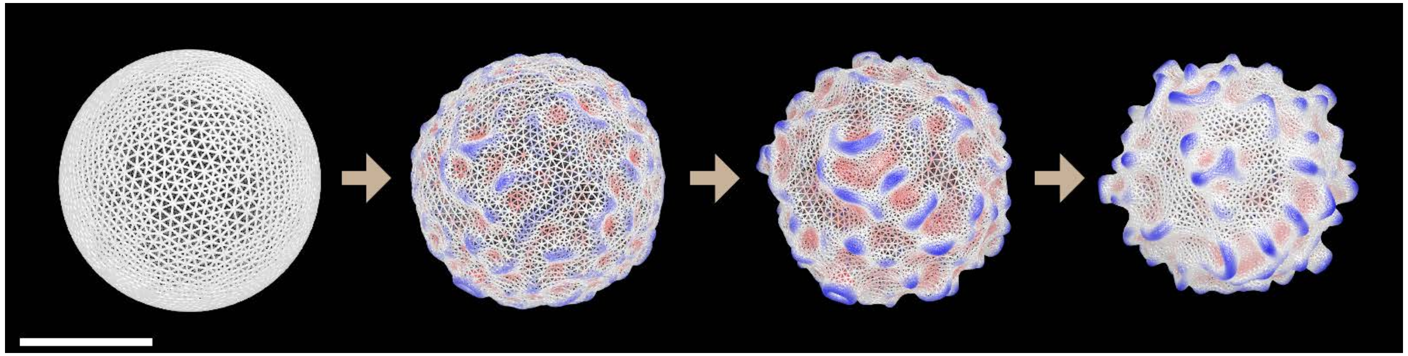
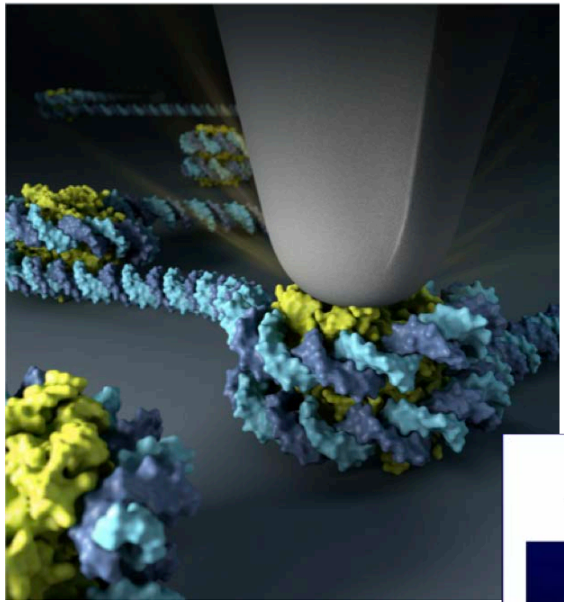
Biological Active Matter. Statistical Mechanics. Protein Physics.

Garegin Papoian

Molecular Modeling of the Cell

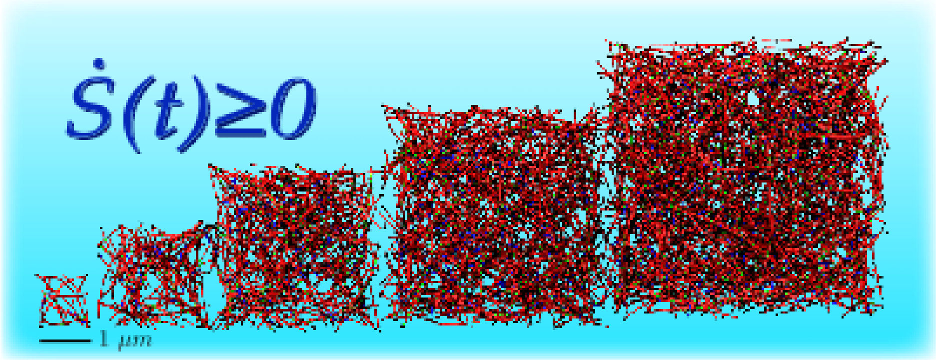


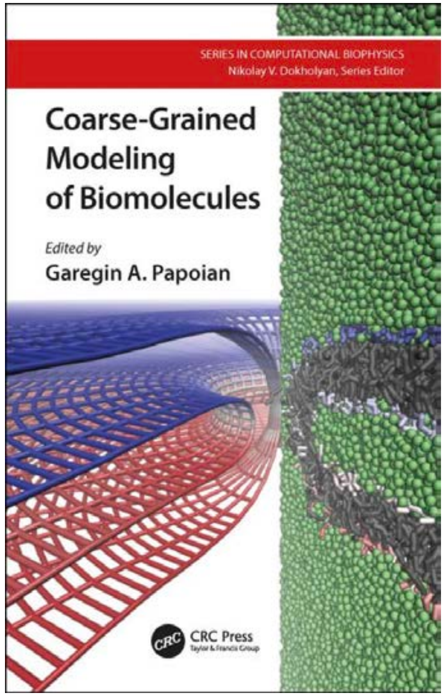
Chromatin



Molecular Dynamics

Entropy Production of the Cytoskeleton





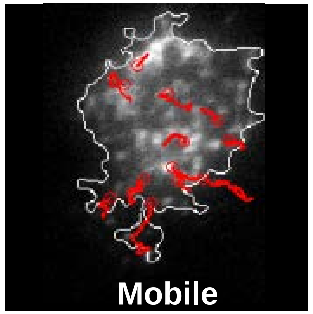
Coarse-Graining

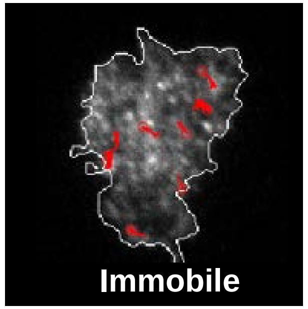
PNAS 2019 DOI: 10.1073/pnas.1911880116; Interface Focus 2019 10.1098/rsfs.2018.0078; "Coarse-Grained Modeling of Biomolecules, Publisher CRC Press, edited by G. A. Papoian

