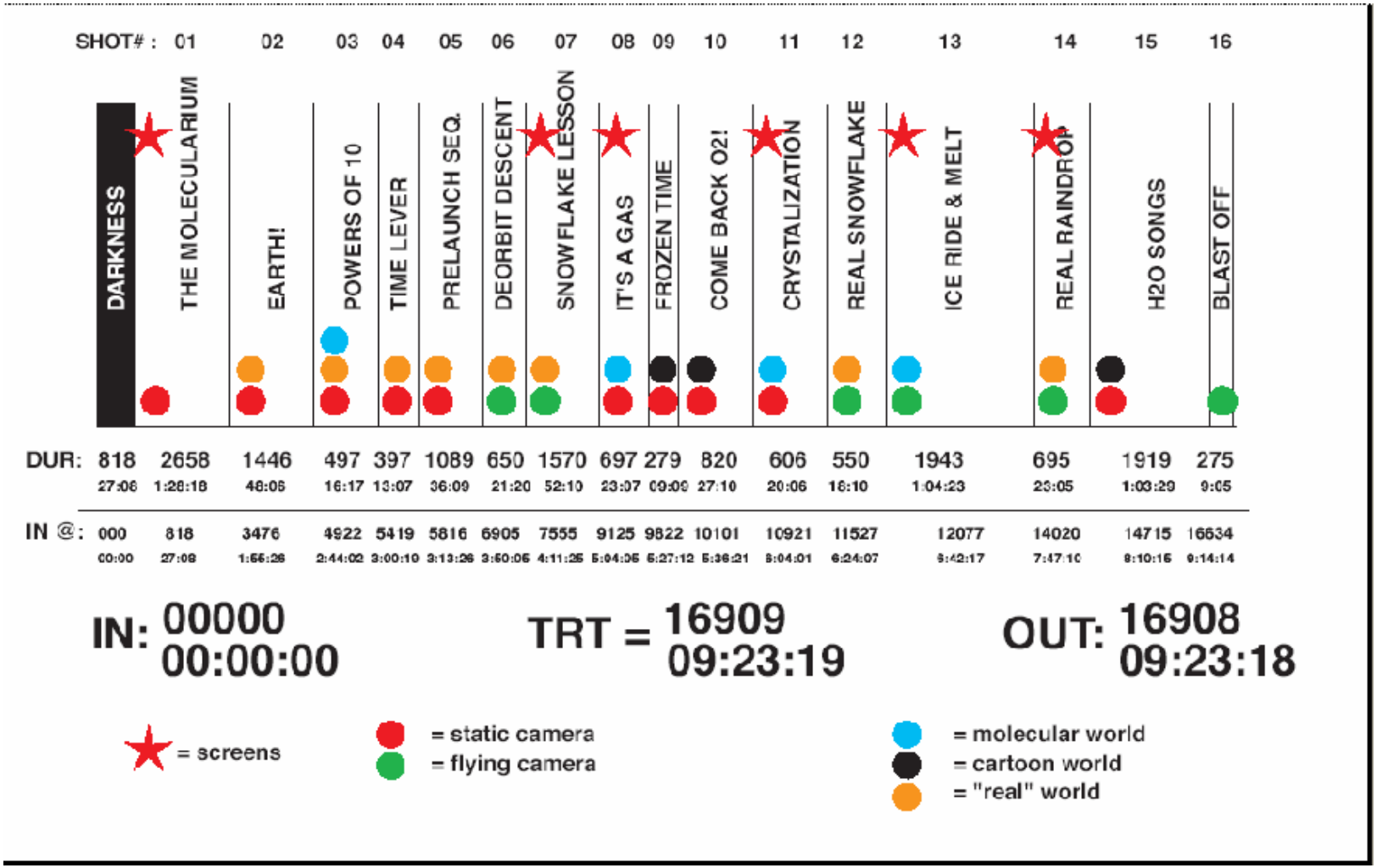
Molecularium: Riding Snowflakes

1. • Meet characters
   • Define Atoms & Molecules
   • Everything is made of Atoms & Molecules
2. • States of Matter
   • Cloud (vapor, rain, snowflake)
3. • Snowflake Ride
   • Melting
   • "solids are slow, liquids flow, gas is fast"
4. • Meet "Carbone"
   • Graphite, Diamond, Buckyballs
   • Polymer Ride to Earth
5. • Inside a Penny (Copper, Zinc)
6. • Recap while inside Gum, Paper, Aluminum, Polymer.
   • End with Carbone loving life ! (DNA)

