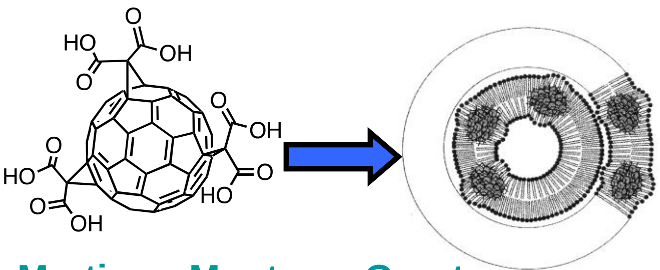
SAND2011-7430 C

Assembly and Reconfiguration of “Soft” Nanomaterials

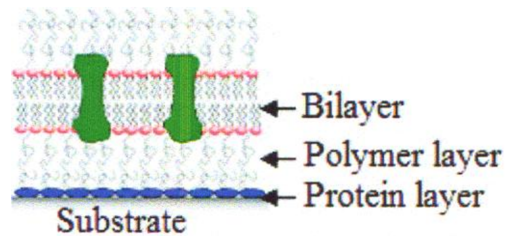
SAND2011-7430C

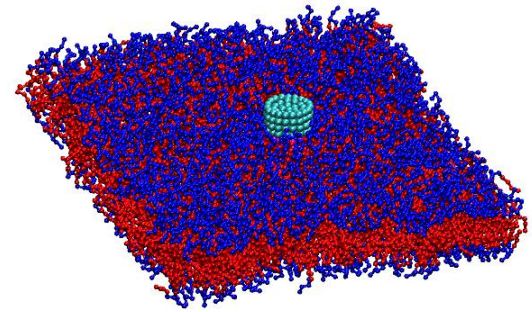
Bruce Bunker, Soft-Bio Thrust Area
The Center for Integrated Nanotechnologies (CINT)

Self-Assembly



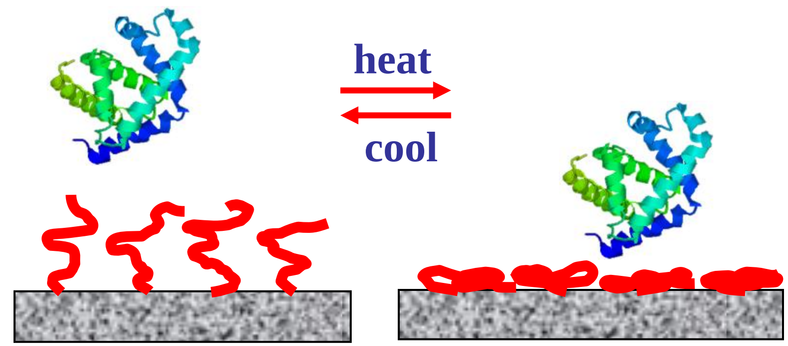
Martinez, Montano, Goertz





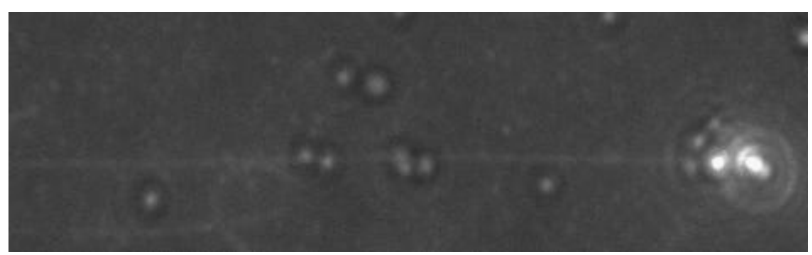
Stevens

Programmed Assembly



Huber

Active Assembly



Bachand, Liu, Spoerke

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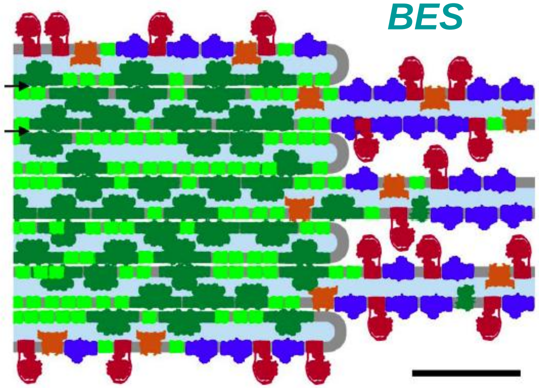
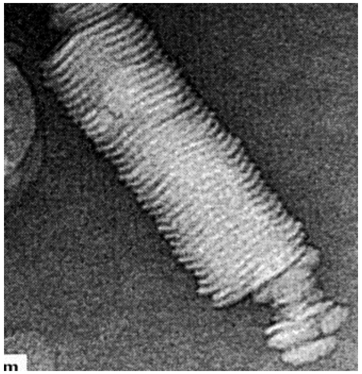
Potential Impact/Applications for Membrane Composites