Mechanobiology of immune response and gene regulation

Immune receptor dynamics

Regulation of T & B cell signaling

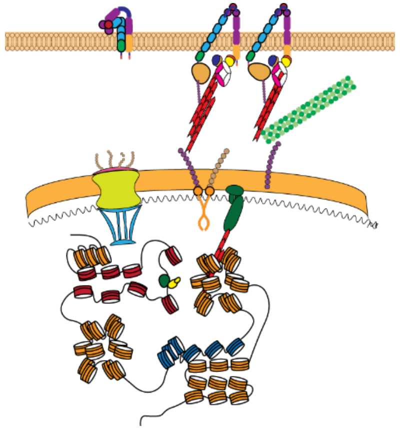


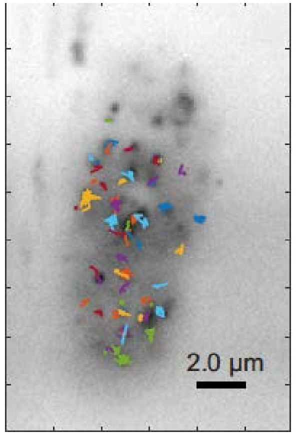


Biophys J. 2014, Nature Comm., 2020

Gene regulation

Imaging of transcription factor dynamics in live cell nuclei

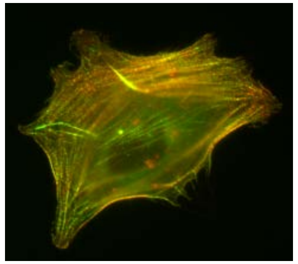




Molecular Cell, 2019

Arpita Upadhyaya

arpitau@umd.edu



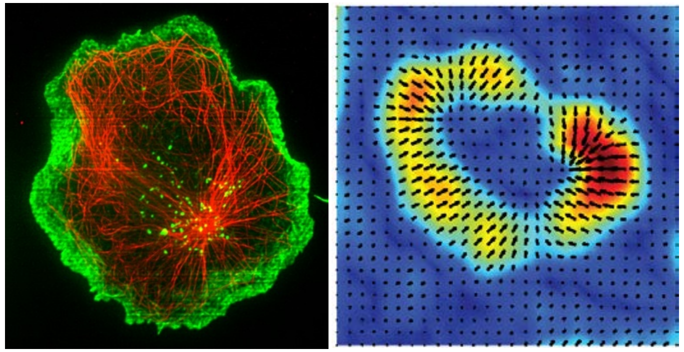
How do cells sense and respond to physical cues?

- **Stiffness**
- **Topography**
- **Mobility**

Techniques:

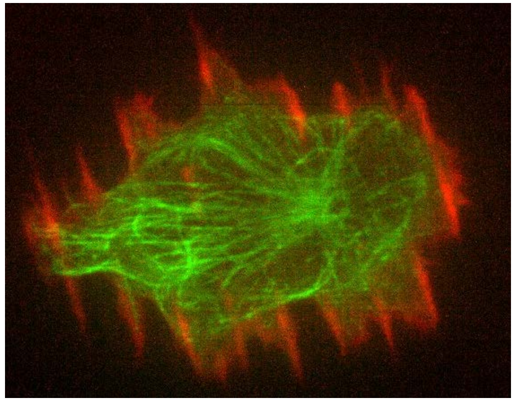
Single molecule imaging
Traction force microscopy
Super-resolution microscopy
Computational image analysis

Cellular Force generation



Mol. Biol. Cell 2015, PNAS, 2018

Cytoskeletal dynamics

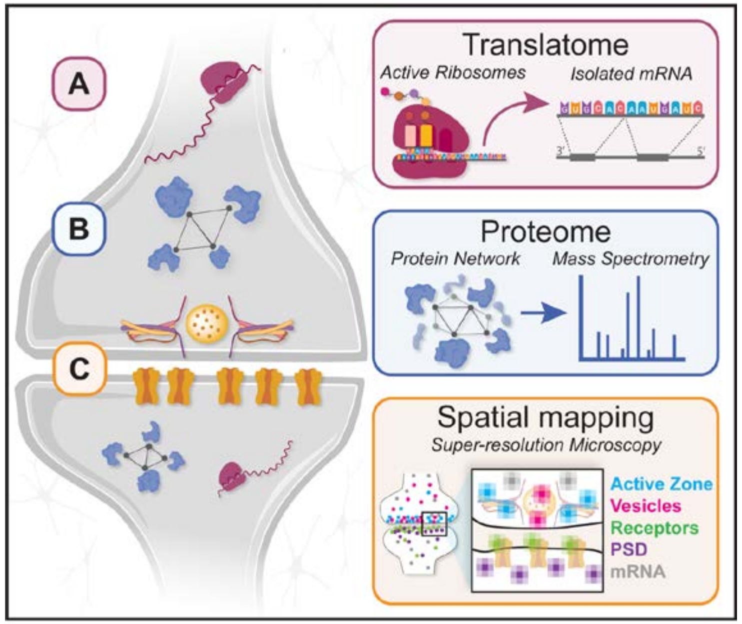


Mol. Biol. Cell 2018

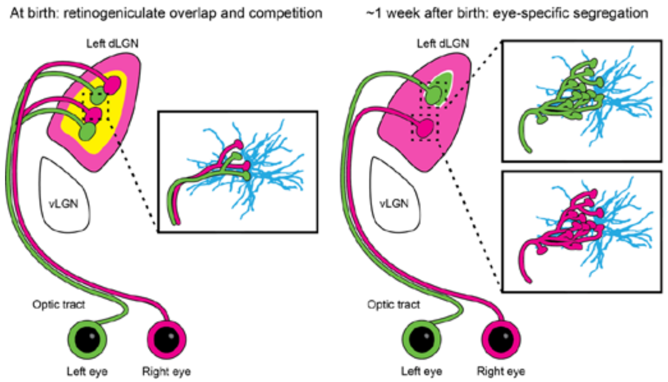
Multi-scale analysis of synaptogenesis and plasticity in developing circuits

SPEER LAB

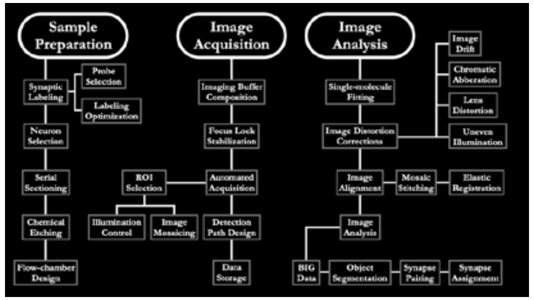
We investigate synapse development from the translatome → proteome → structure.



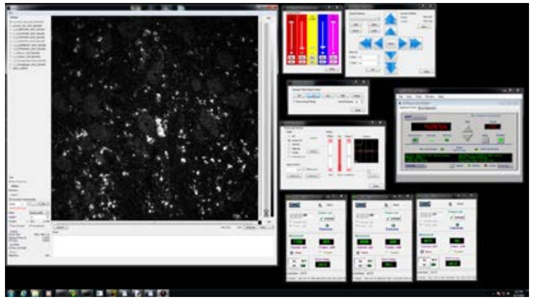
Using mammalian visual circuits as a model system…



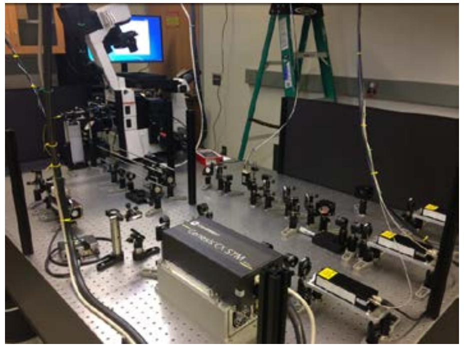
we build and validate new tools…



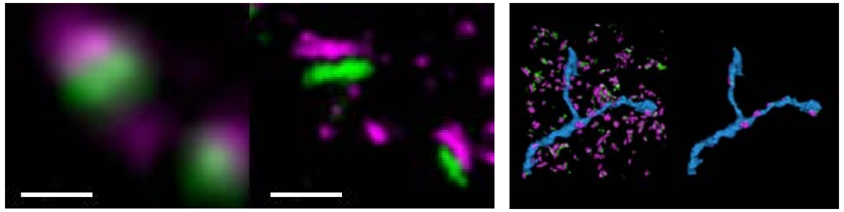
including image analysis and control software…