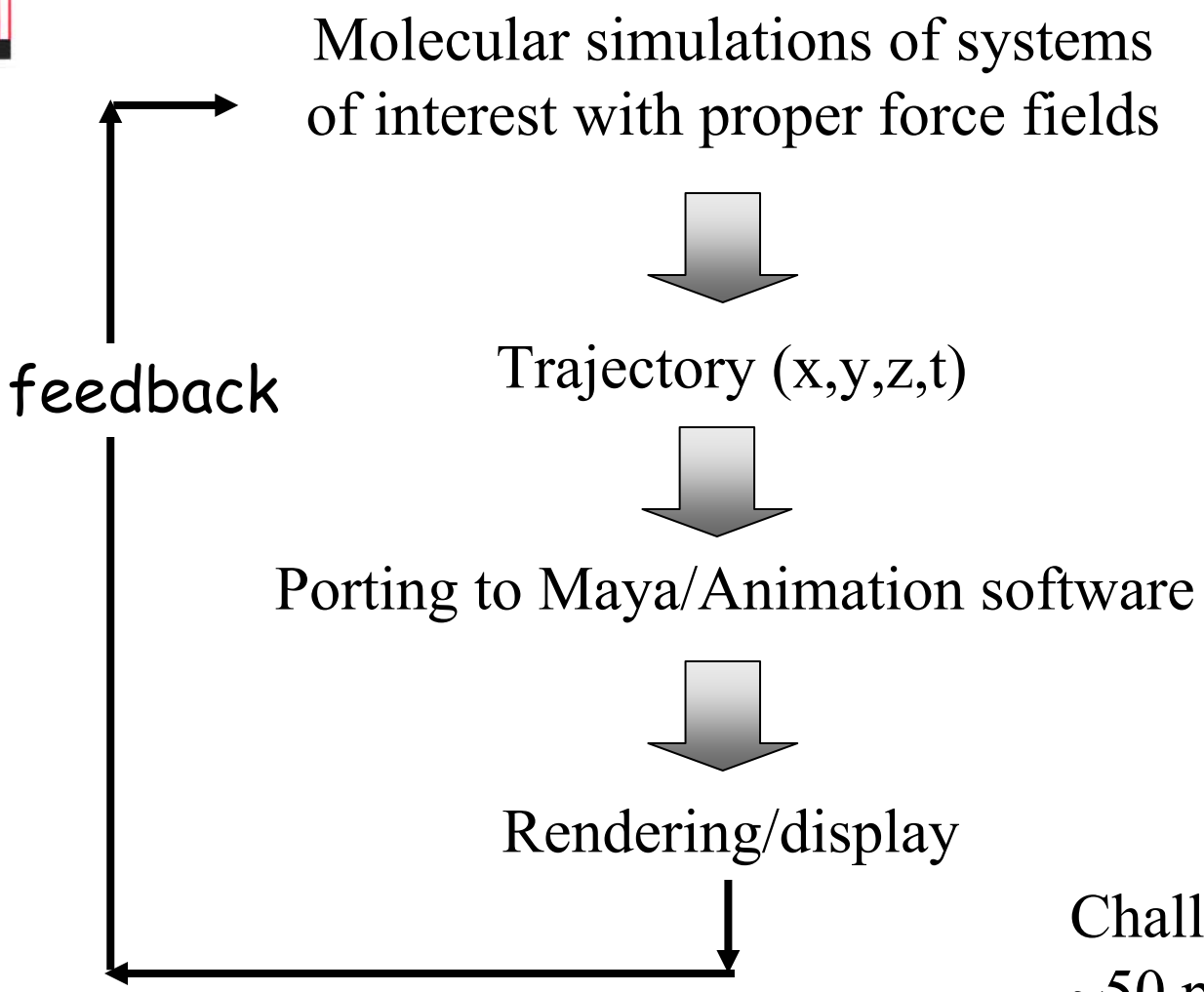


Opportunity for molecular simulation in Mollywood!

ACT-I



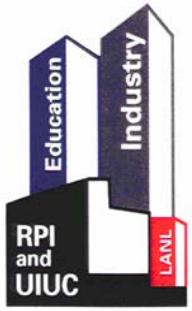
The process…. (partial)



Challenges?…Many!!
~50 people

Administrative…(Schadler/Siegel)

The process…. (partial)



Molecular simulations of systems of interest with proper force fields

feedback

Trajectory (x,y,z,t)

Porting to Maya/Animation software

Rendering/display

Software/hardware infrastructure

How does one send MD coordinates to Maya? formats, representations, (spheres, ribbons, sticks) connectivity of atoms.

Art/visual: nonflatscreen rendering, colors, feel, flight paths, backgrounds, Interpolations.

Audio, visual etc.

