Brandeis MRSEC BioInspired Soft Materials

21 Primary Participants

International Laboratory Primary Collaborators

Secondary Participants

color code:
- theory
- computation
- soft matter experiment
- biology / chemistry

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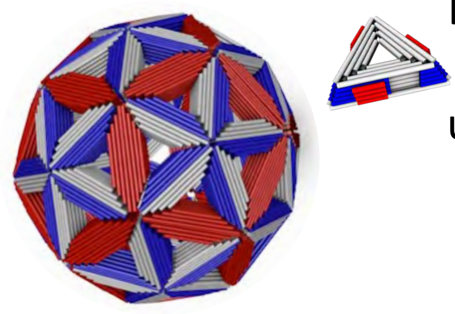
Center Vision

Elucidate the *Rules of Life* to engineer new materials that capture the remarkable functionalities found in living organisms.

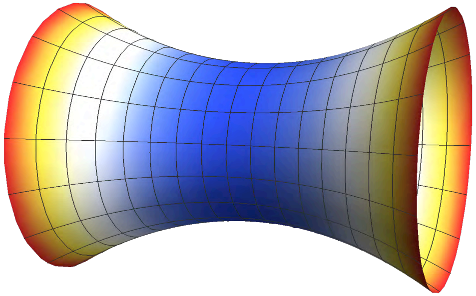
IRG1: **Self-Limiting Assembly**

curved blocks



Build multiple classes of structures of arbitrary, but self-limited size using a minimal number of distinct building blocks.

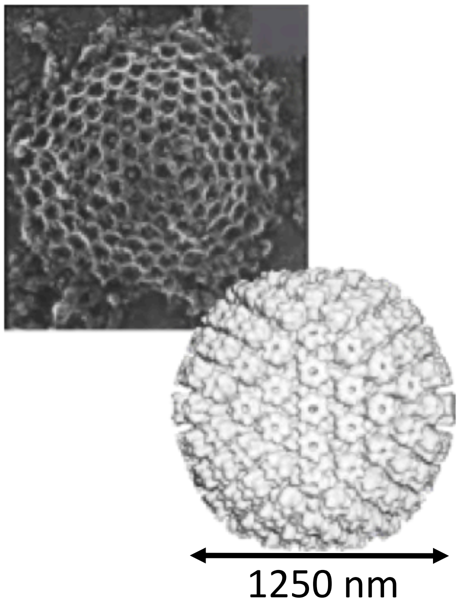
frustrated blocks



Geometrically-programmed, self-limiting assemblies

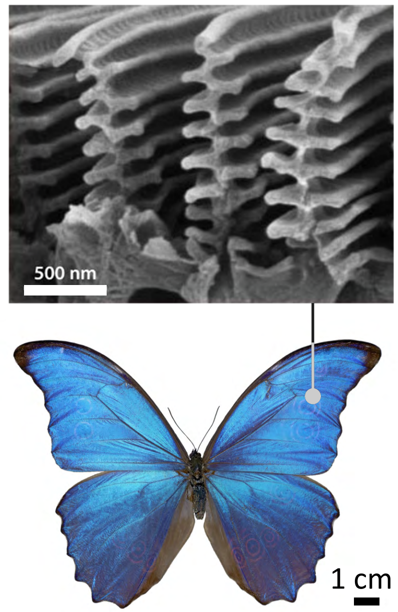
Functional size-controlled nanostructured materials from biology

shells/capsules



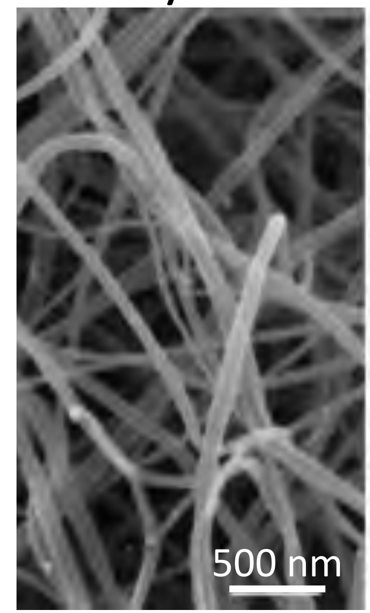
transport & delivery

nanostructured dielectrics



photonics

fibers/bundles



mechanics

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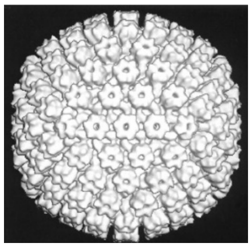
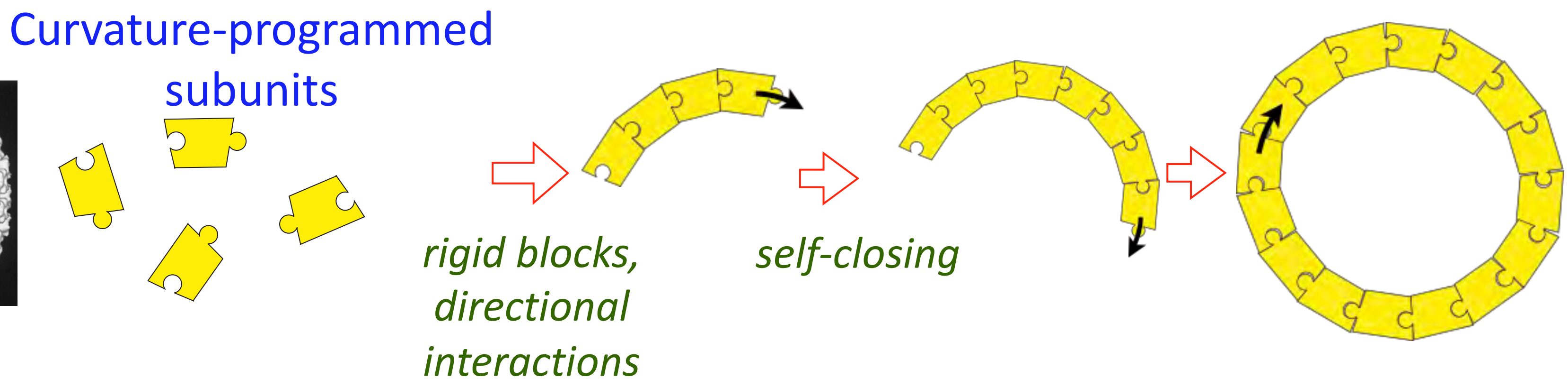
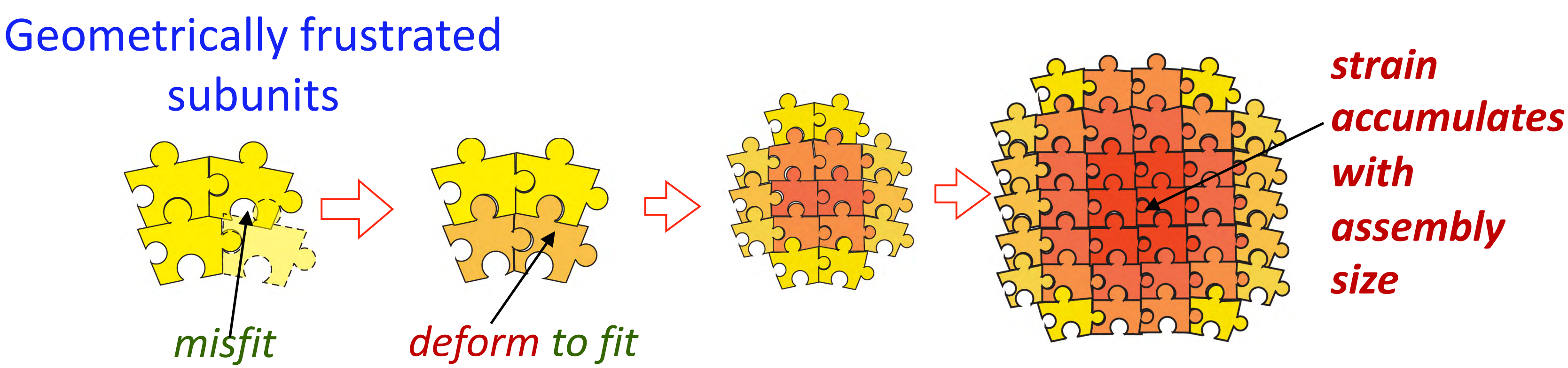
Geometrically-programmed, self-limiting assemblies

Thrust 1: Curvature-Controlled assembly (self-closing assembly)



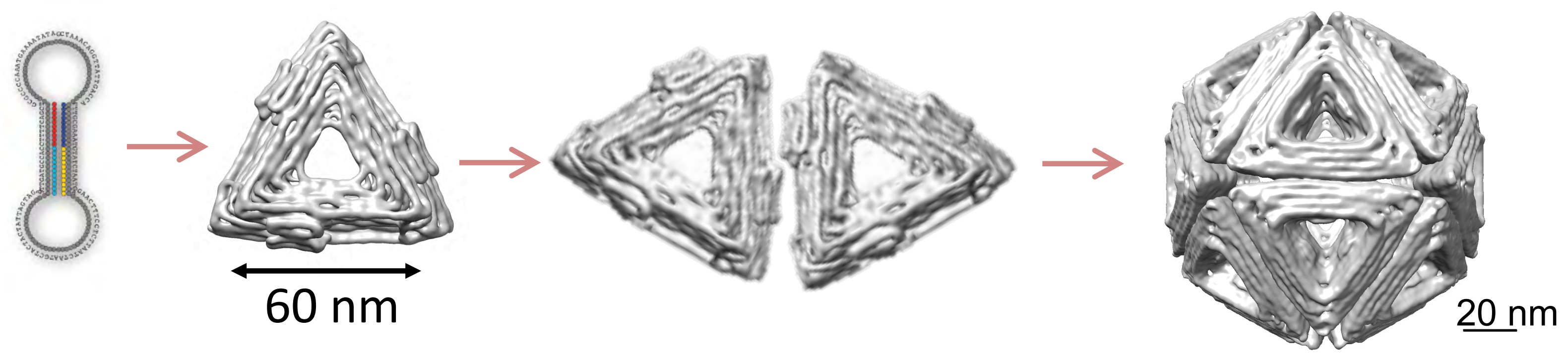


Thrust 2: Frustration-Controlled assembly (finite assembly with open edges)