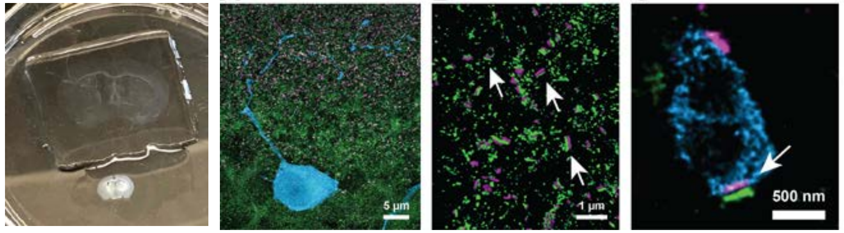


super-resolution image acquisition hardware…

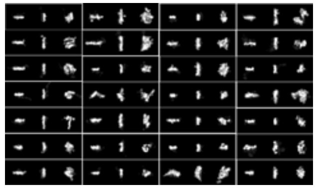


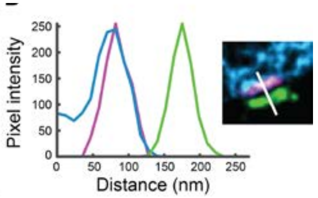
and labeling wetware for synaptic and cellular imaging.

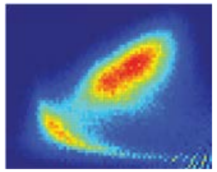


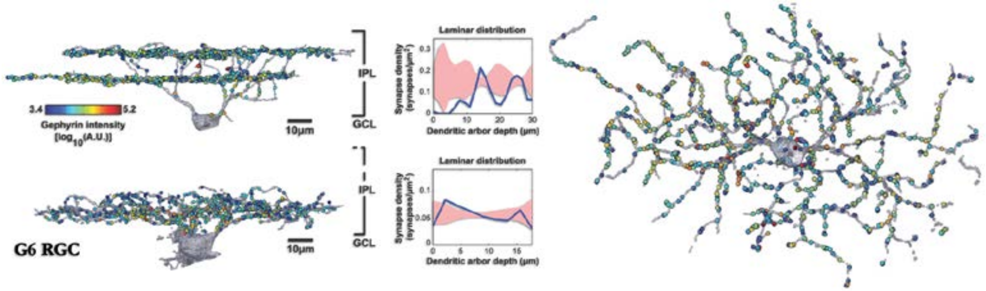


Using automated image classification and analysis, we investigate the molecular basis of synaptogenesis.





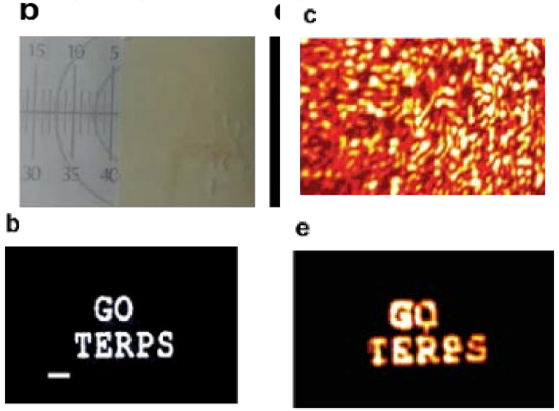




Light-Matter Interactions in the Bio-Universe

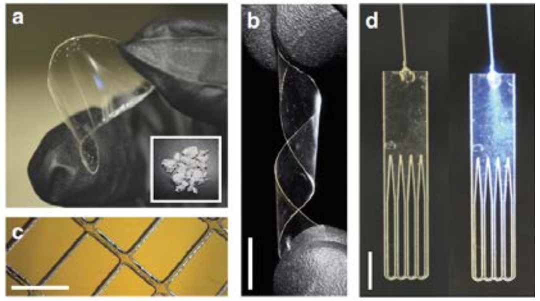
G. Scarcelli

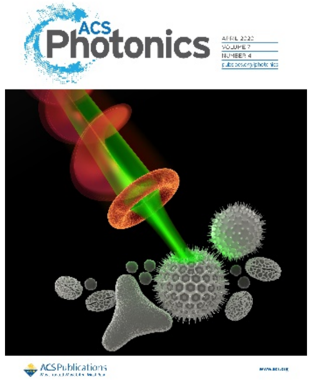
Imaging through turbid media



Edrei & Scarcelli, Optica (2016)

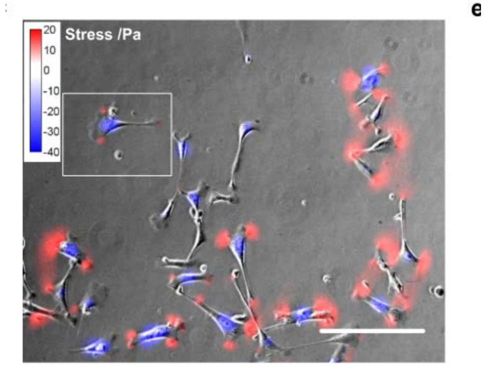
Bio - Optics





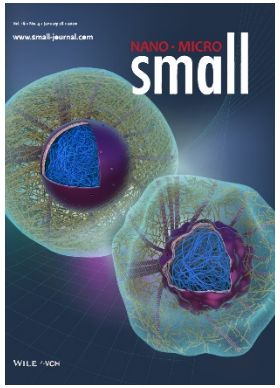
Nizamoglu et al. Nature Comm. (2016)
Edrei & Scarcelli, ACS photonics 2020

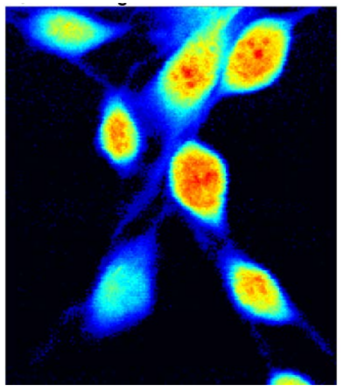
Soft-matter resonators to map forces



Kronenberg et al, Nature Cell Bio (2017)

Photon-phonon probe to map stiffness

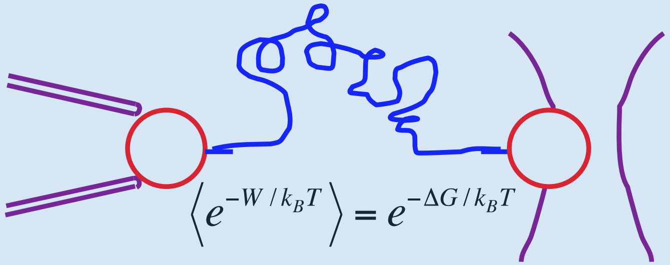


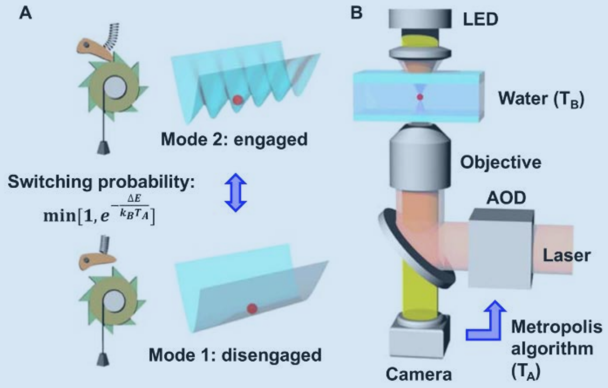


Scarcelli & Yun, Nature Photonics (2008)
Scarcelli et al, Nature Methods (2015)