Computational requirements

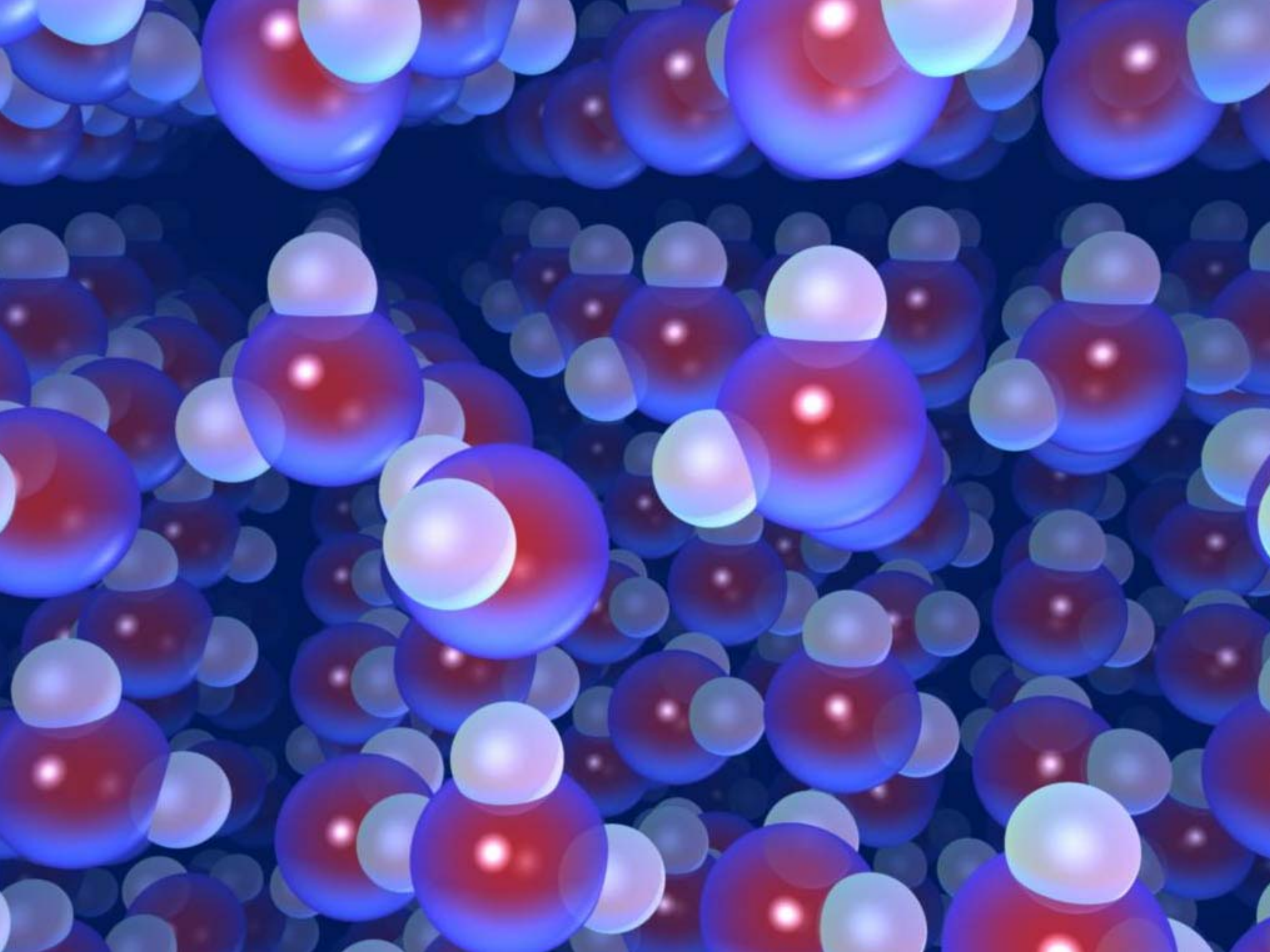
Molecular simulations