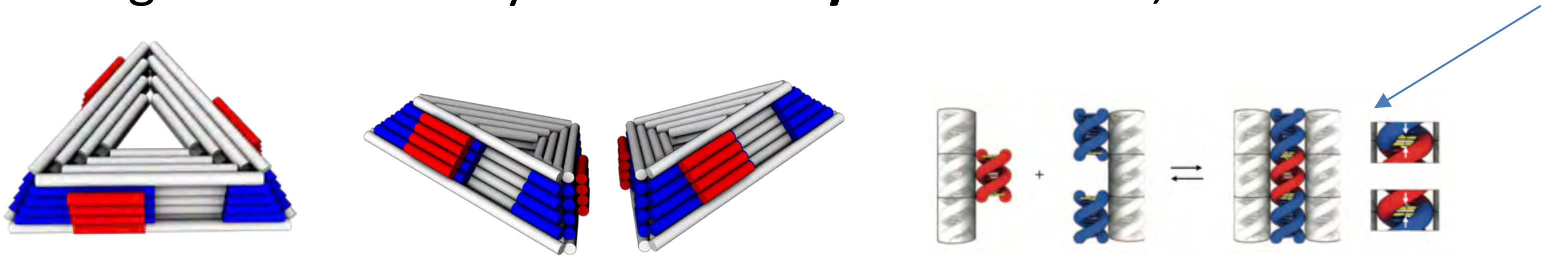


Core material platform: DNA origami

DNA folds into self-assembling triangle building block



triangles assemble by **lock-and-key interactions**, via blunt-end stacking



key attributes:

- sub-nm-precision geometry
- interactions are: valence-limited, chemically specific, $k_B T$-precision
- programmed **deformability**

Fraden, Hagan, Dietz

Thrust 1: Curvature-Controlled (Self-Closing) Assembly

<u>Goals:</u>

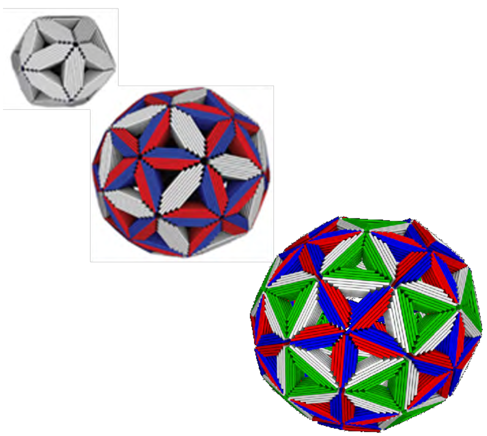
-Target self-closing architectures with arbitrary curvature

-Maximize **economy** = assembly size / min # block species

(Enabled by generalized symmetry-based theory)

K_{G} = Gaussian curvature

$K_{\mathrm{G}} > 0$

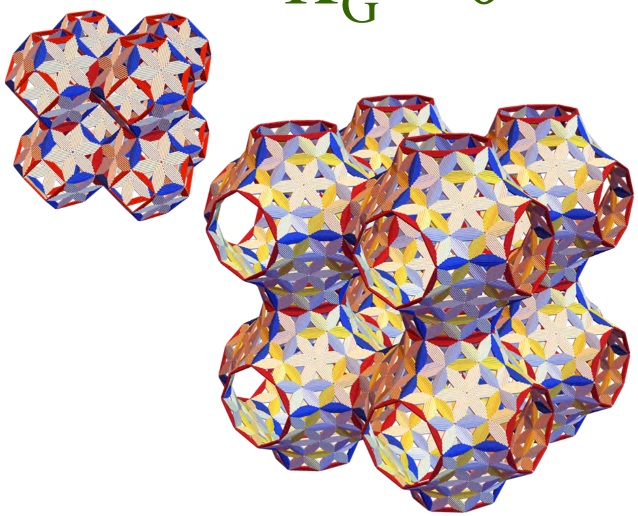


icosahedral capsids

$K_{\mathrm{G}} = 0$

tubules

$K_{\mathrm{G}} < 0$

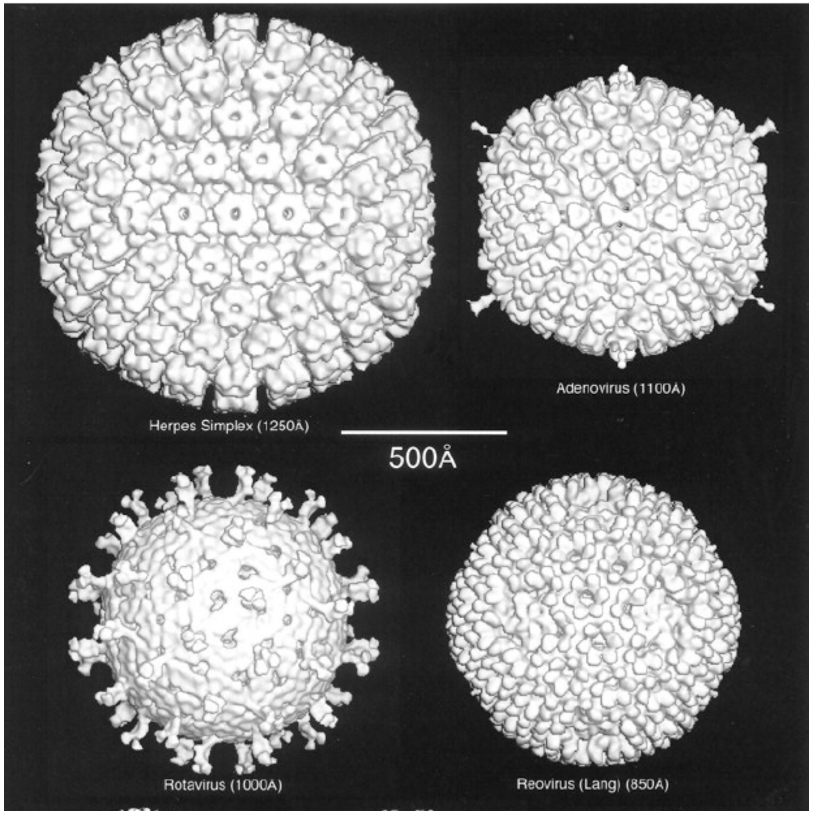


periodic negative curvature framework (photonics)

Dietz, Fraden, Rogers, Rodal, Hagan, Ivanovic, Santangelo, Xu

Quasi-equivalence: Icosahedral body plan

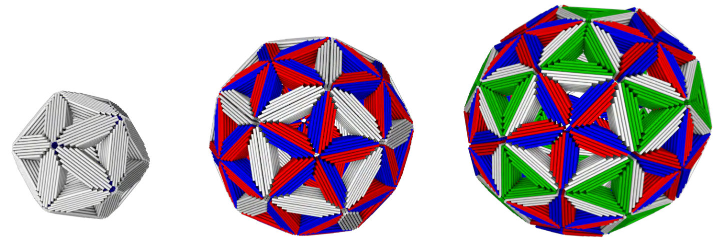
Caspar & Klug (1962)
Cold Spring Harbor Symp. Quant. Biol. **27,** 1-24



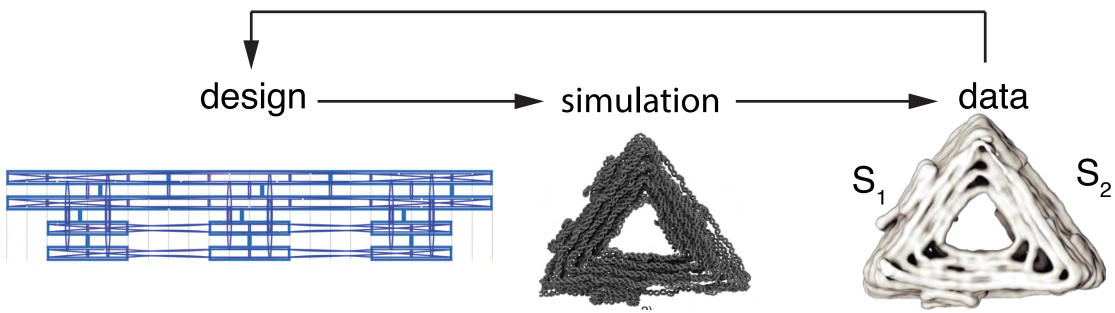
Buckminster Fuller 1967 Montreal World' Fair