Energy Systems

BES



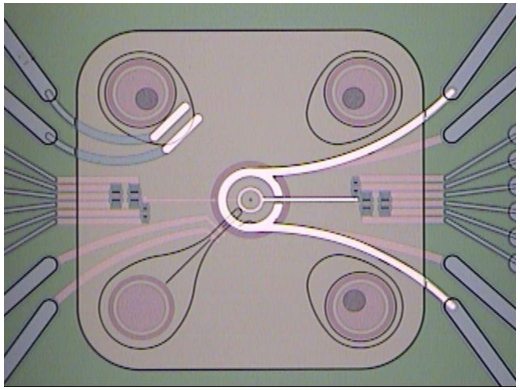
Darryl Sasaki



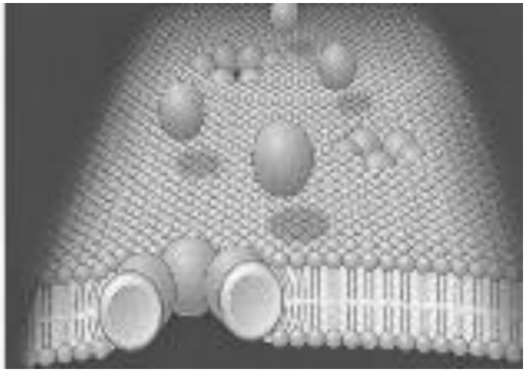
BES

Sensors

Intellegence



Membrane Composites



Murat Okandan

Homeland Defense

DTRA, LDRD

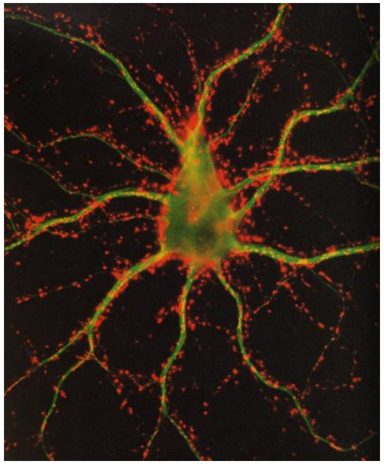
Nano-Toxicology

LDRD, BES, NIH

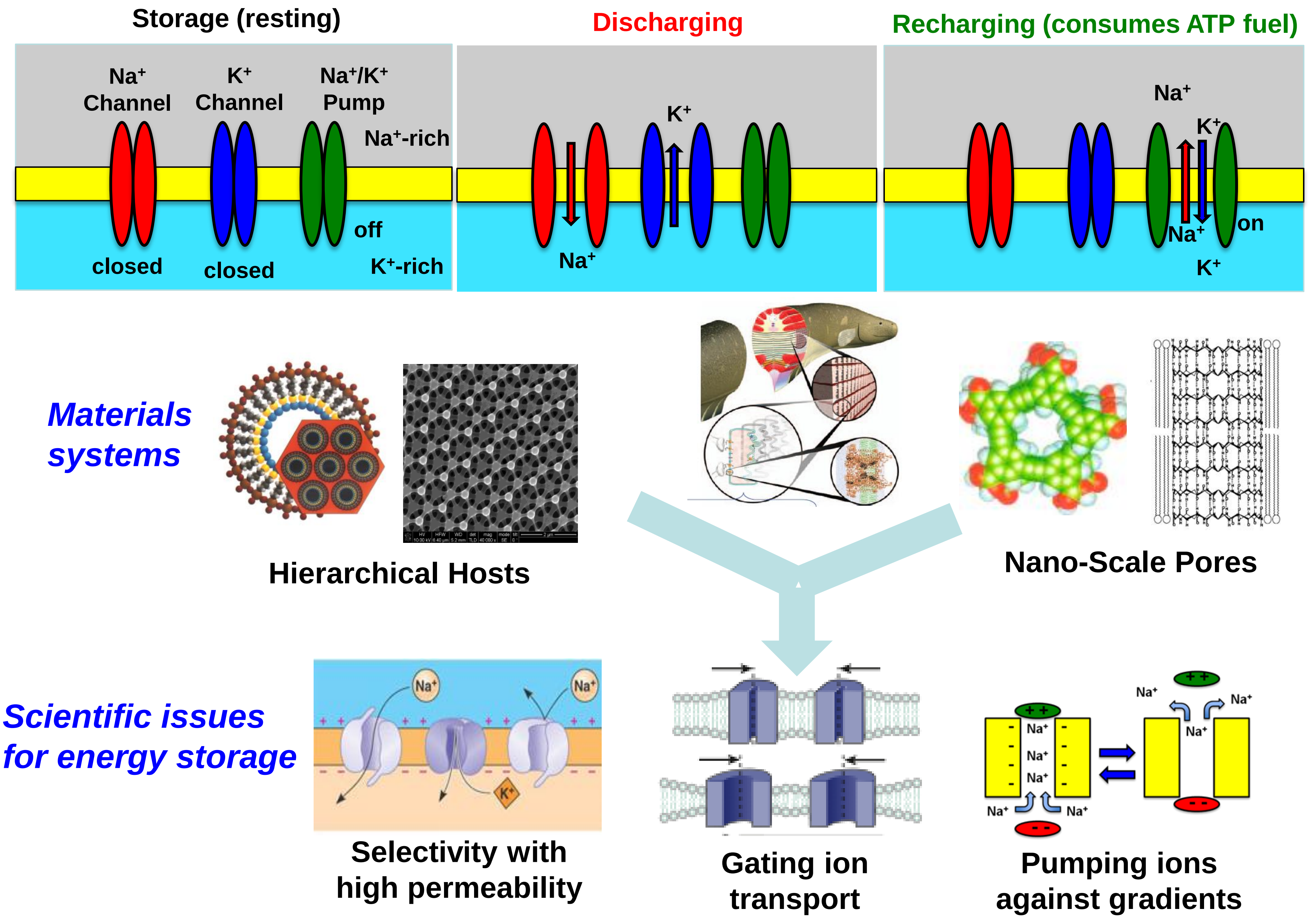
Responsive and reconfigurable materials represent a new frontier in materials science, providing access to the complex functionality found in living systems.