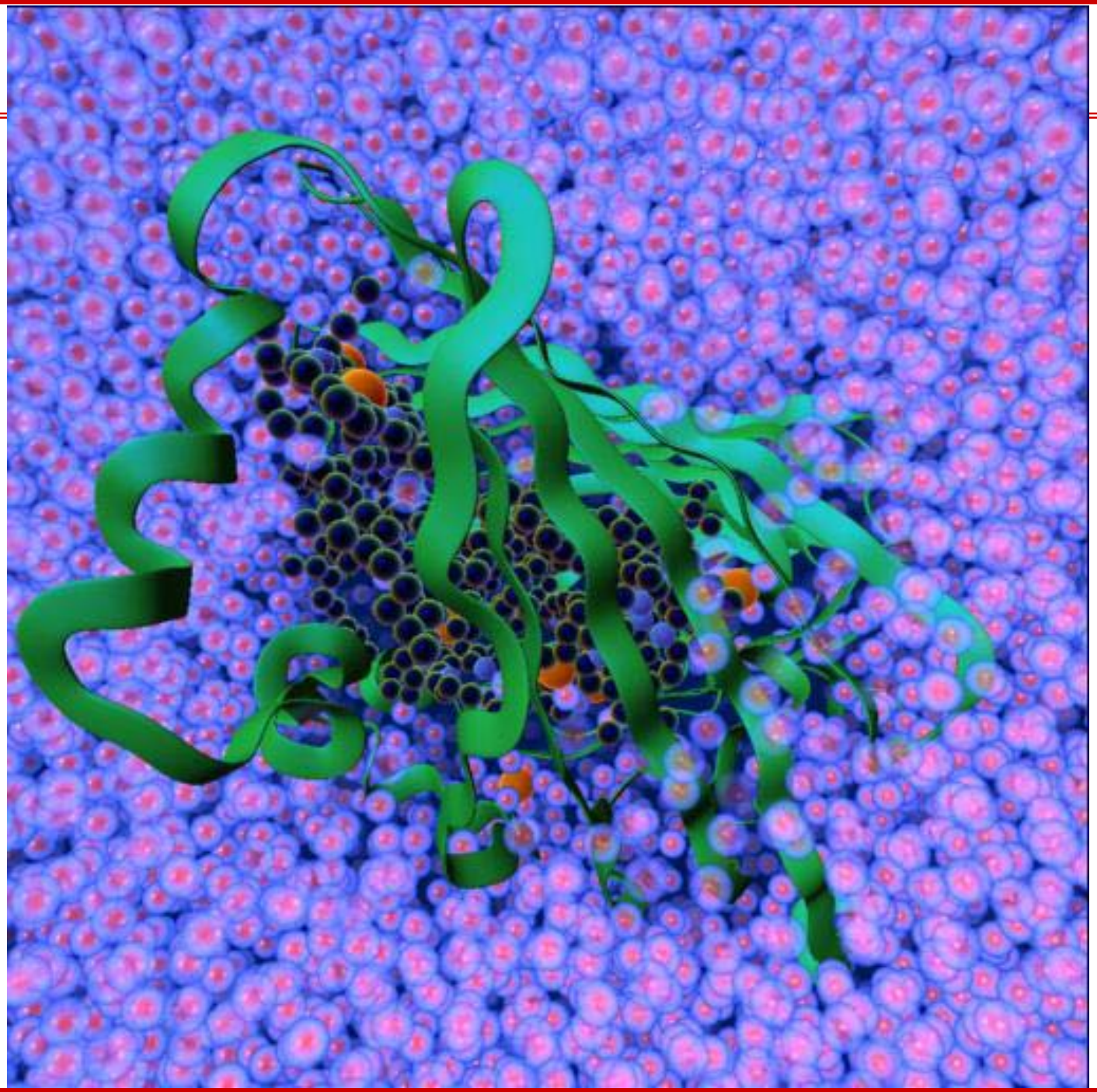
Rendering process

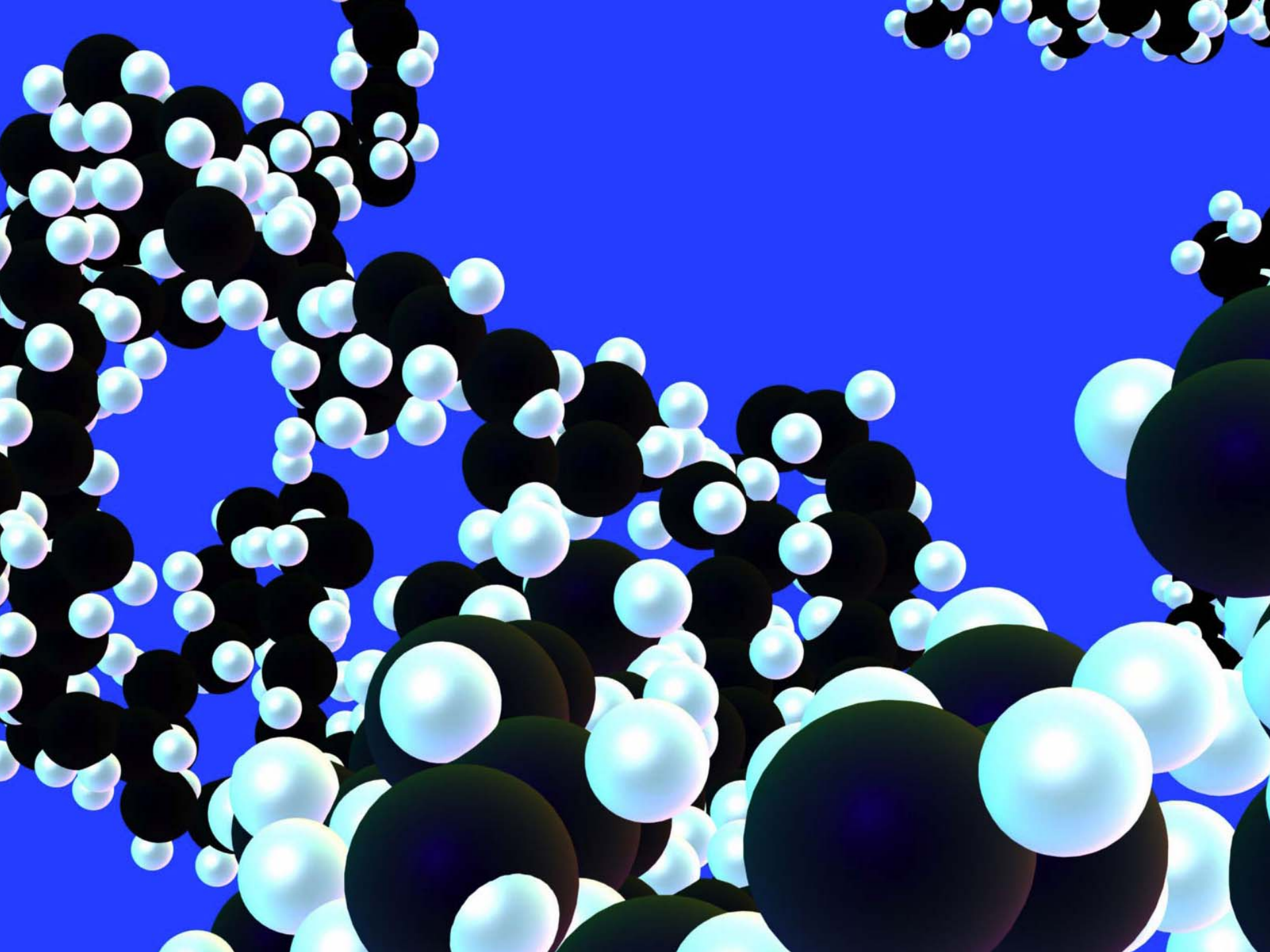
Large images (10-20MB/frame) ~30 