Synergy: Theory / Computation / Experiment

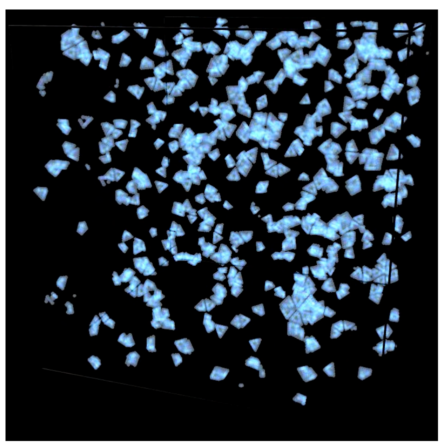
Theoretical Principles



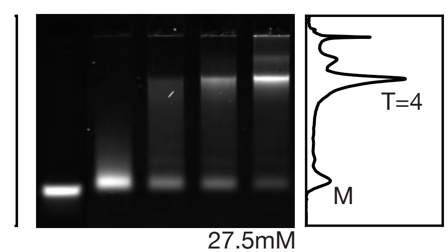
Data-driven block design

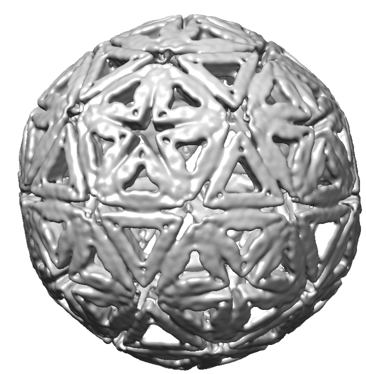


Computational modeling of assembly



Experimental characterization of assembly

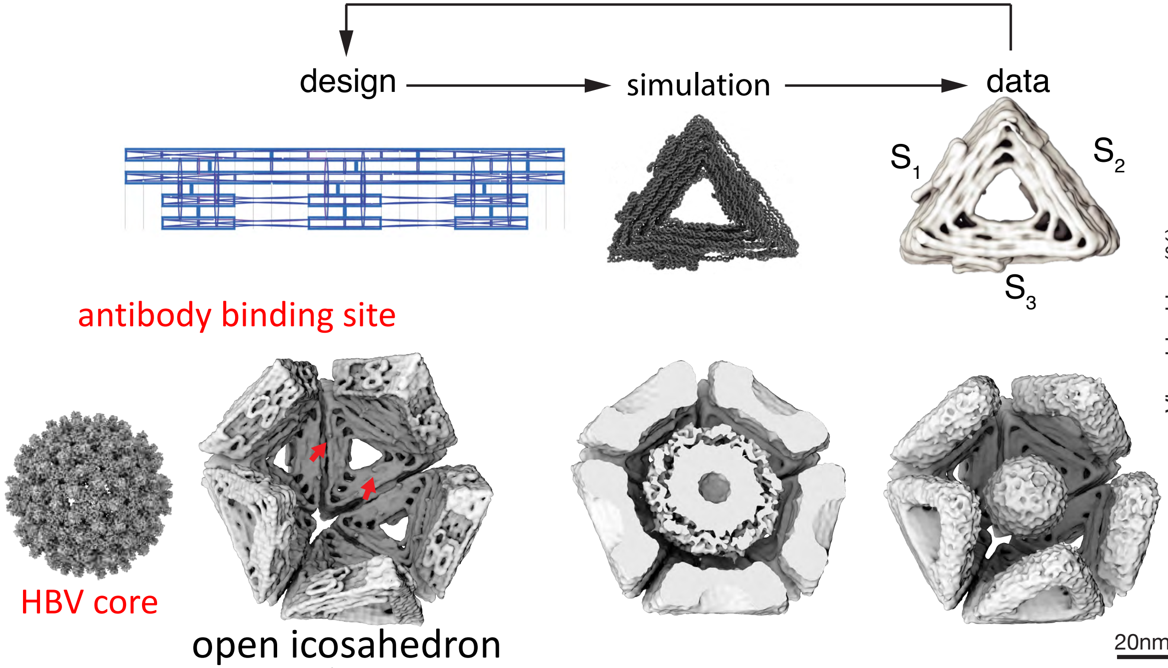




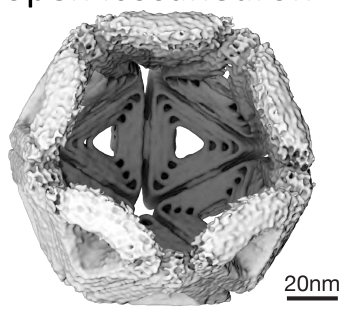
Dietz, Fraden, Rogers, Rodal, Hagan, Ivanovic, Santangelo, Xu

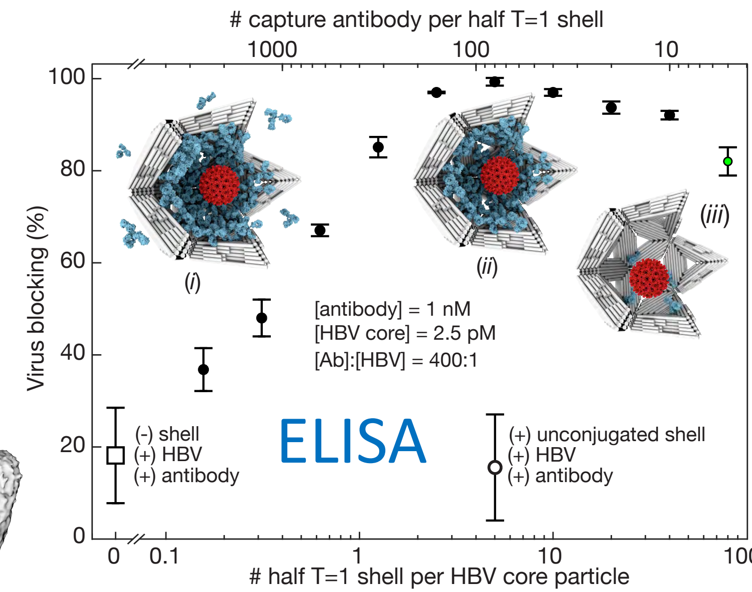
IRG1: Using viral assembly principles to deactivate virus

DNA origami capsids deactivate hepatitis B virus core

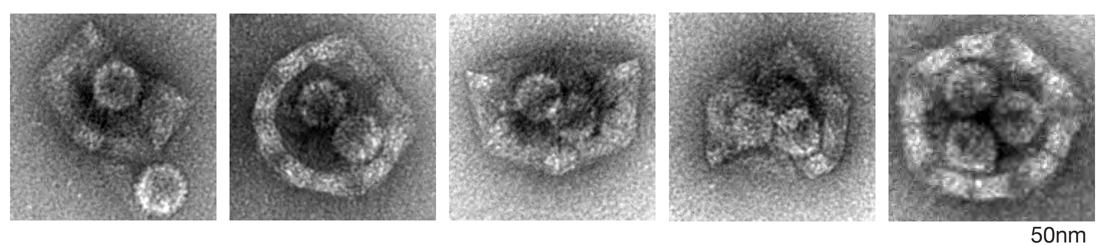


open icosahedron





enzyme-linked immunosorbent assay



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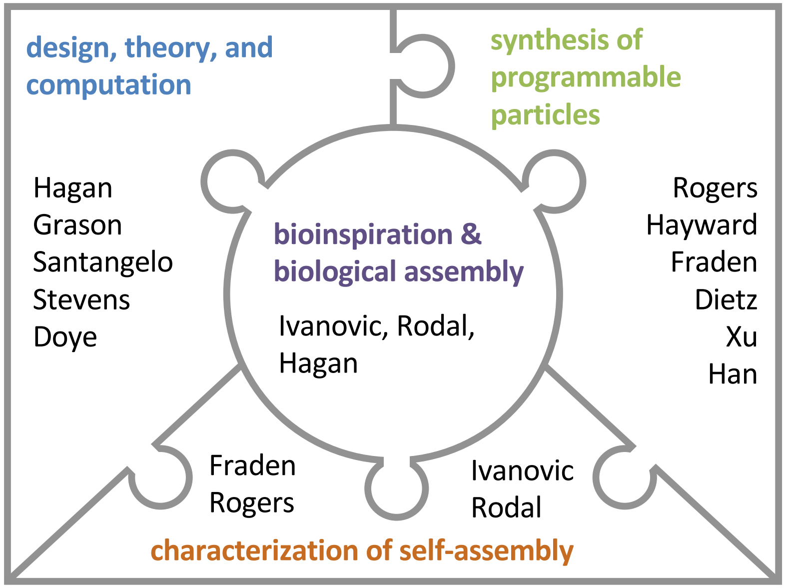
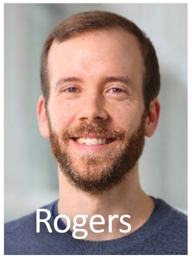
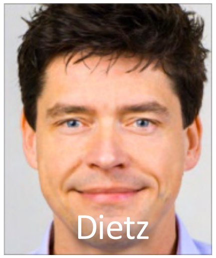
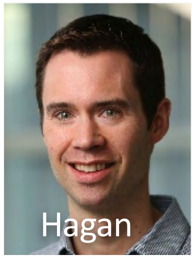
Creating a new assembly paradigm requires teamwork

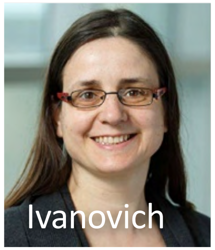
IRG1: **Self-Limiting Assembly**

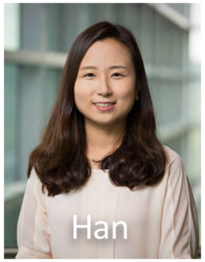












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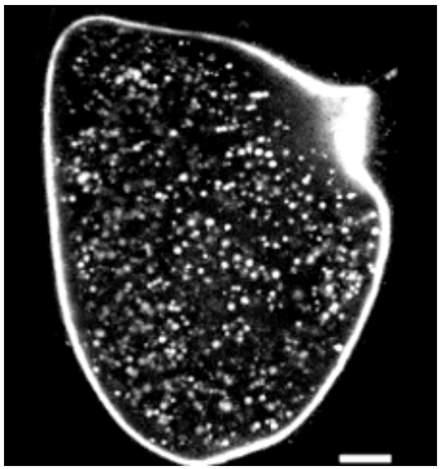
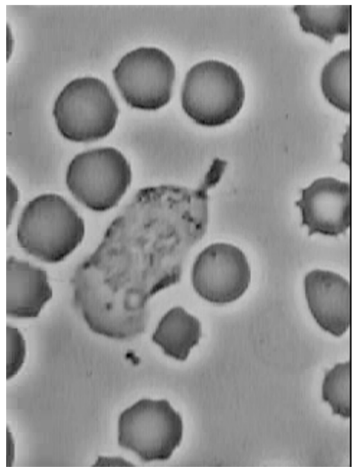
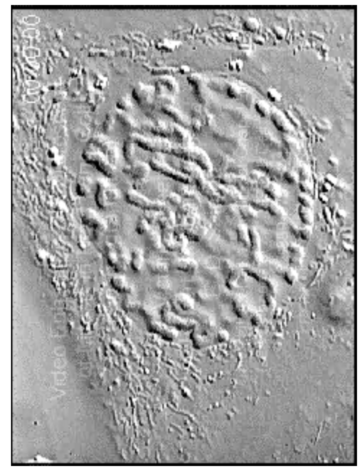
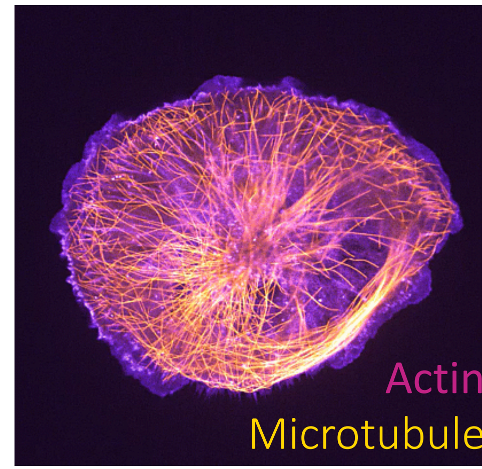
IRG2: **Soft Active Materials** - Bioinspiration

Vision: Animate the Inantimate









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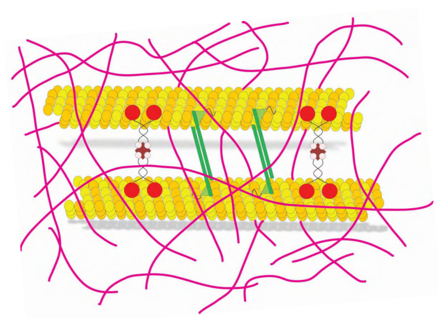
Center Vision

Elucidate the *Rules of Life* to engineer new materials that capture the remarkable functionalities found in living organisms.