Biomedicine

NIH

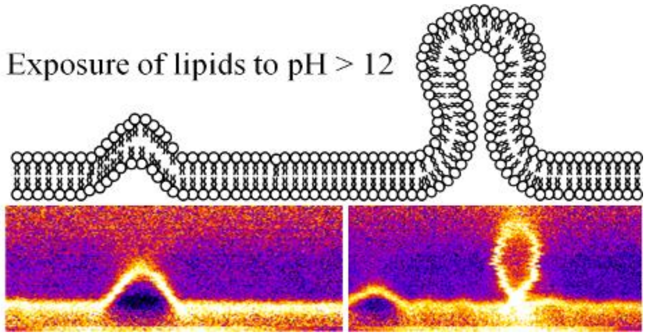


Bio-Inspired Ion Transport Materials for Energy Storage



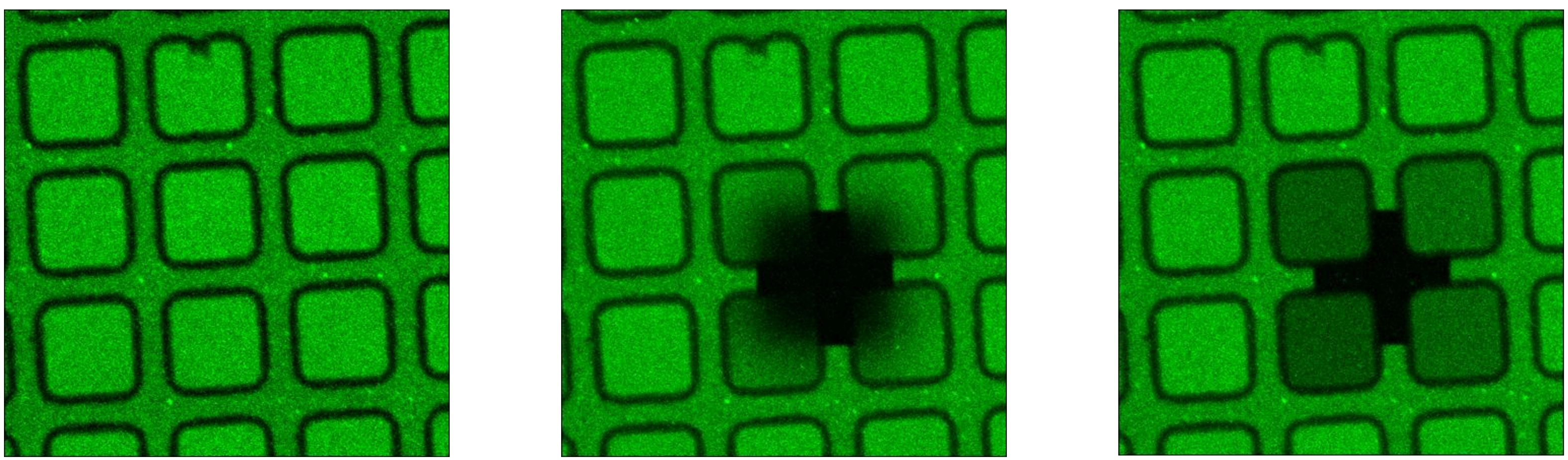
Substrate Interactions

Lipid:Substrate Interactions



Disruption of substrate interactions triggers vesicle nucleation.

Polymersome:Substrate Interactions

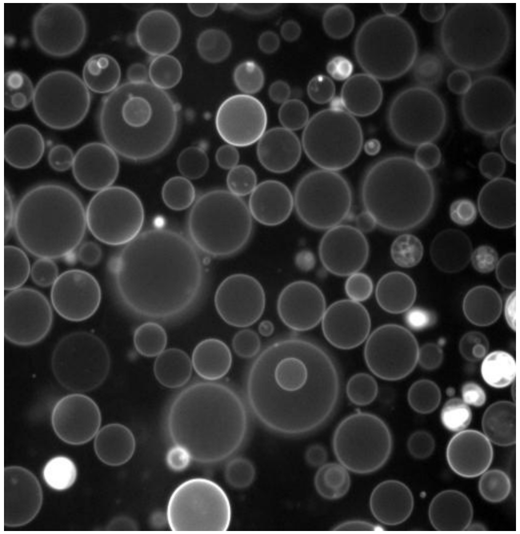


Monolayers on hydrophobic squares are mobile.
Bilayers on hydrophilic interstices are immobile.

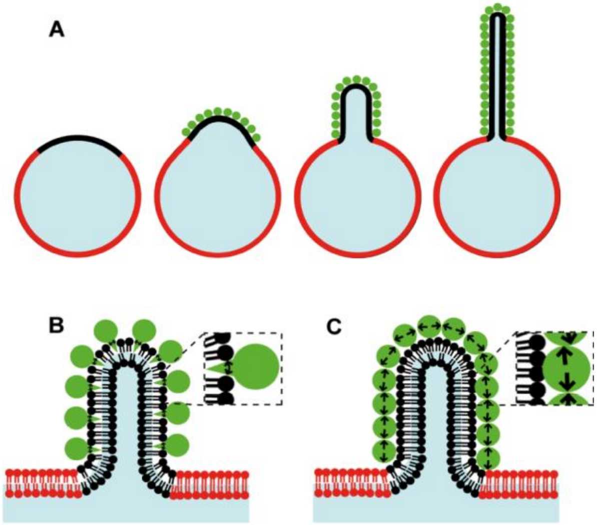
Highlight: Steric Crowding in Vesicle Assemblies

Baseline Studies: Morphology effects promoted by sterics (not programmed).

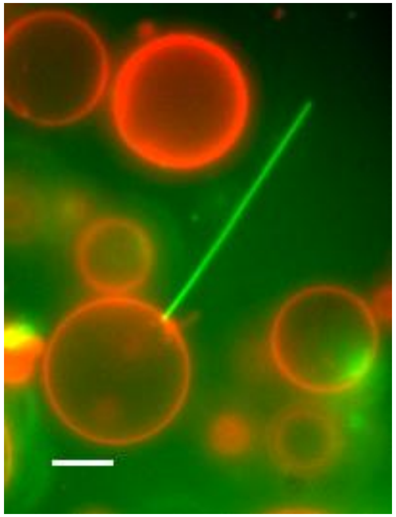
Lipid Vesicles



Protein-Induced Crowding



Nanotube Formation



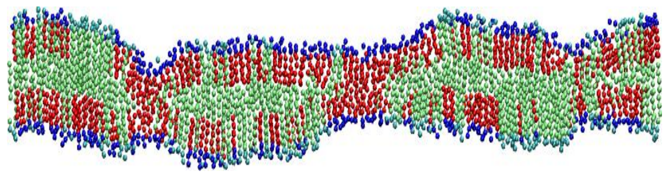
Darryl Sasaki

Morphology induced by programming component sizes.

Programmed Assembly: Adaptive and Reconfigurable Nanocomposites

Basic Energy Sciences

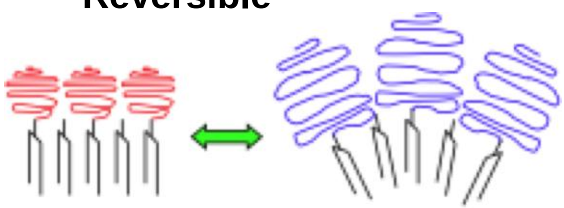
Mobile Host



Attributes:
- **Fluidity**
- **Functionality**
- **Deployment**

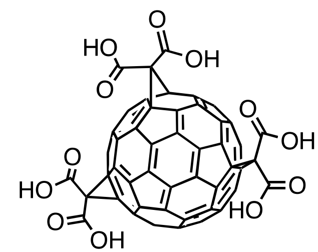
Switchable Molecule

Attributes:
- **Energy activated**
- **Reversible**

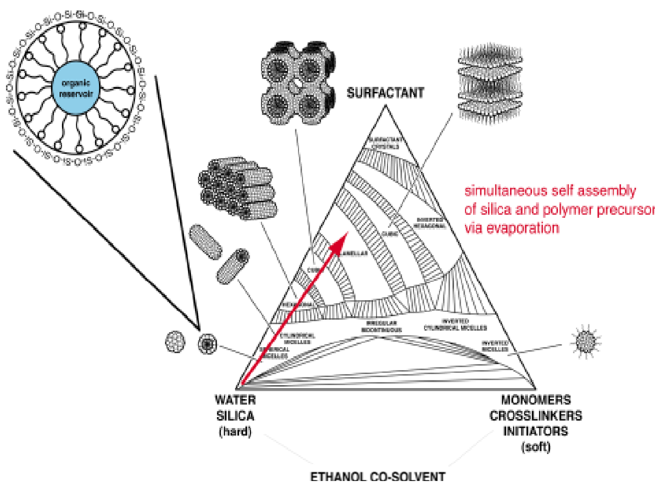


Programming of:
- **Size**
- **Shape**
- **Conformations**
- **Interactions**

Active Nanoparticle



Variables:
- **Size**
- **Shape**
- **Function**



Reconfigurable Nanocomposite

Goal: Combine programmable molecules, reconfigurable matrices, and nanomaterials to create reversibly switchable nanocomposites.