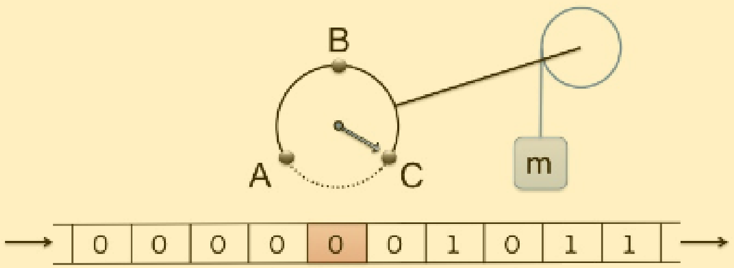
Theory and Computation in the Jarzynski group

Thermodynamics at the nanoscale

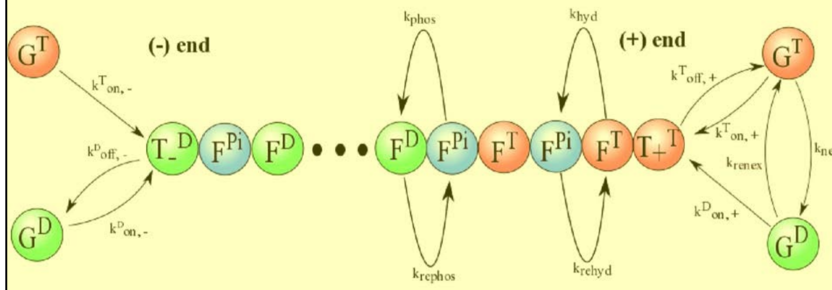




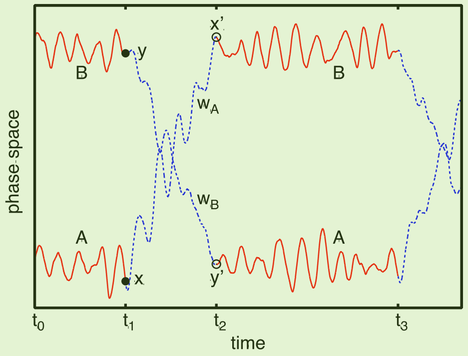
Physics of information processing



Biophysics out of equilibrium



Computational thermodynamics



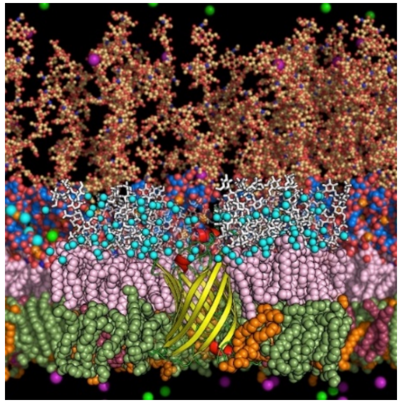
Chris Jarzynski
cjarzyns@umd.edu
(301) 405-4439

Molecular Modeling: *Cell Membranes and Associated Proteins*

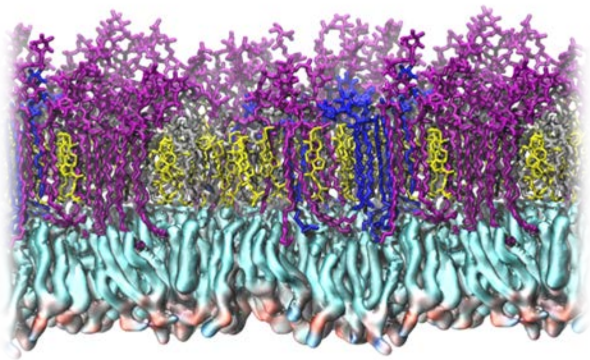
Cell Membranes

Jeff Klauda

Outer Membrane of E. Coli[1]



Plasma Membrane of Yeast

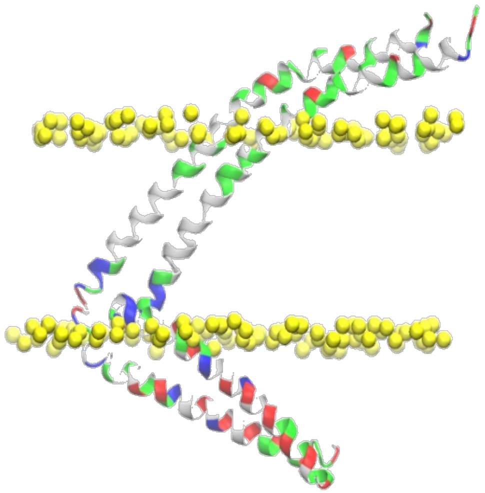


Stratum Corneum Layer of Skin[2]

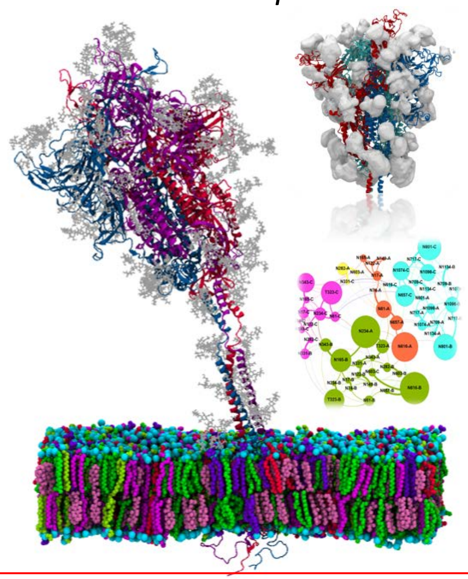
- Modeling of organism and organelle membranes at physiological concentrations[1,2]
- Dimerization of proteins involved in neuronal, bone and cancer growth[3]
- COVID-19 Research on Spike Protein[4]
- Activation of the Serotonin Receptor[5]
- Peptide-membrane interactions with applications to anti-microbial peptides (AMPs)[6]

Membrane-Associated Proteins

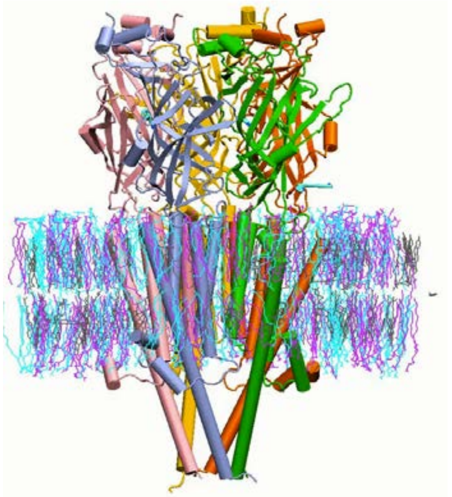
PlexinA3 homodimerization[3]