IRG2: **Soft Active Materials**

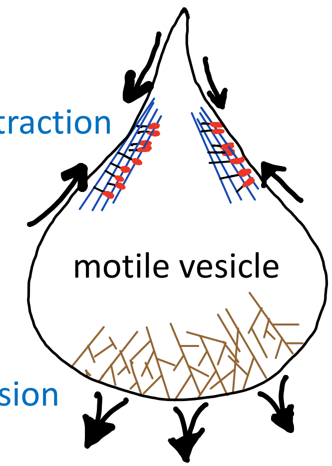
active composites



Design active stresses through 3D active composites

Measure active stresses

Control active stresses in space and time to generate desired functions.



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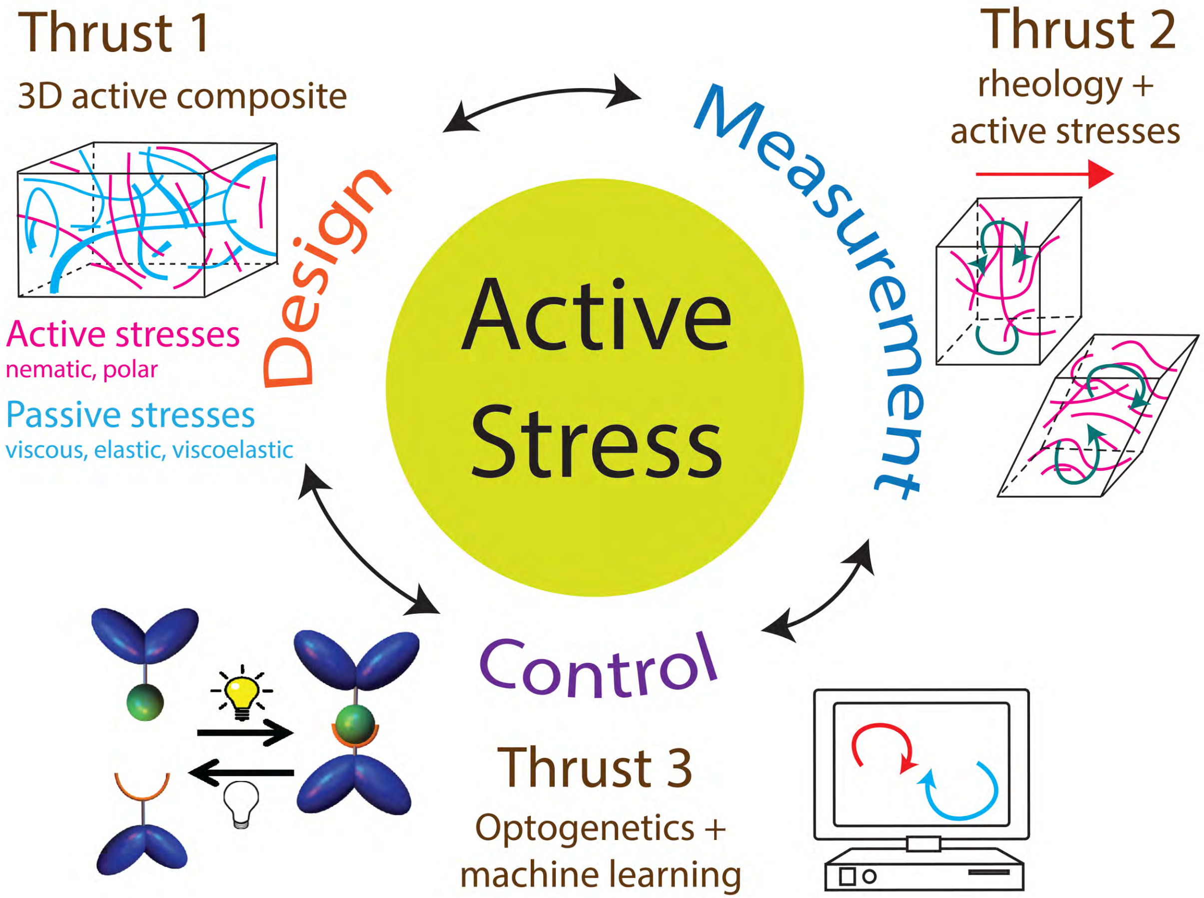
IRG2: Soft Active Materials



Vision: Active and passive building blocks can be rationally engineered to build robust 3D active materials, whose dynamics and mechanics can be tuned in situ using control theory.

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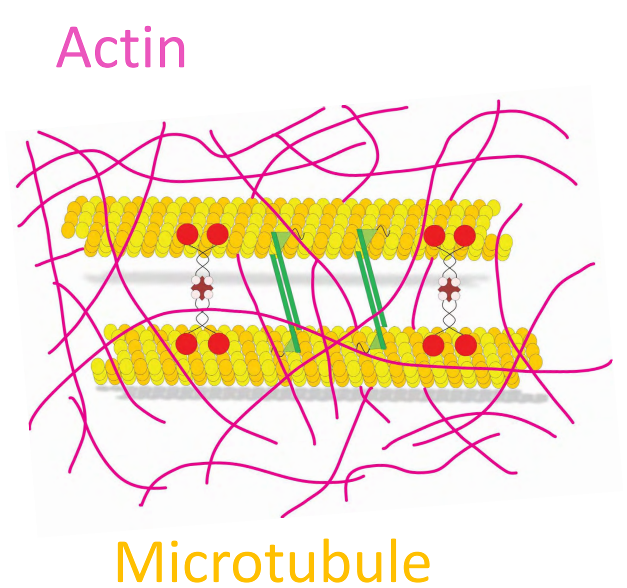
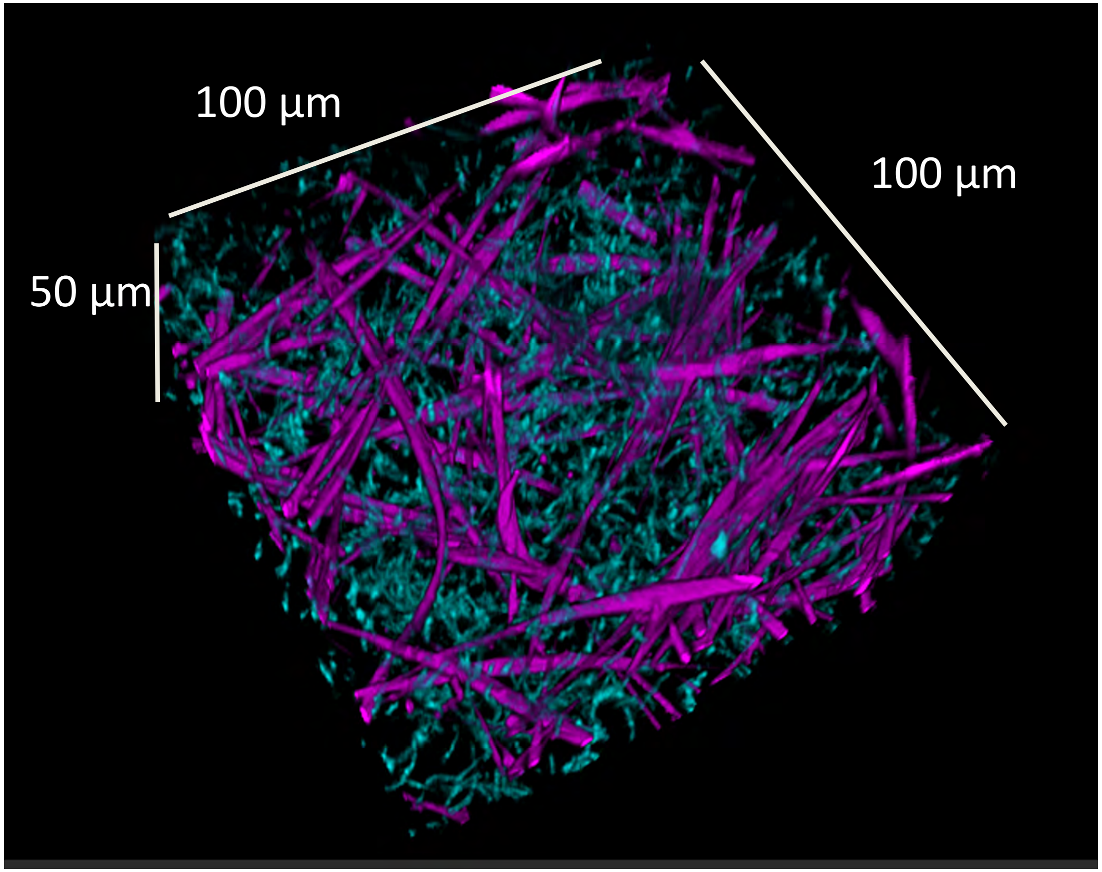
Thrust 1 : Active Viscoelastic Gel

Integration of soft matter expertise and biochemistry expertise yielded a designer active viscoelastic gel