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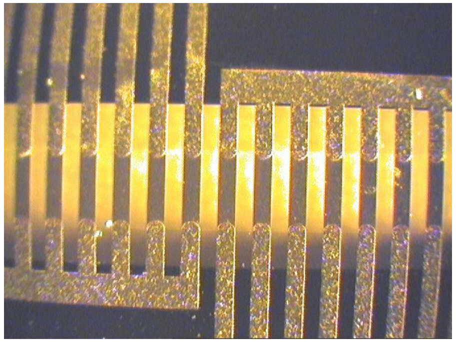
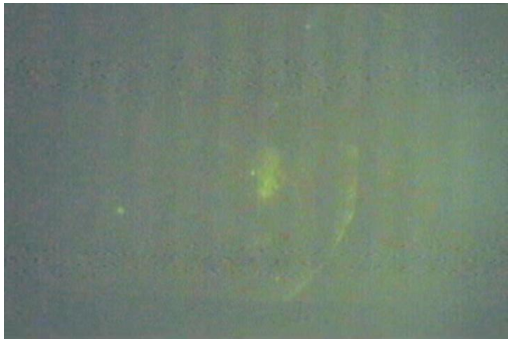
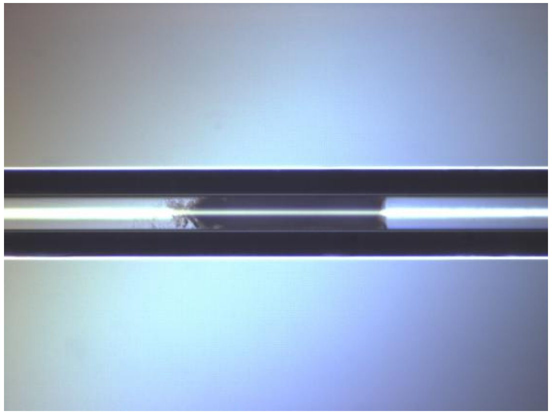
PNIPAM for Protein Capture/Release

Router





Preconcentrator



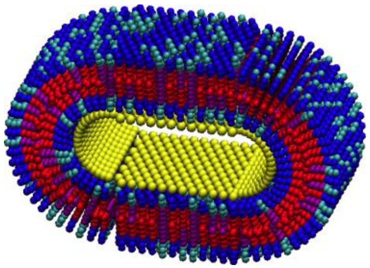
Thermal programming of PNIPAM monolayers promotes the reversible capture and release of proteins, cells, and other biological species.

Highlight: Monolayers on Gold Nanorods

Basic Energy Sciences

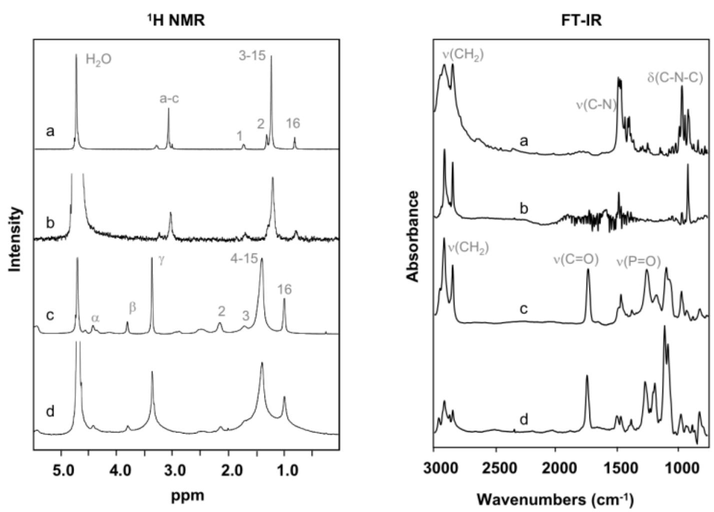
Monolayers and lipids create fluid, functionalized coatings.

Attributes:
- **Fluid, mobile**
- **Exchangeable**
- **Functionizable**



Mark Stevens (modeling)

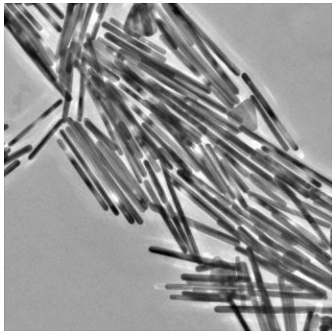
Observations of Exchange (CTAB → POPC lipid)



Todd Alam (characterization)

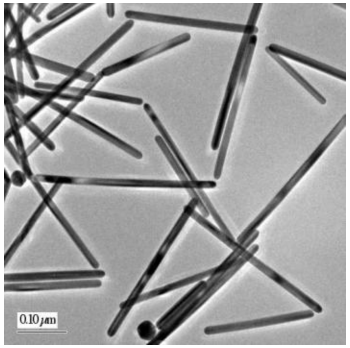
Monolayers mediate interactions + assembled architectures.

CTAB (cationic)



Chris Orendorff (Au nanorods)

POPC (zwitterionic lipid)



Status: moving from static to programmable interactions.

ACS Nano, 3, 971 (09)

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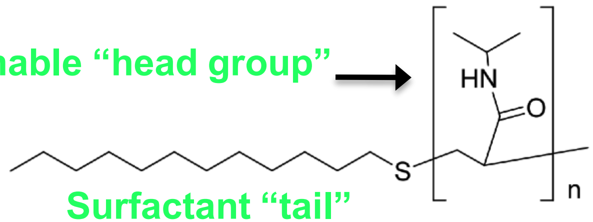
Highlight: Molecular Assemblies Containing Programmable Surfactants

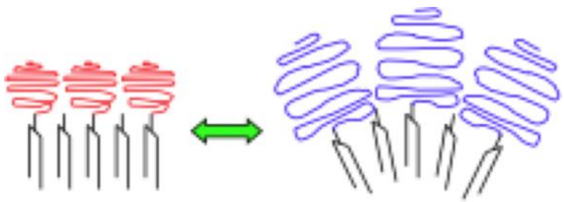
Programmable attributes of PNIPAM: hydration forces, size.