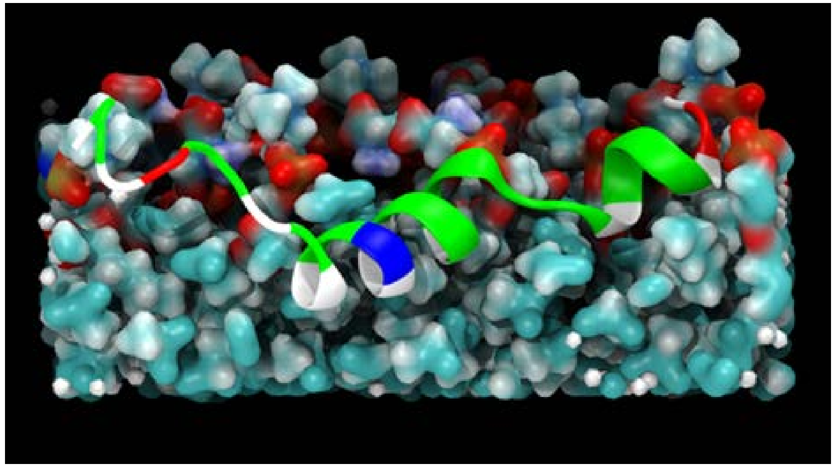
COVID-19 Spike[4]



Serotonin Receptor[5]



Peptide-membrane Binding[6] *and AMPs*



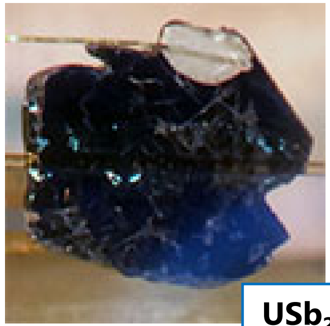
[1]*Biophys. J.* **106**: p2493 (2014). [2]*JACS*. **141**: p16930 (2019). [3]*Biochem*. **55**: 4928 (2016). [4]https://doi.org/10.1101/2020.09.28.317206. [5]*PNAS*. **117**: p405 (2020). [6]*JPCB*. **122**: p9713 (2018).

Quantum Materials: Magnetism, Superconductivity, Topology

Materials Synthesis

Cu_2OSeO_3

UTe_2

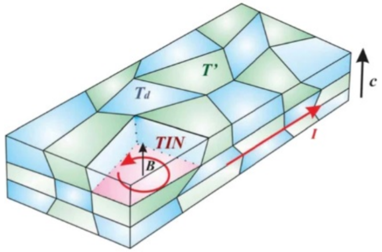


USb_2

Quantum + Topological Physics

"Lazarus" extreme high field reentrant superconductor (UTe_2)

Chiral surface states in a topological superconductor (UTe_2)



Topological Interface Network under pressure ($MoTe_2$)

Extreme Environments, Big Experiments

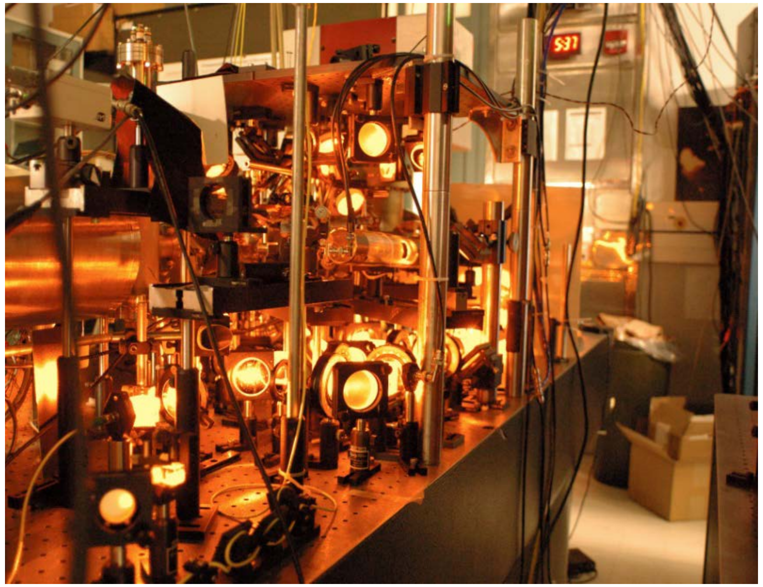
Pulsed Field Facility, Los Alamos National Lab – high magnetic field experiments to 65 T and up

NIST Center for Neutron Research (nearby) – studying quantum magnetic excitations

Nicholas Butch
NIST & Physics

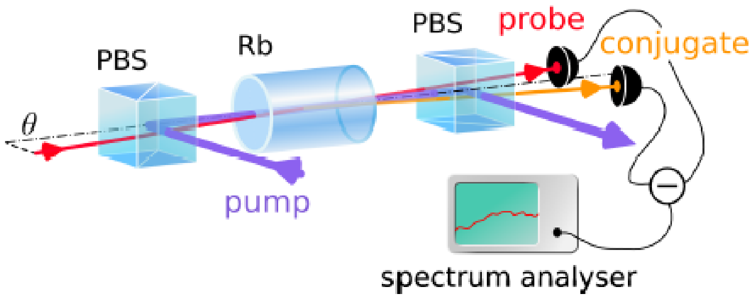
Cold atom physics and Nonlinear/Quantum Optics

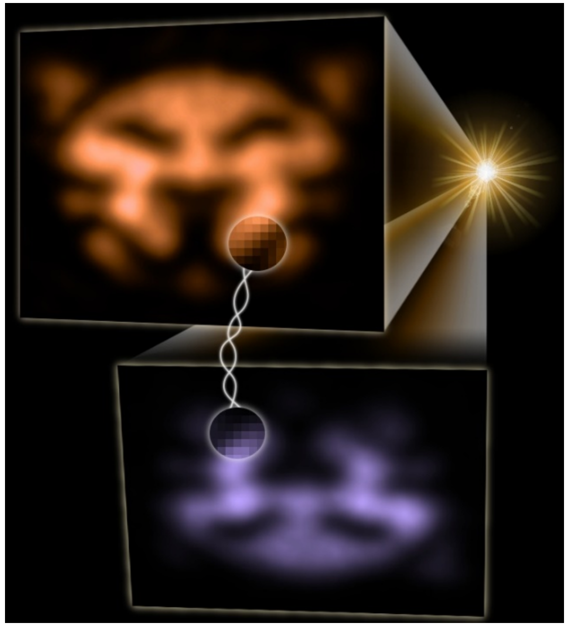
Paul D. Lett – National Institute of Standards and Technology / Joint Quantum Institute
UMD Chemical Physics Program

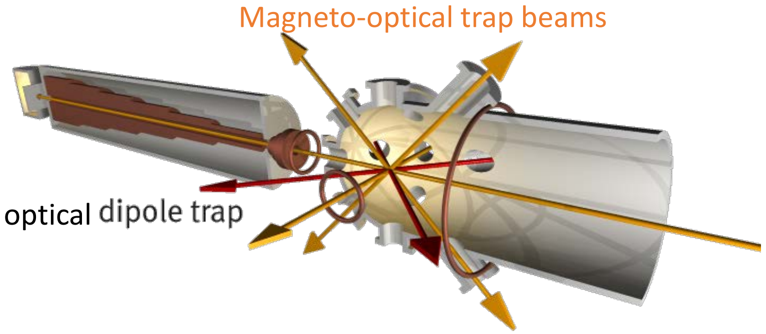


Spinor Bose-Einstein condensate Investigations in sodium vapor. Atoms in a superposition of spin states evolve and interact as a complex quantum many-particle system.

4-wave mixing in atomic vapors to generate quantum-entangled images and improve optical measurements.