frames/second

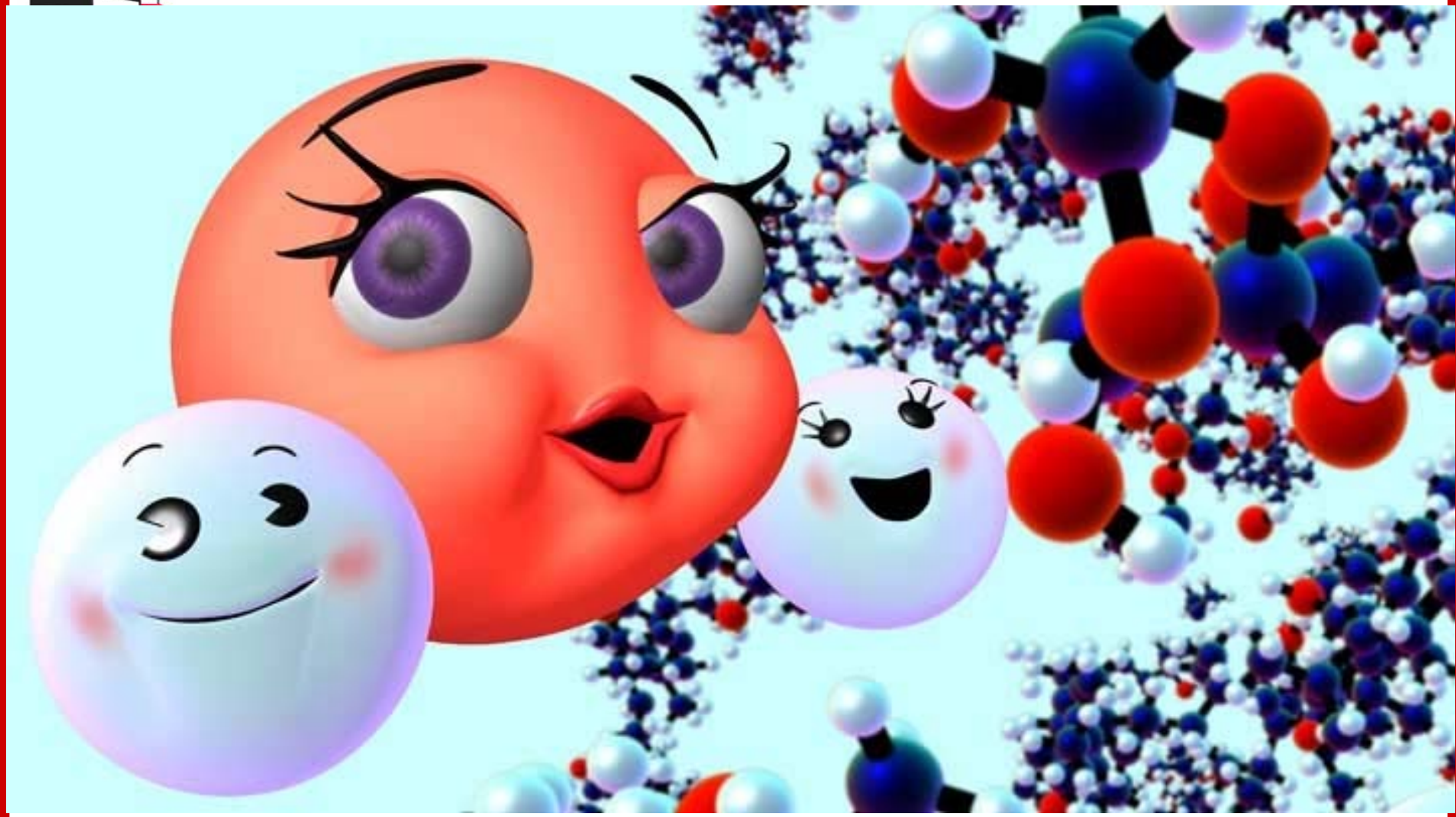
Each image can take 10-20 mins to render!