Programmable "head group"

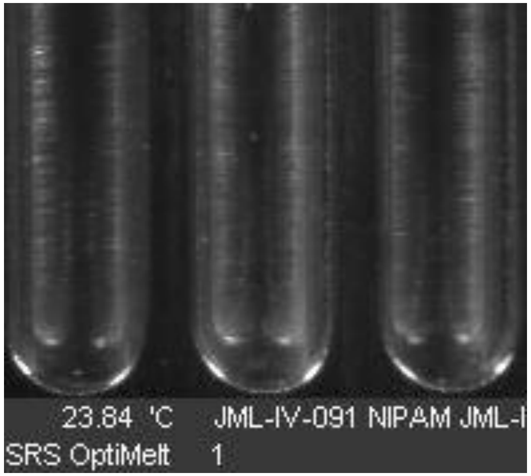


Surfactant "tail"

Hot: Hydrophobic Collapsed



Cold: Hydrophilic Swollen

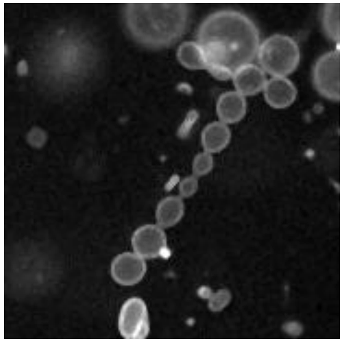


Dale Huber

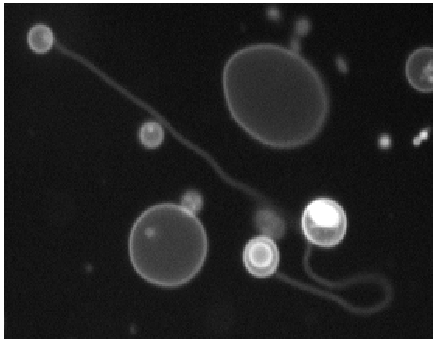
Programming reconfigures surfactant vesicles.

"peanuts"

"pearls"



lipid nanotubes

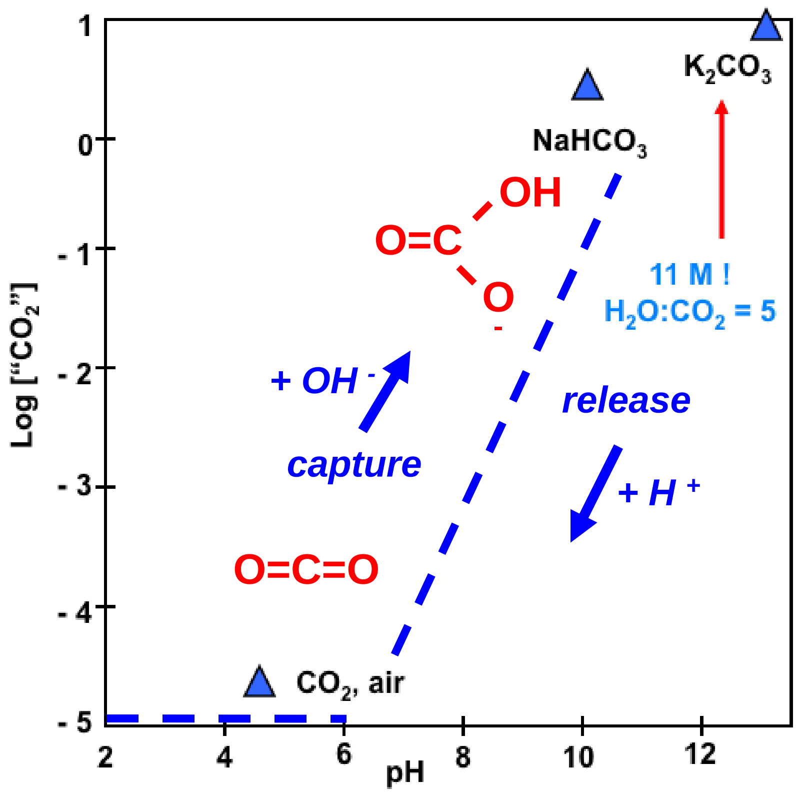


Darryl Sasaki

Reversible Sequestration of CO_2 by Water Requires the Inter-conversion between "Insoluble" CO_2 and Soluble Carbonates

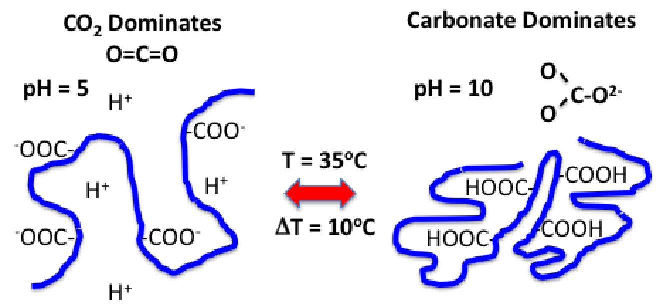
Carbonates for capture <-> CO_2 for release