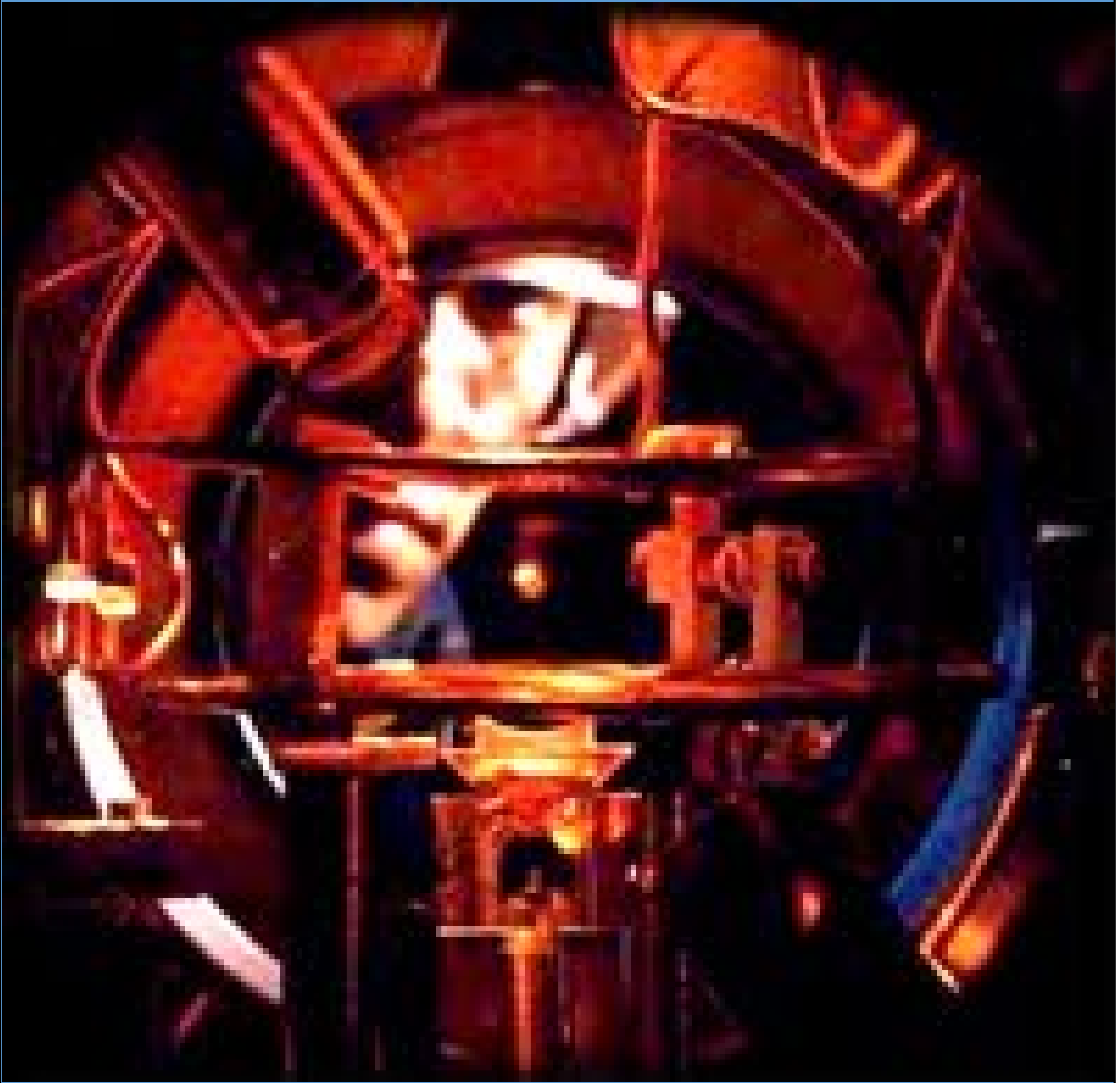






We study both the fundamental physics of entangled atoms and photons, as well as their applications to precision measurements and quantum sensing.

microkelvin atoms suspended in vacuum



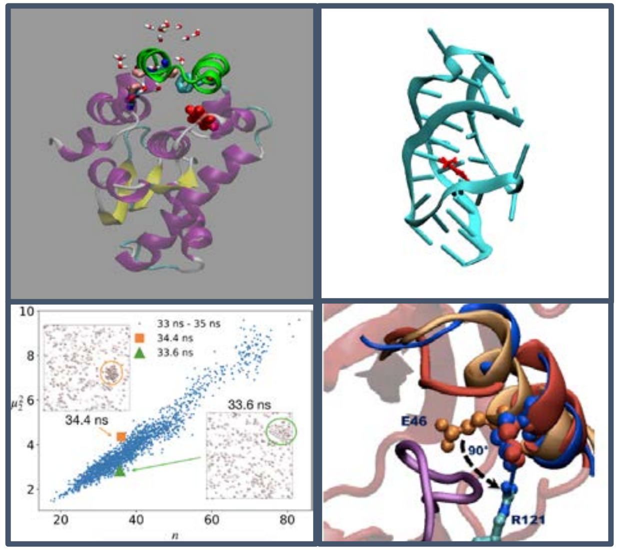
william.phillips@nist.gov wdp@umd.edu

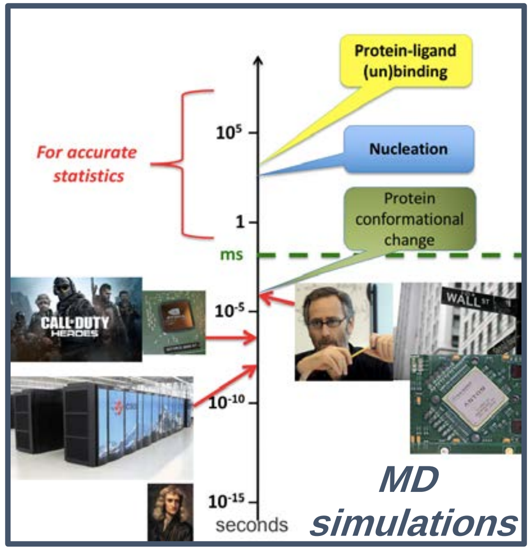
Laser Cooling and Trapping Group: NIST/JQI

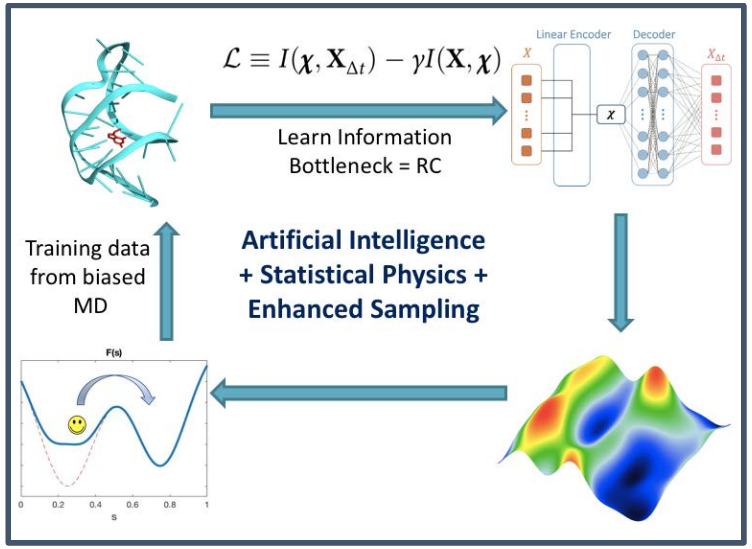
In laboratories on both the National Institute of Standards and Technology and University of Maryland campuses of the Joint Quantum Institute, our group studies the coldest materials in existence. Cold atoms and quantum degenerate gases are the starting points for a variety of research directions in experimental and theoretical quantum science:

- Cold quantum chemistry
- Quantum Information Science
- Quantum simulation and computing
- Squeezed light—beyond quantum limits
- Topological matter
- Quantum thermodynamics
- Atomtronics
- More…

From atoms to mechanisms: with a little help from AI and Stat Phys







Complex problems in chemical and biophysics

We develop & apply new simulation methods

Tiwary research group, University of Maryland

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

@tiwarylab

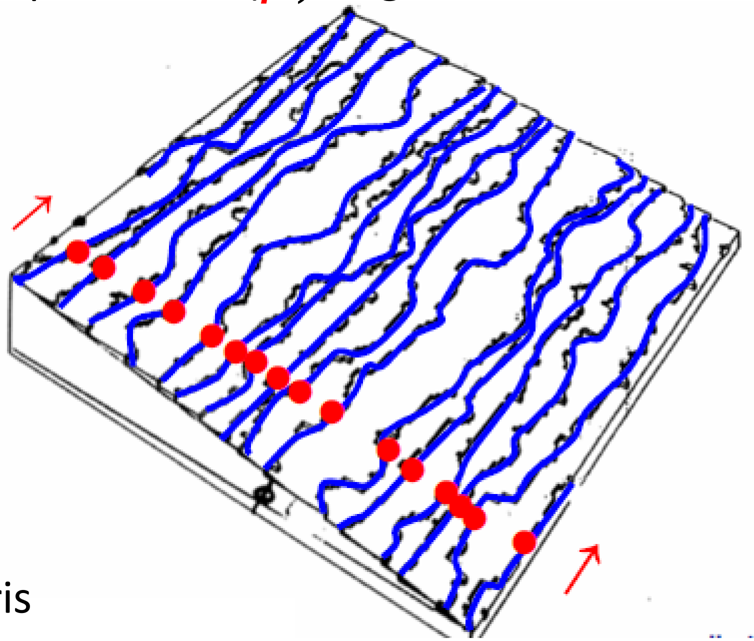
Institute for Physical Science & Technology IPST

Ribeiro, Bravo, Wang, Tiwary ***J. Chem. Phys. 2018***
Wang, Ribeiro, Tiwary ***Nature Comm. 2019***
Smith, Ravindra, Wang, Cooley, Tiwary ***J. Phys. Chem. B 2020***
Tsai, Smith, Tiwary ***J. Chem. Phys. 2019***
Ravindra, Smith, Tiwary ***Mol. Sys. Des. Engg. 2020***
Tsai, Kuo, Tiwary ***Nature Comm. 2020***

Analyzing Distributions at the Nanoscale & Human Scale with a Celebrated Formula for Fluctuations

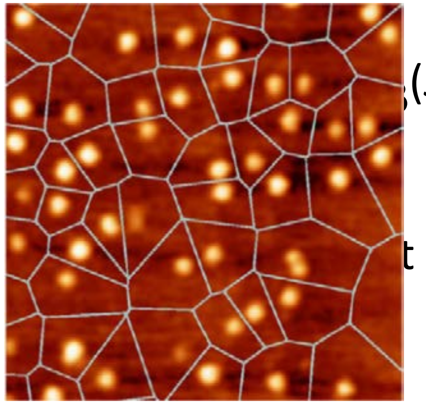
Distributions of spacings between energy levels in nuclei depend only on symmetry → single parameter (β) Wigner surmise:

$P_\beta(s) = a_\beta\, s^\beta \exp(-b_\beta s^2)$, $\beta = 1, 2, 4$, where s is spacing/⟨spacing⟩



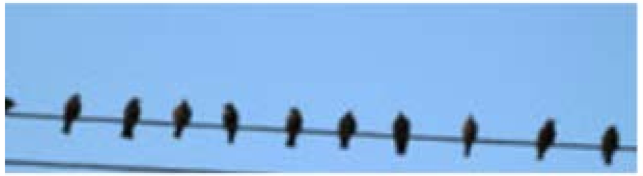
Next consider 2D config'ns of [non-crossing] steps on vicinal (tilted, stepped) surfaces maps to world lines of repelling fermions in 1D (evolving in time)

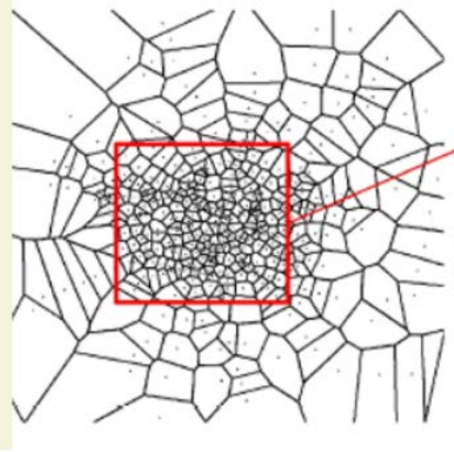
Describe step-separation distribution by $P_\beta(s)$, $\beta \geq 1$: β from arbitrary step repulsion

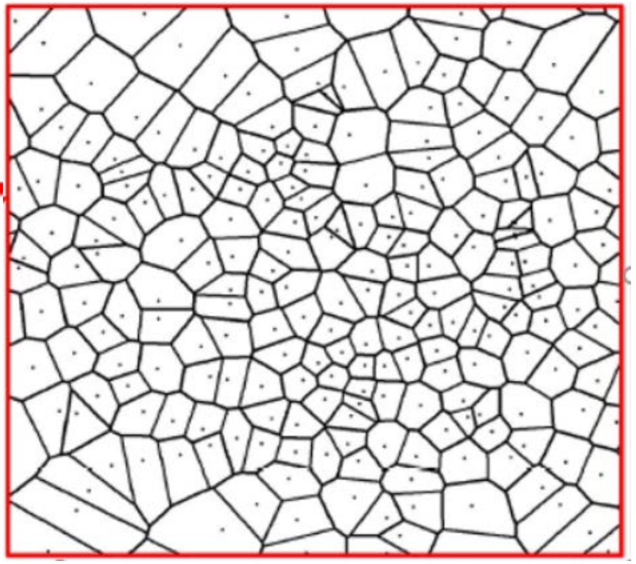


(s) describes distribution of areas of proximity (Voronoi) cells around random points, e.g. quantum dots

t human scale, it can describe spacings between parked cars, between birds on a wire, distributions of subway stations (e.g. Paris Metro), areas of counties in SE USA or French districts







Ted Einstein

Complex Fluids and (Soft) Nanomaterials

COMPLEX FLUIDS & NANOMATERIALS

http://complexfluids.umd.edu

Prof. Srinivasa R. Raghavan

Patrick & Marguerite Sung Professor
Dept. of Chemical & Biomolecular Engineering
University of Maryland, College Park

Office: 1227C Chem-Nuc Building

Phone: (301) 405-8164

Email: sraghava@umd.edu

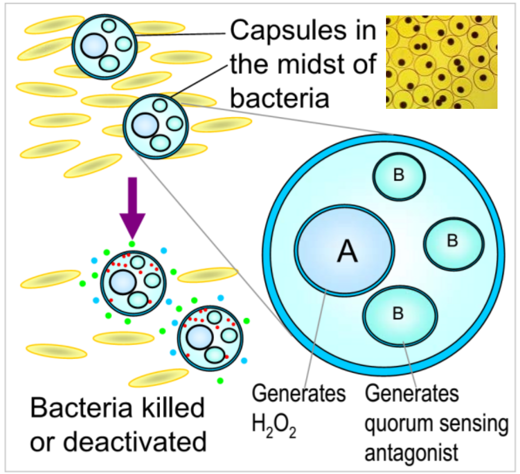
Bio | CV | Google Scholar

Group Photo: 2019

Amphiphilic polymers that stop bleeding.