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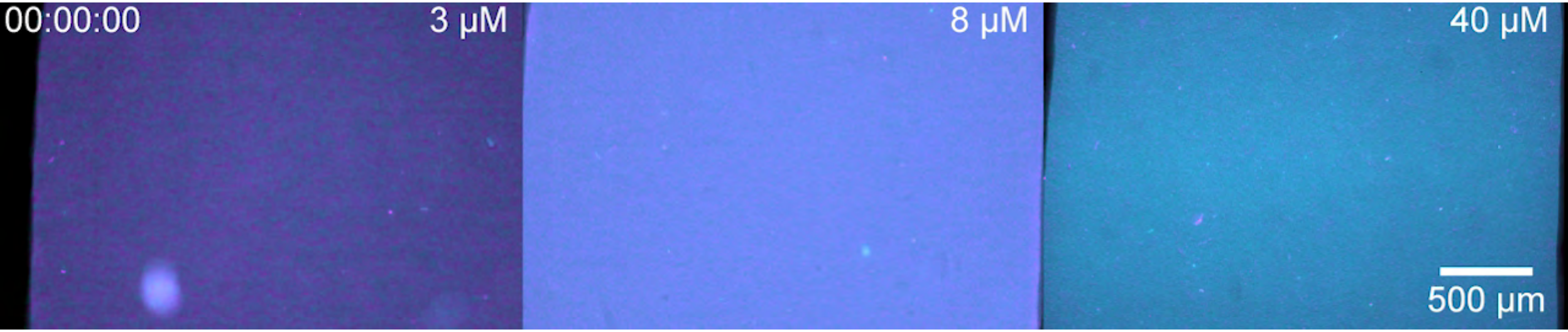
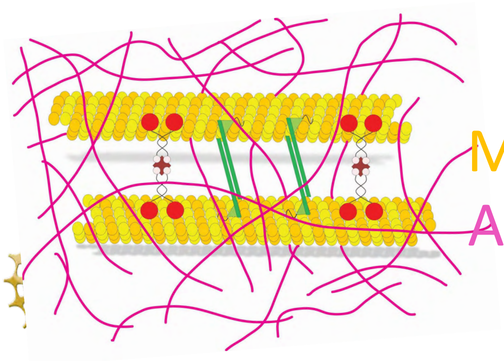
Thrust 1 : Active Viscoelastic Gel

Dramatic change in the mesoscale stress as a function of one continuously changing material parameter

Extensile active gel **Aster formation** **Contractile active gel**



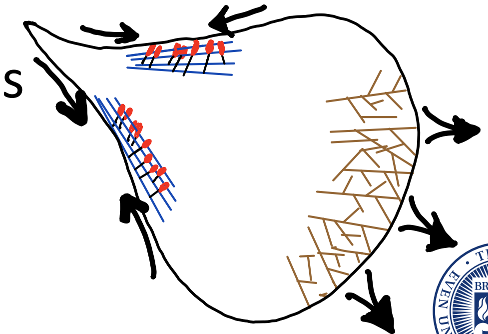
Increasing actin concentration



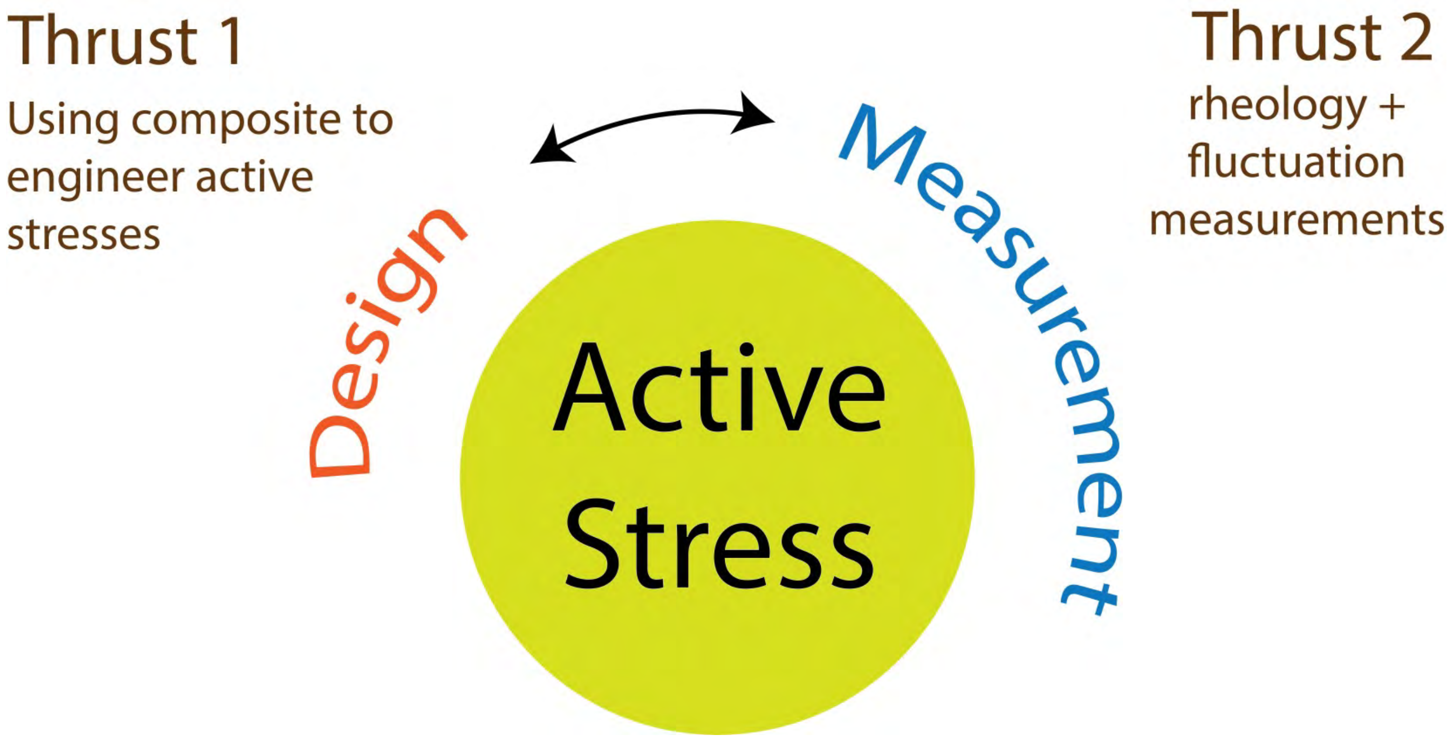
Microtubule

Actin

First step towards making a vesicle capable of directed motility

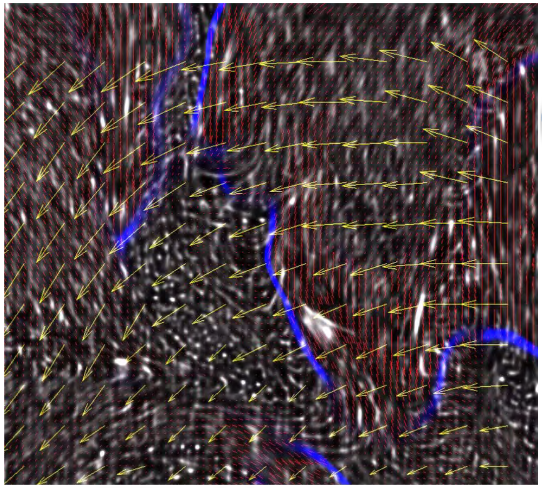


Thrust 2 : Measuring active stress



Quantifying Mesoscale active stress is essential

3D active nematic



$[\rho, \vec{v}]$

50um

Flows
Defects
Microtubules
Orientation

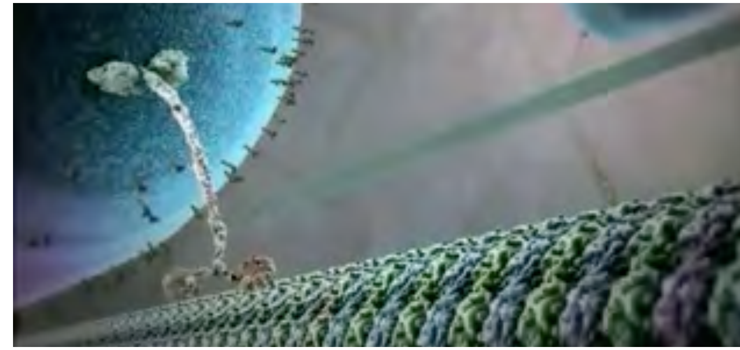
Structure/ dynamics

Stress/Mechanics

$\vec{F}[\rho, \vec{v}]$

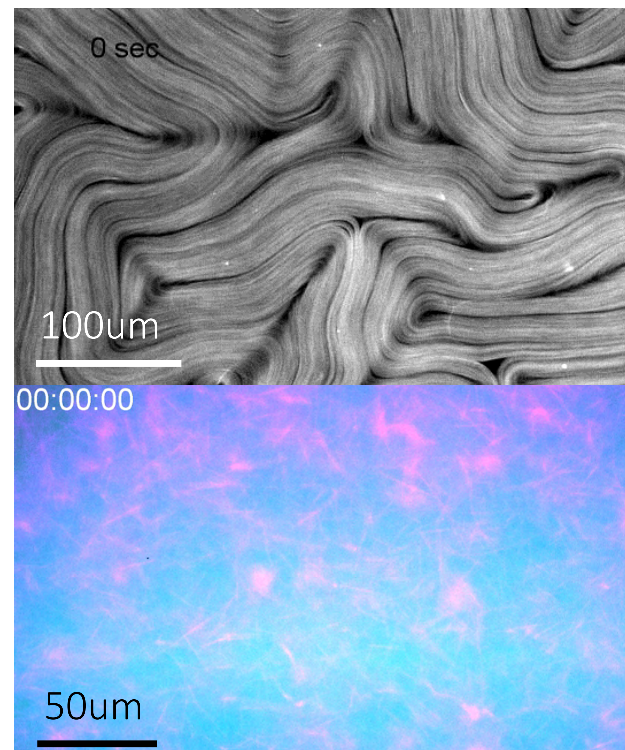
Force

Nano-scale



Extensile (top) or contractile (bottom)