Solubility



Materials and Mechanisms

Programmable Polymers



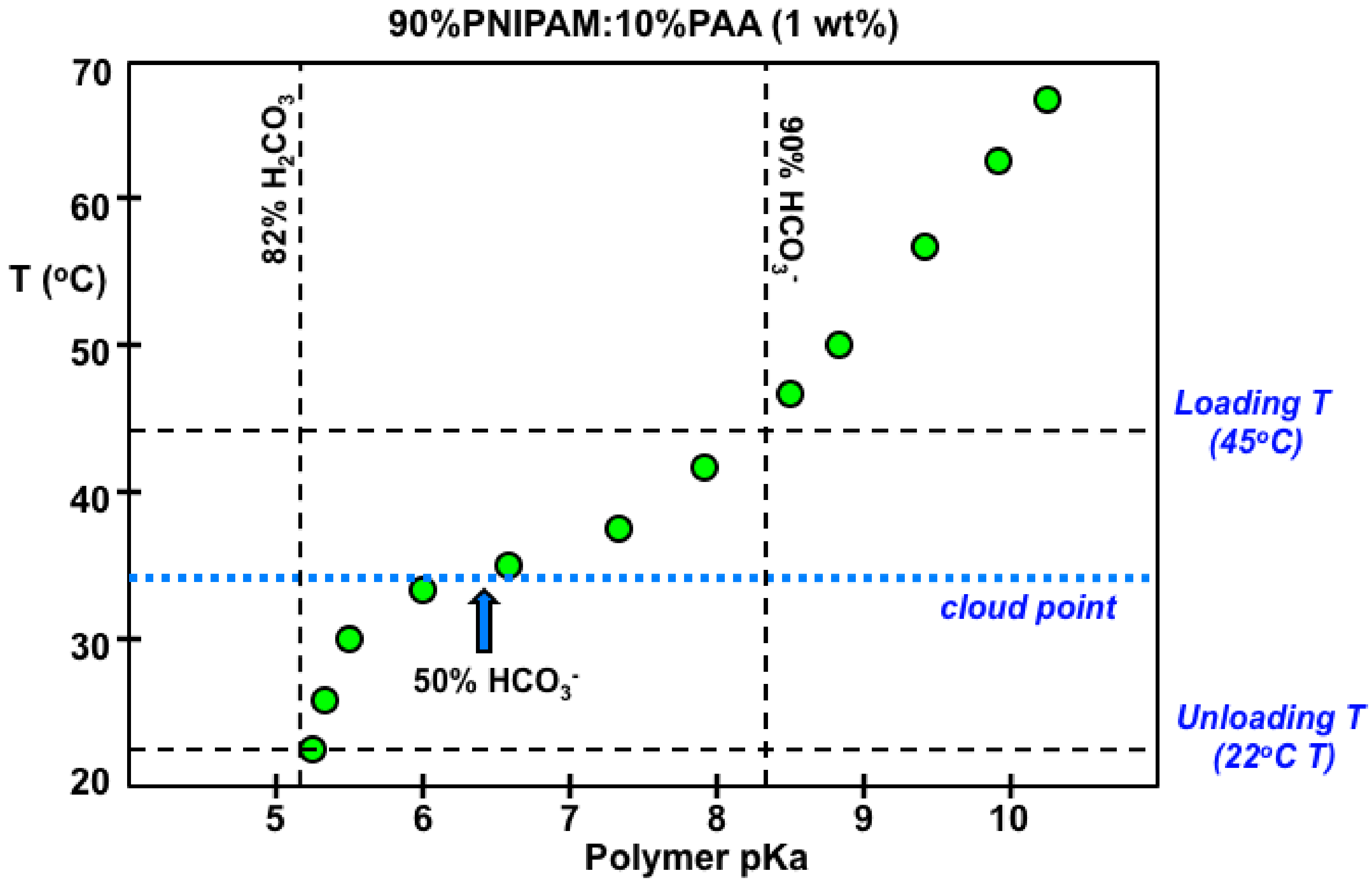
Catalytic Enzymes

Nature has developed a process!
Can we adapt it to our needs?

Research Goal: Develop nano-materials that can be used to catalyze reversible CO_2:carbonate inter-conversions.

Programmable Polymers: Results to Date

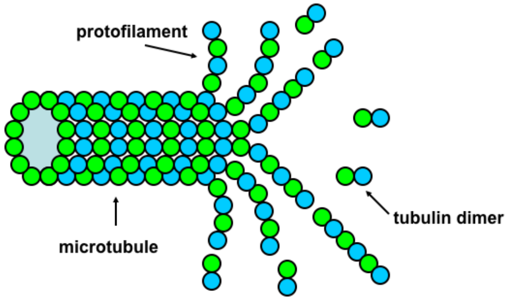
SAND 2010-5443C



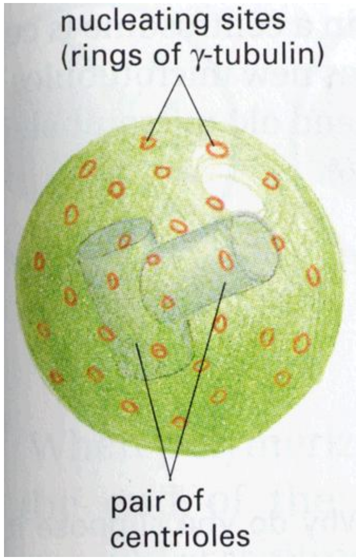
1) The initial polymer formulation (PNIPAM/PAA) has been synthesized.
2) Large concentrations of the polymer can be dissolved into water (> 5%).
3) The polymer transition temperature in water is 34°C.
4) The transition induces large, reversible changes in solution pH.
5) *Programming of the polymer should suffice for loading/unloading of CO_2.*

Active Assembly of Dynamic and Adaptable Materials

Microtubule

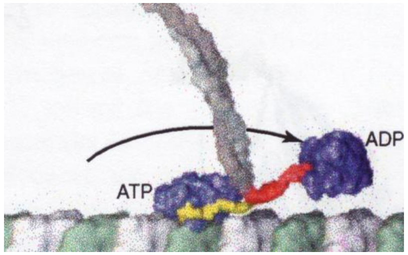


Microtubule Organizing Center



Active Proteins in "Action"

Motor Protein



Video Credits: "Inner Life of Cell"
Conceptualized by *Dr. Alain Viel Ph.D.*, and *Dr. Robert Lue Ph.D.*, Molecular and Cellular Biology, Harvard University
Animated by *John Lieber* of XVIVO, Inc.
Funded by the *Howard Hughes Medical Institute*

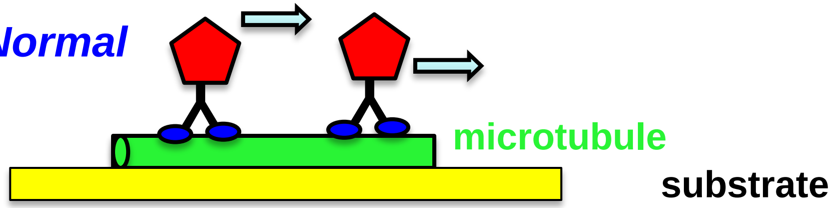
Goal: Explore the extent to which energy-consuming proteins can be used in artificial systems for the active transport, assembly, and reconfiguration of nanomaterials.