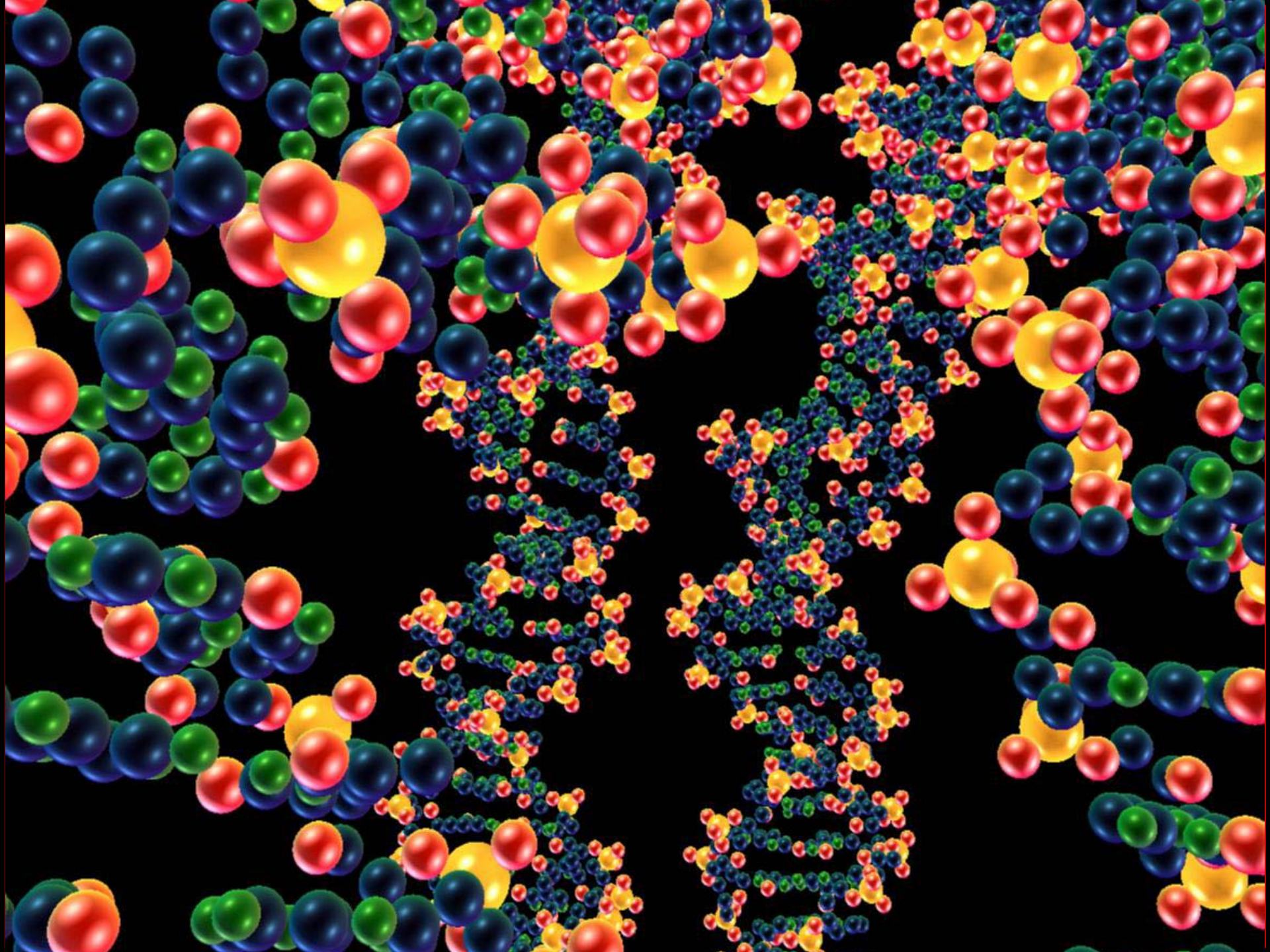
Needs a cluster...