Meso-scale



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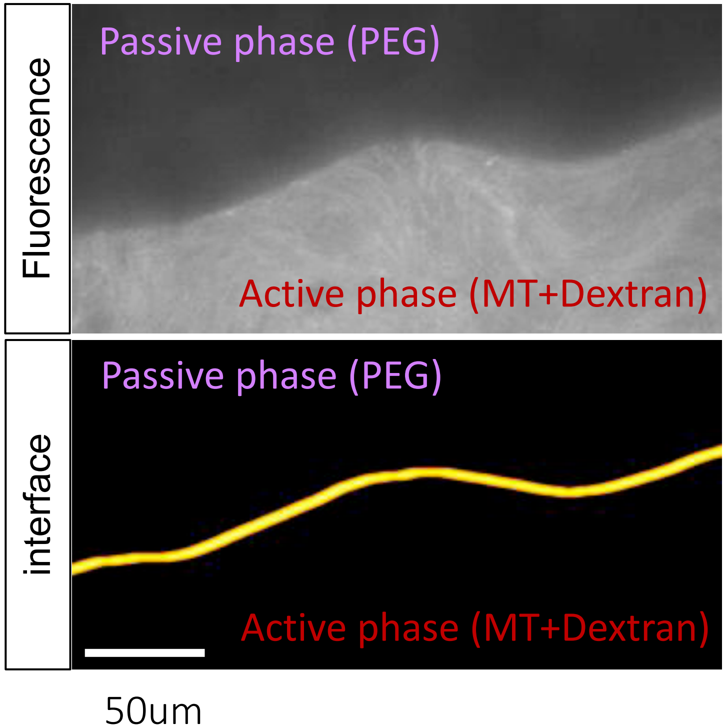
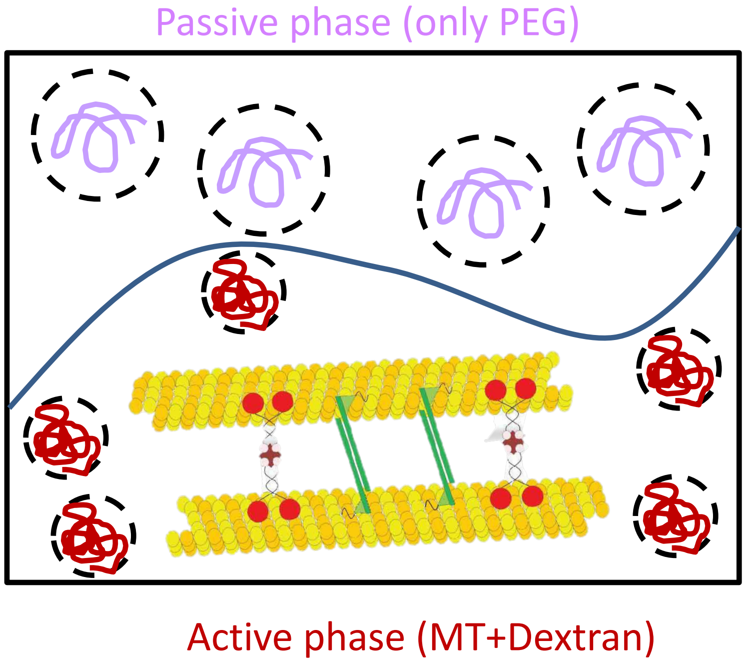
Thrust 2: Using interface fluctuations

2 phase mixture of PEG + Dextran





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Thrust 3 : Control of Active Stress

Vision: Establish rational design principles for building 3D adaptive active matter through engineering measurement and control of emergent active stresses

Thrust 1
Using composite to engineer active stresses

Thrust 2
rheology + fluctuation measurements

Thrust 3
Optogenetics + machine learning

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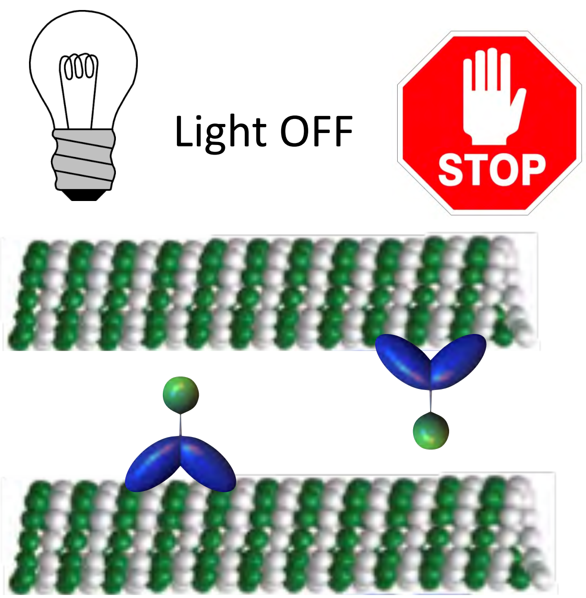
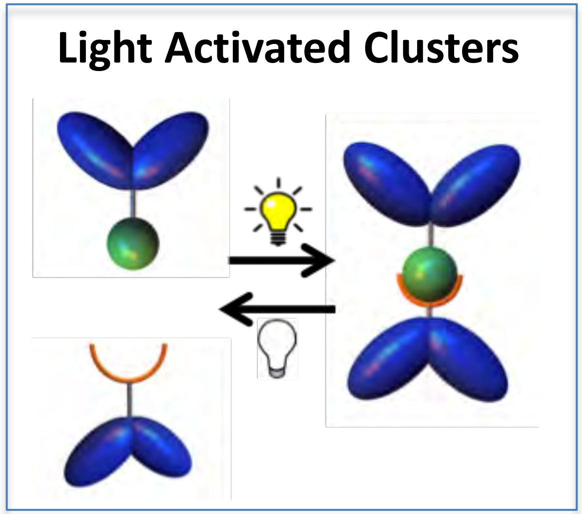
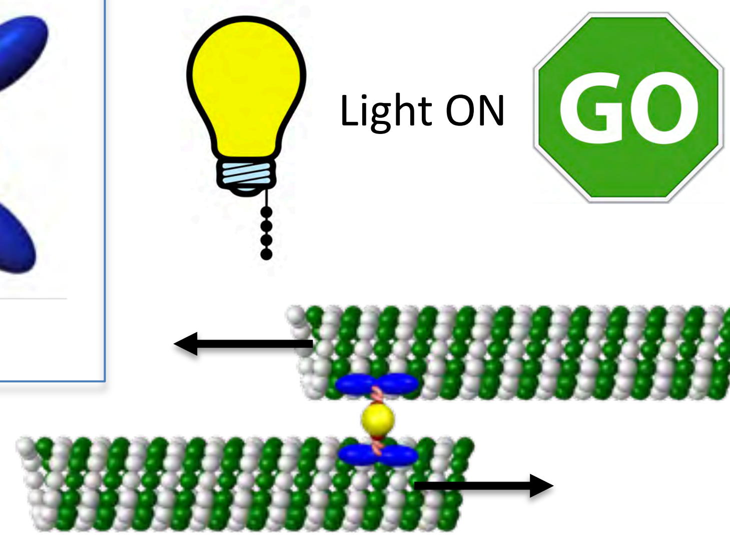
Light as the control signal

Optogenetics: Active fluid with light activated motor proteins







Crosslinking Force Generating

No cross linking, no force

Biomolecular Engineering

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Light as the control signal

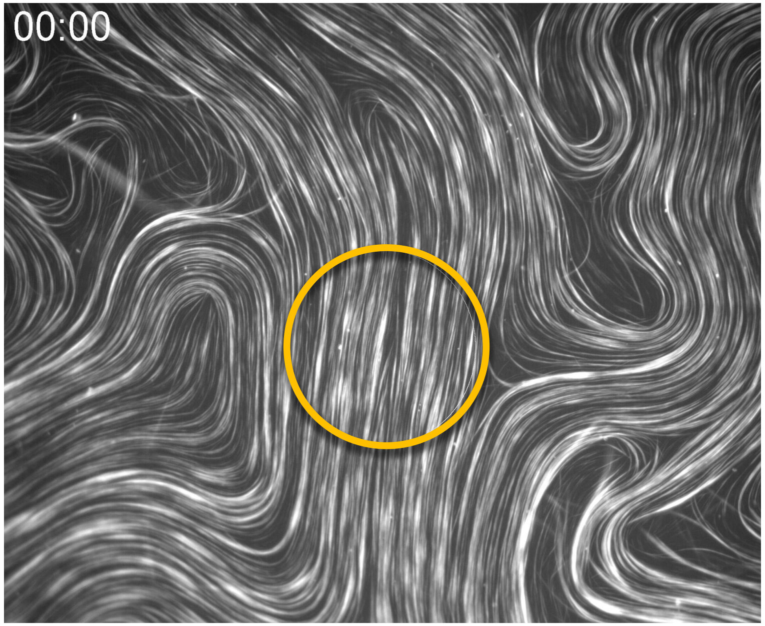
Optogenetics: Active fluid with light activated motor proteins