Highlights: Active Transport

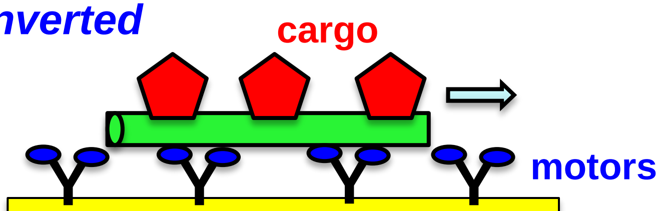
Basic Energy Sciences

Transportation Modes

Normal

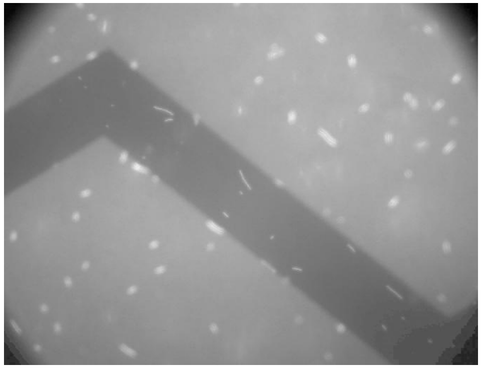


Inverted

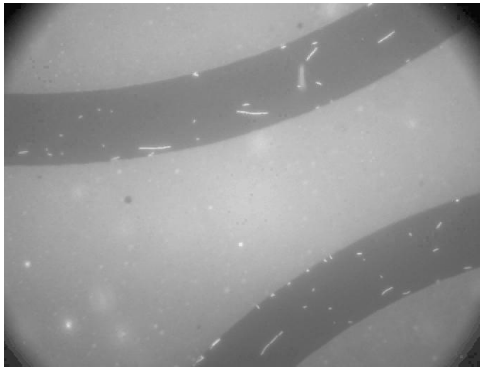


Patterned Transportation Networks (Engineered Bio-Interfaces)

Physical Alone



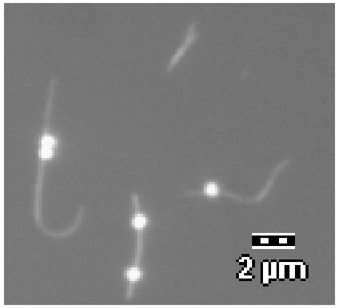
Physical + Chemical



Cargo Handling

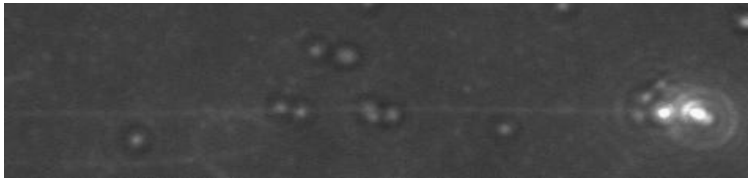
Boal, Bunker

Inverted



Boal, Bunker

Normal



Haiqing Liu

Motor-driven transport has evolved from one to two to three dimensions.
Integrated transport: explored in both normal and inverted motility modes.
Motor variations: stabilization, functionalization, switching, and directionality.

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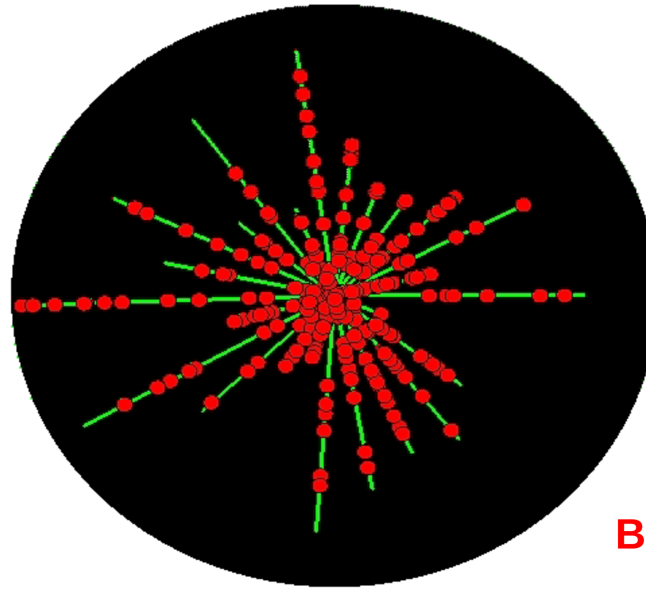
Motor-Driven Reconfigurations

Requirements for Artificial “Chameleon”

Chromatophores in Action (Caldwell, UC-Berkeley)

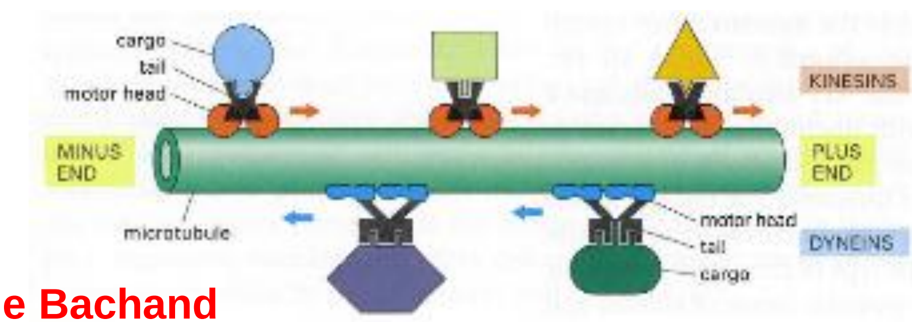
Simulation of Artificial Chameleon



Bouchard

- **Stable retrograde (dynein) motors**
- **“Start-stop” kinesin motors***
- **Motor functionalization***
- **Polar microtubule organizers***
- **Integration**