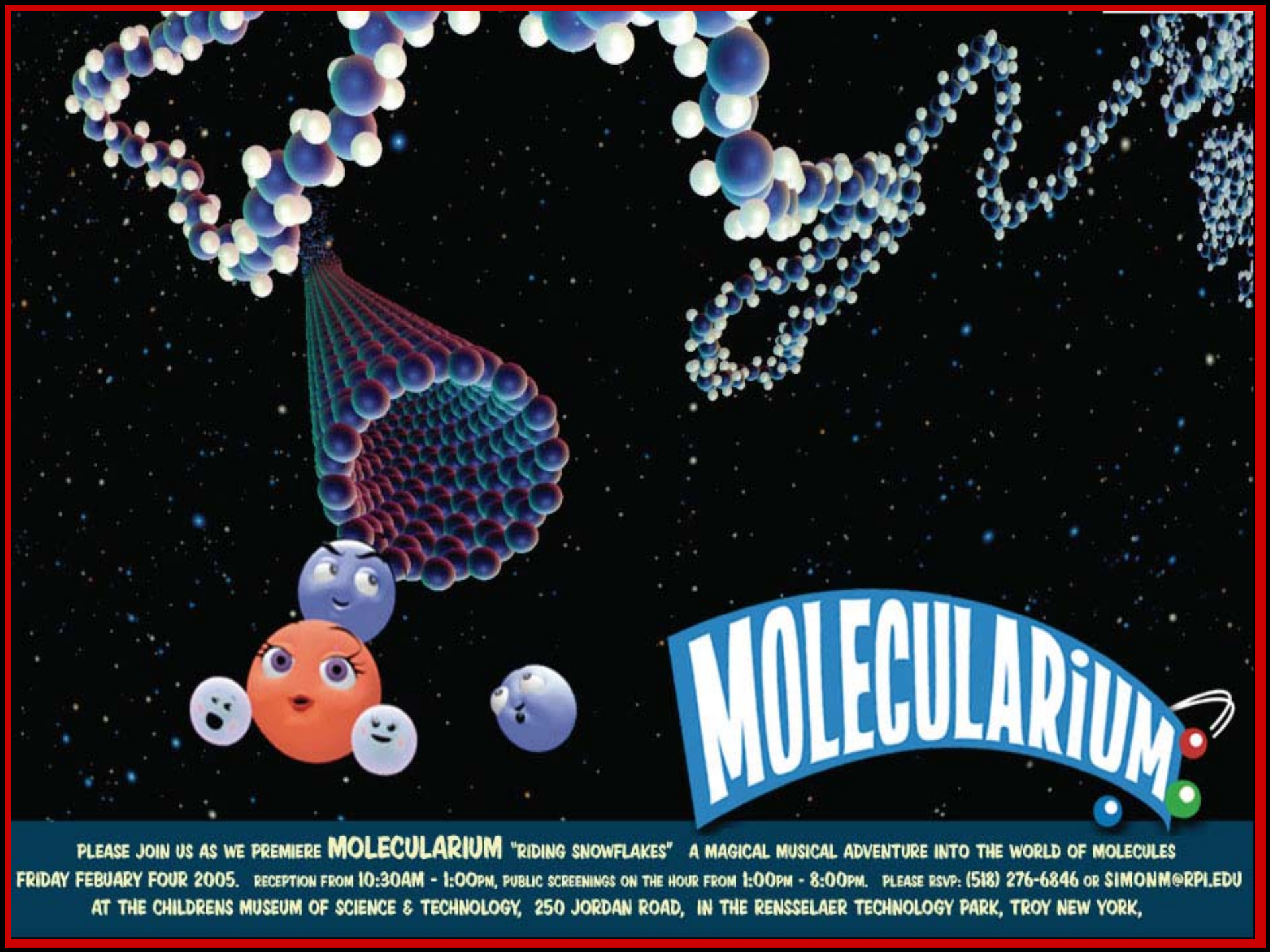



Education
Industry
RPI
and
UIUC
LANL







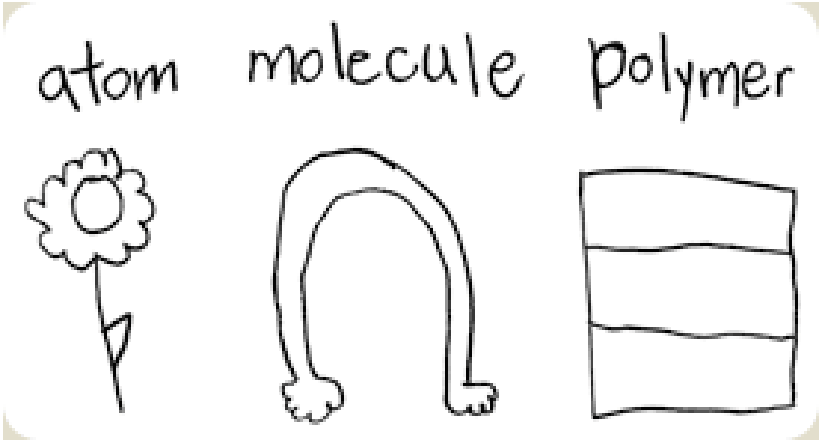


PLEASE JOIN US AS WE PREMIERE **MOLECULARIUM** "RIDING SNOWFLAKES" A MAGICAL MUSICAL ADVENTURE INTO THE WORLD OF MOLECULES
FRIDAY FEBUARY FOUR 2005. RECEPTION FROM 10:30AM - 1:00PM, PUBLIC SCREENINGS ON THE HOUR FROM 1:00PM - 8:00PM. PLEASE RSVP: (518) 276-6846 OR SIMONM@RPI.EDU
AT THE CHILDRENS MUSEUM OF SCIENCE & TECHNOLOGY, 250 JORDAN ROAD, IN THE RENSSELAER TECHNOLOGY PARK, TROY NEW YORK,

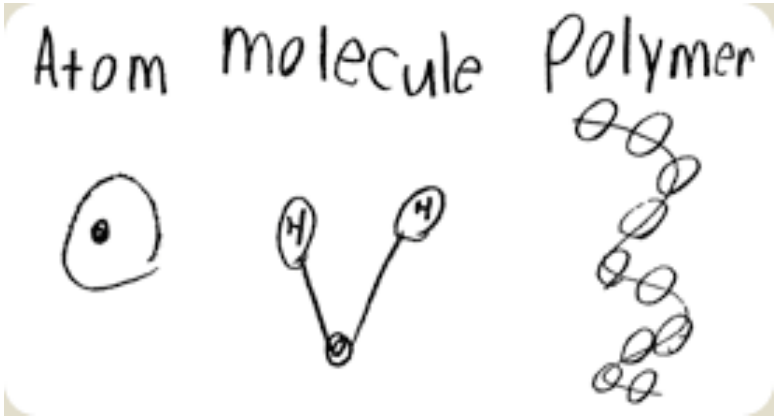
Assessment

Pilot show assessment

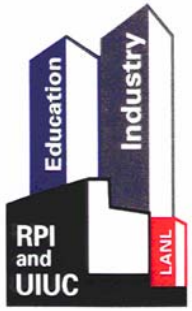
Before



After



- Assessment is being performed.
- Pre and post show activities emphasize the concepts learned during the show.



Future plans for the molecularium?

--- nationwide distribution (planetariums, school districts,..)

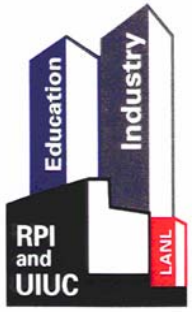
--- next show (biologically oriented)

Thoughts:

--- Introduction of molecular ideas early on to children actually works. We need to use the right tools.

--- incorporation of molecular concepts into undergraduate curriculum (texts? problem sets? Hard work!)

--- raising awareness of the general public about science and technology issues.



Acknowledgments

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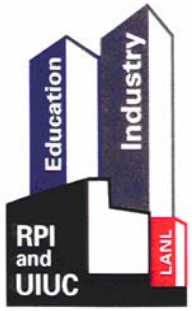
NIH



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Many UG students

http://www.molecularium.com
http://www.rpi.edu

See Materials Research Society Bulletin, Feb 2005

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Please see Prof. Chang Ryu's poster on other NSEC related education/outreach activities