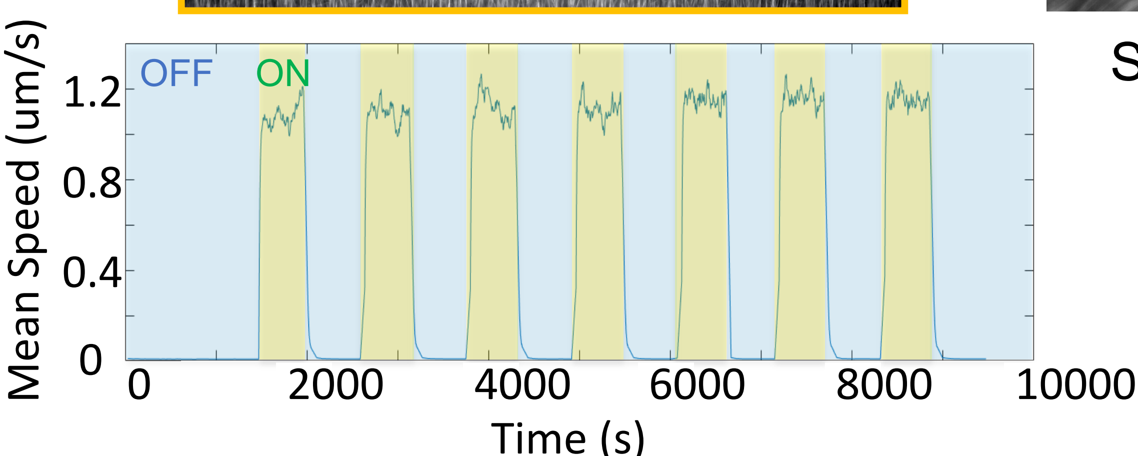
Temporal control

3D active gel

Spatial control

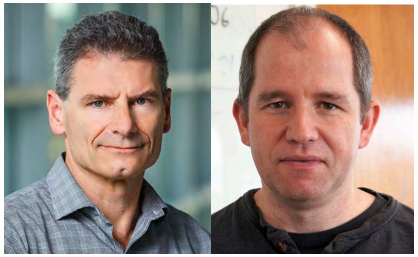
2D active nematic



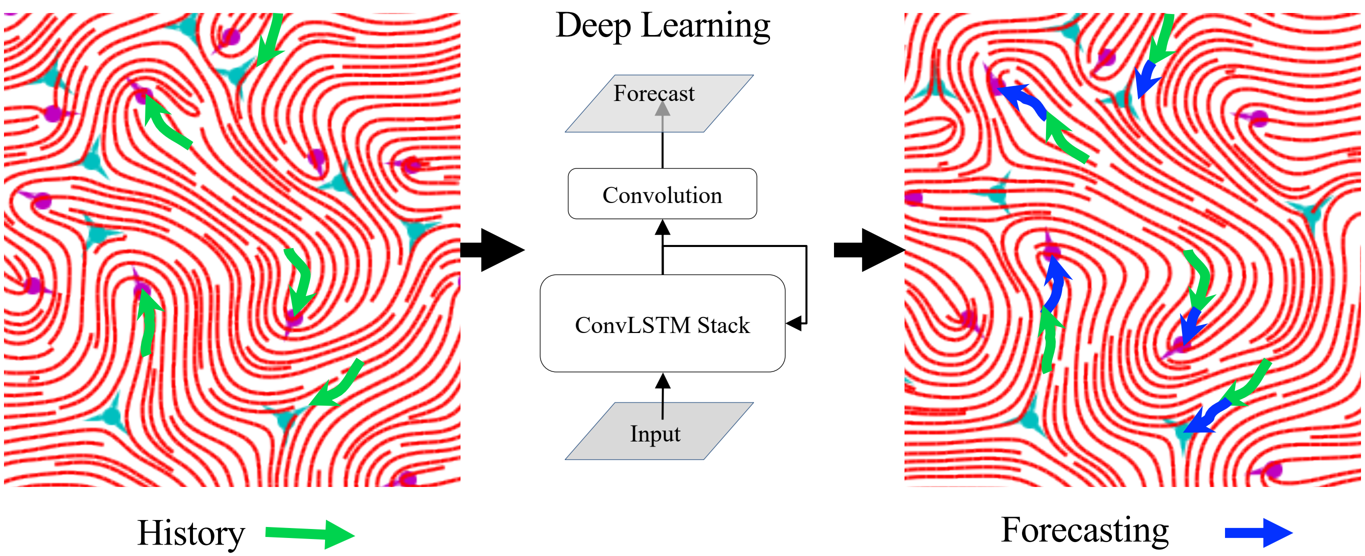


Spatiotemporally patterned light

Fraden, Dogic



Machine learning forecasting of active nematics



Zhou Z, et al. Machine learning forecasting of active nematics. Soft Matter. Published online 2021:10.1039.D0SM01316A. doi:10.1039/D0SM01316A

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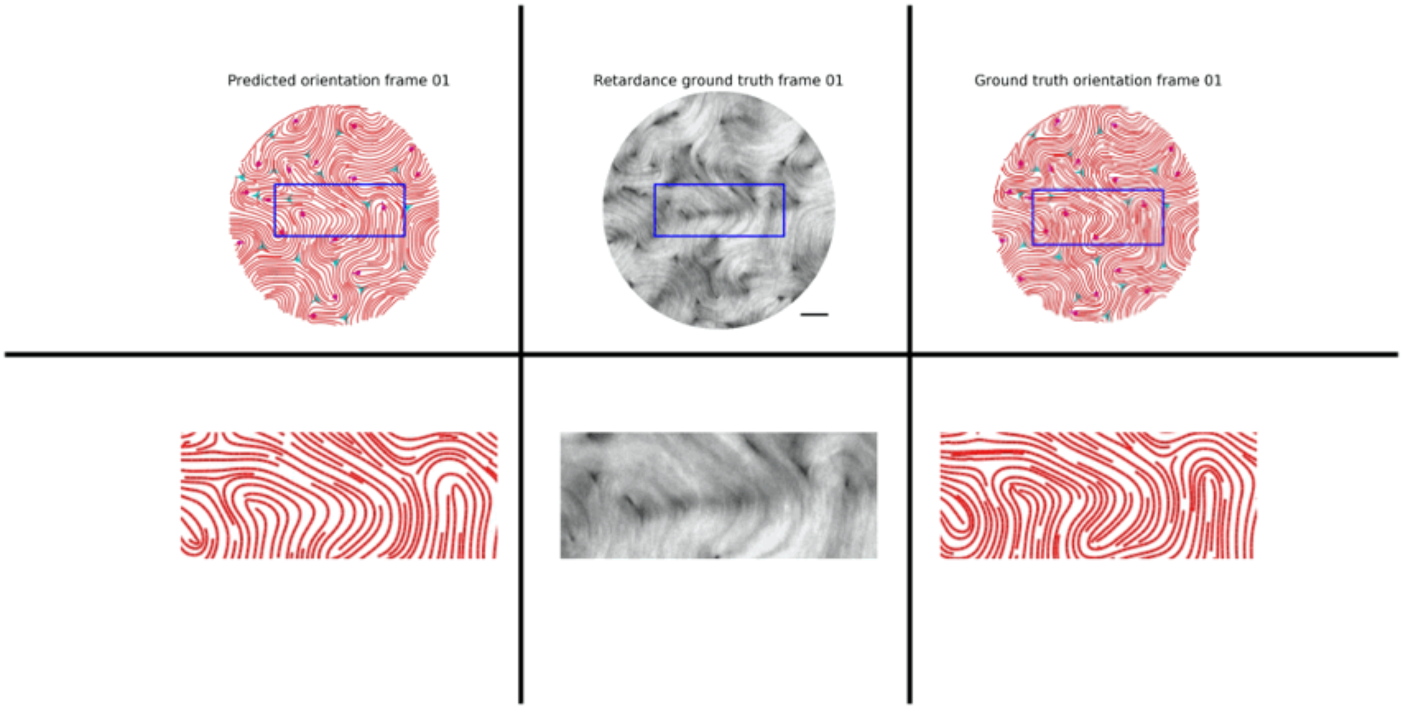
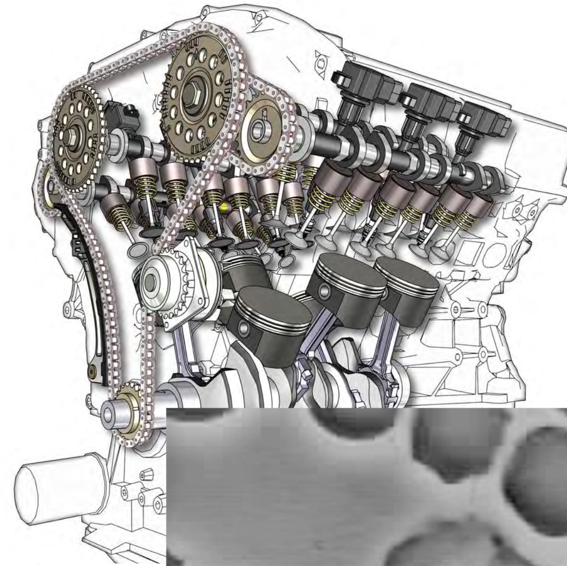
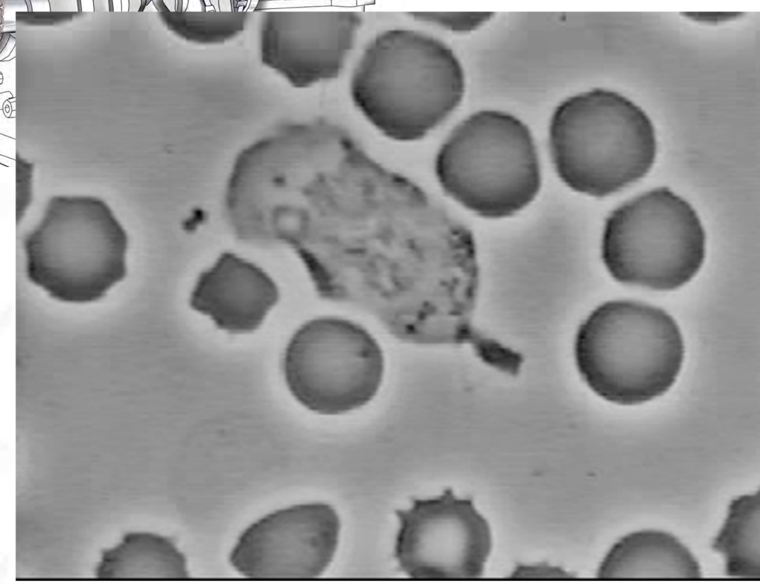
Forecasting model predicts key events



Zhou Z, et al. Machine learning forecasting of active nematics. Soft Matter. Published online 2021:10.1039.D0SM01316A. doi:10.1039/D0SM01316A

Thrust 3: Control of Active Stress





Active control of cell migration/polarization

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Thrust 3: Control of active stress