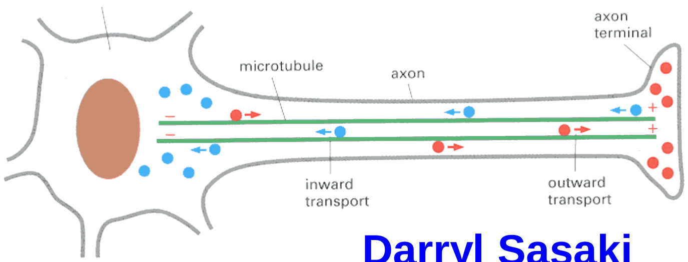
***Already demonstrated.**



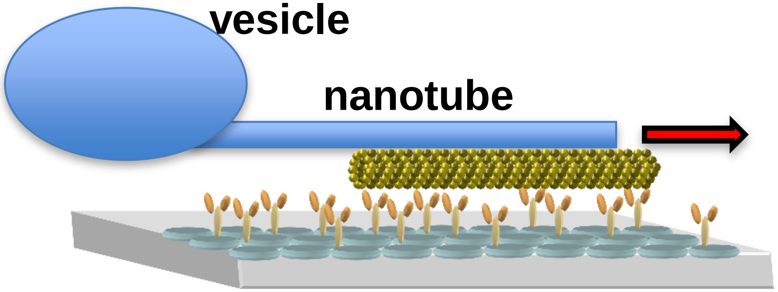
George Bachand

Highlight: Pulling Lipid Nanotubes from Vesicles

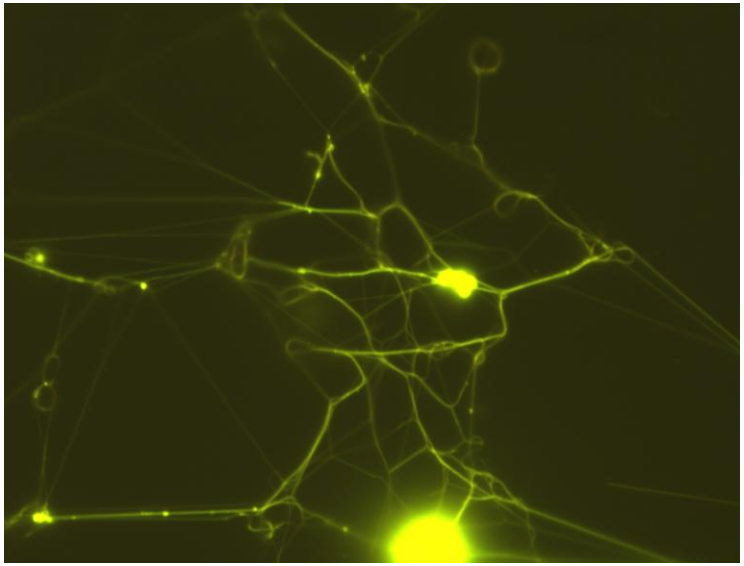
Strategy: Use microtubules as "needles" to pull nanotube "thread".

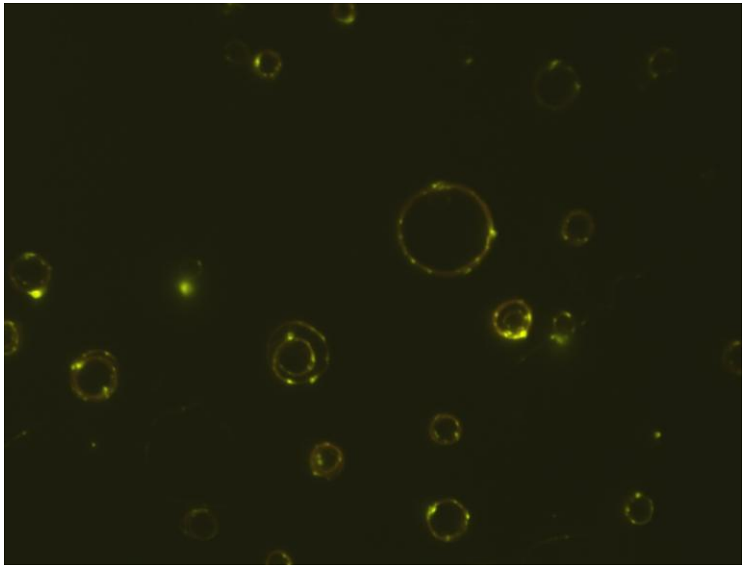


Darryl Sasaki



Results: Formation of Nanotube Networks and Rings



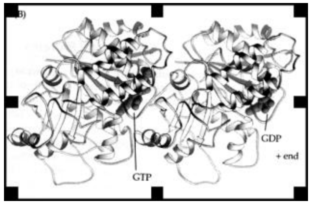


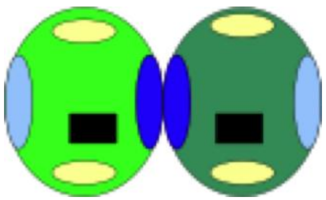
Lipid nanotubes are potential conduits for fluids and directed motor transport.

D. Sasaki, A. Carroll-Portillo, H. Liu, G. Bachand

Dendrimers as Artificial Tubulin

Attributes of Tubulin

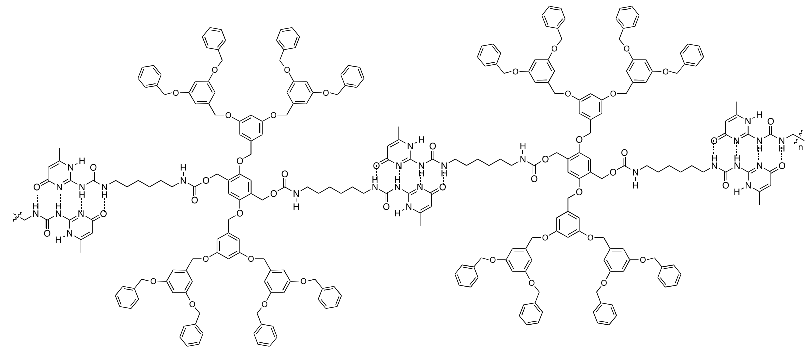




- **Axial binding sites**
- **Programmable glue**
- **Lateral binding sites**
- **Stabilizer anchors**
- **Motor binding sites**

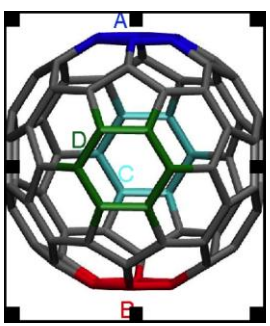
Programmable Dendrimers

Jim McElhanon

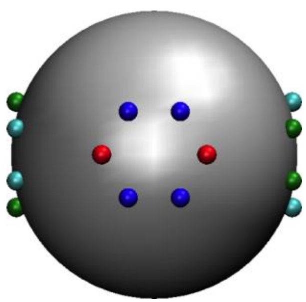


Programming based on pH, temperature, etc.

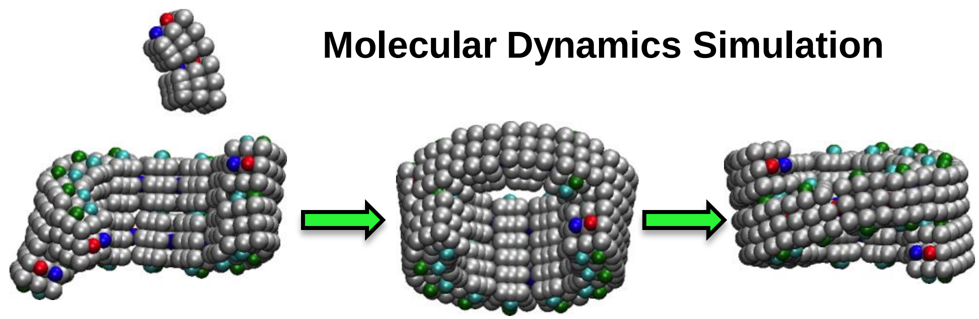
Theory/Modeling



Designer Monomers



Molecular Dynamics Simulation



Mark Stevens

Goal: Create artificial analogues to active proteins such as tubulin that can undergo programmed polymerization yet are more robust than their biological counterparts.