Model predictive optimal control theory

based on hydrodynamic theory of the active fluid

Reference state penalty

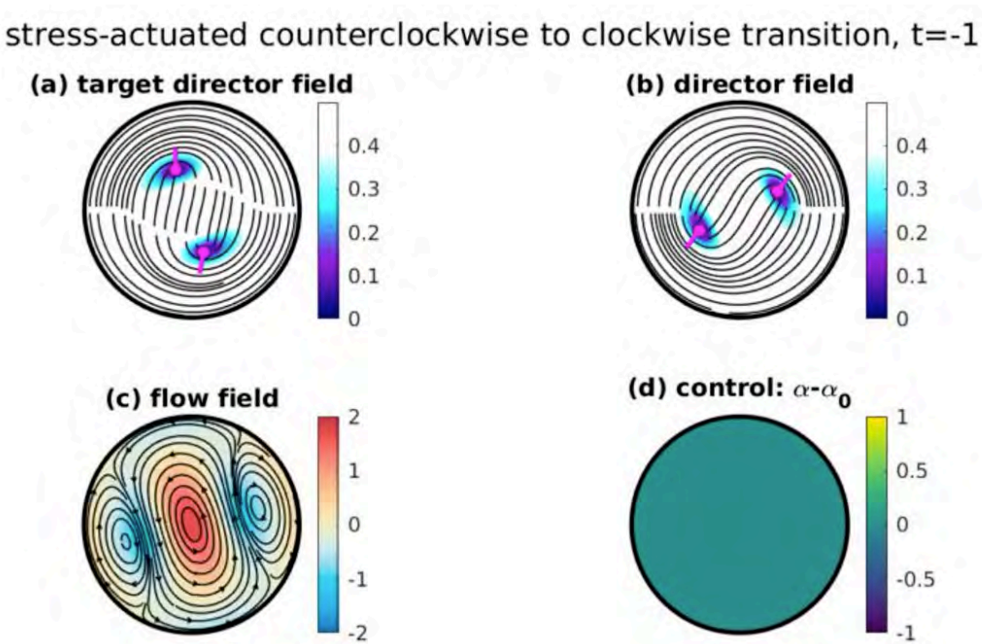
$$\mathscr{H} = \frac{1}{2}\left(\mathbf{Q}-\mathbf{Q}^*(\theta)\right)^\top \mathbf{C}\left(\mathbf{Q}-\mathbf{Q}^*(\theta)\right) + \frac{1}{2}\left(\mathbf{u}-\mathbf{u}^*(\theta)\right)^\top \mathbf{D}\left(\mathbf{u}-\mathbf{u}^*(\theta)\right)$$

Control penalty

$$+\frac{1}{2}(\alpha-\alpha_0)^2 + \boldsymbol{\nu}\cdot\left(-R\partial_t\mathbf{u} + \nabla^2\mathbf{u} - \nabla P - \nabla\cdot\alpha\mathbf{Q}\right) +$$

control input

$$\phi\left(\nabla\cdot\mathbf{u}\right) + \boldsymbol{\psi}\cdot\left(\partial_t\mathbf{Q} + \nabla\cdot(\mathbf{u}\mathbf{Q}) - (\mathbf{Q}\boldsymbol{\Omega} - \boldsymbol{\Omega}\mathbf{Q}) - \lambda\mathbf{E}^\tau - \mathbf{H}\right)$$



M. M. Norton, ***PRL 125***, 178005 (2020)

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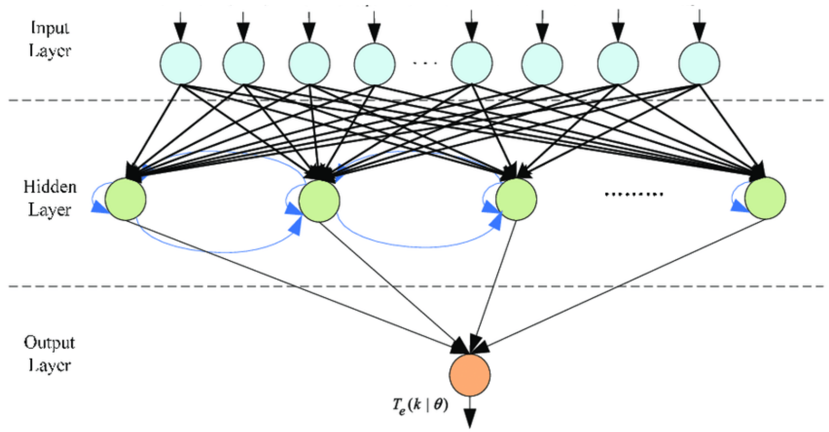
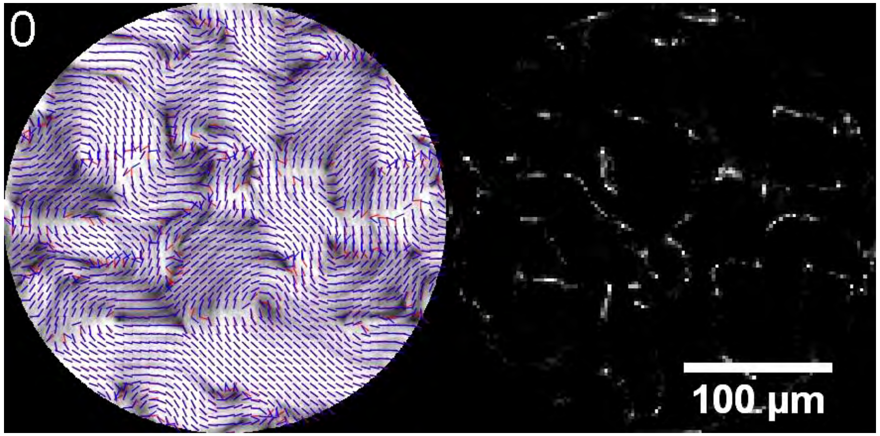
Thrust 3: Control of active stress

Model independent control

Machine learning based forecasting





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IRG2 team

Vision: Establish rational design principles for building 3D adaptive active matter through engineering measurement and control of emergent active stresses

Synergy:

Biomolecular Engineering

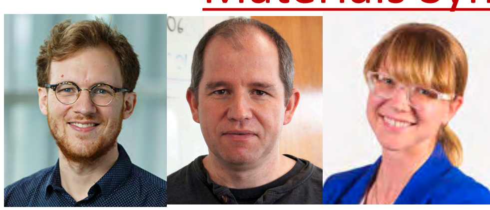
Bisson, Bradshaw, Ramirez San-Juan, Goode

Theory

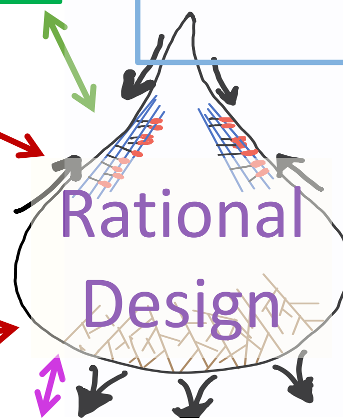
IRG2 leader

Baskaran, Chakraborty, Kondev, Powers, Ramaswamy

Materials Synthesis



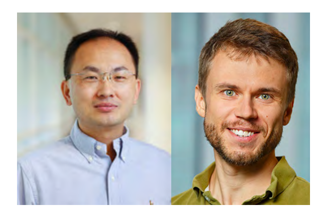
Dogic, Duclos, Ross



Engineering/Microfluidics

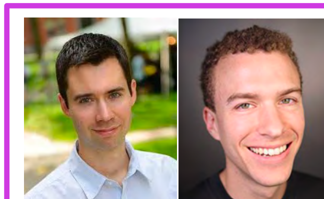
Blair, Fraden

Machine learning



Hong, Wilmes

Computation

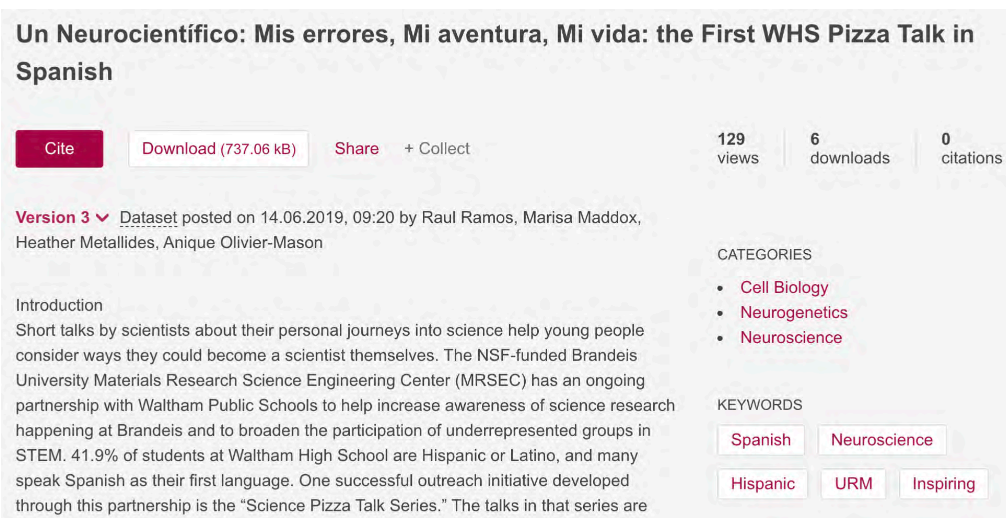


Fai, Hagan

MRSEC iSuperSeed2 update: SciLinkR

SciLinkR is a national web-based tool that simplifies outreach and promotes science:

- SciLinkR matches scientists with the public and creates a repository of outreach reports that credit the scientist who engage in outreach, document best practices, and inspire new science outreach
- Recruited 250 active users to platform through talks and social media, made nationwide connections.



Brandeis bioinspired MRSEC

NSF

MRSEC iSuperSeed2 update: SciLinkR cont.

SciLinkR most benefits outreach professionals

- Outreach professionals seek a platform that organizes and shares coordination, description, and assessment of events/engagements.

Recommendations for next steps

- Collaborating with a national organization for outreach professionals, like ARIS, for recommendations on how to utilize and scale SciLinkR.
- SciLinkR as a database of engagements that collect metrics
- Utilizing a SciLinkR-type platform for the coordination and reporting of volunteer opportunities.

Center for Advancing Research Impact in Society (ARIS)
https://www.researchinsociety.org/

Brandeis bioinspired MRSEC