We have discovered polymers that convert liquid blood into a gel via hydrophobic interactions.

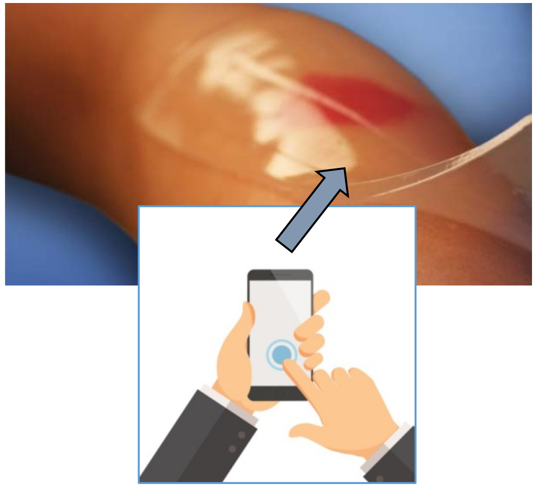
These are being used to stop bleeding from massive injuries.



Microcapsules mimicking the architecture of cells.

We have made capsules with many inner compartments, similar to organelles in a cell.

These are being used as agents to kill or deactivate bacteria.



Drug delivery triggered by external stimuli.

We are using electrical signals as well as irradiation by X-rays to induce drug delivery.

One use is in wireless delivery of drugs through skin to treat pain.

Keywords associated with research:

- *Self-assembly; smart fluids; nanostructured fluids; micelles; vesicles; rheology; neutron scattering*
- *Bionanotechnology; drug delivery; hydrogels; microcapsules; stimuli-responsive/smart materials*

Dynamics of Living Systems

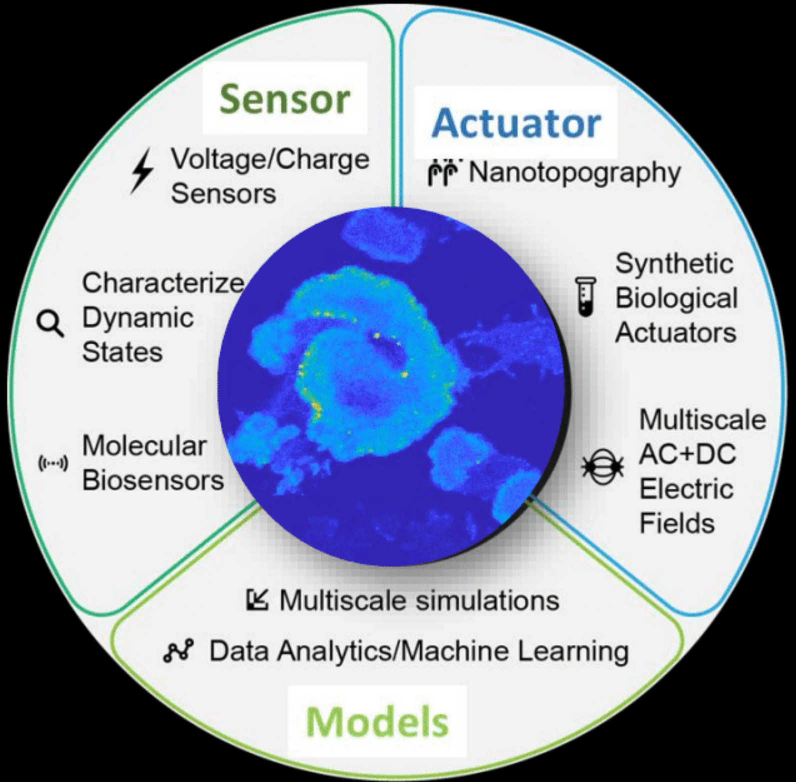
Wolfgang Losert

University of Maryland

MURI

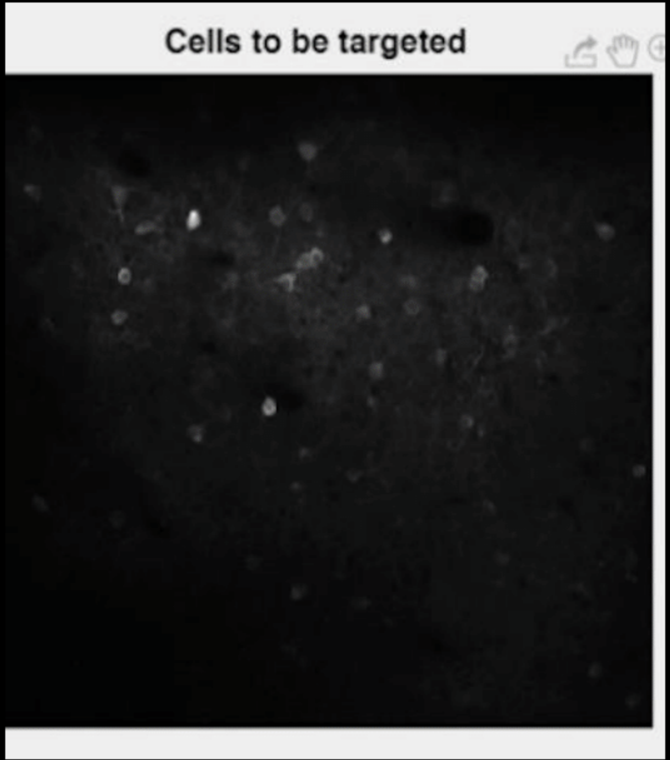
Excitable Systems in Cells

Precise control of Intracellular Biochemical Waves



Dynamic Neural Networks

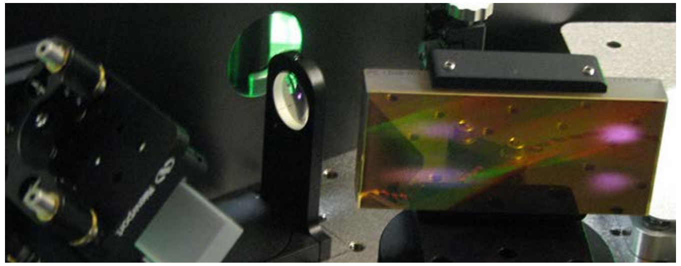
Analysis and Control of Neural systems in vitro and in vivo



Dynamics of Living Systems Team

- Life Cell Microscopy
- Data Analytics and AI
- Models

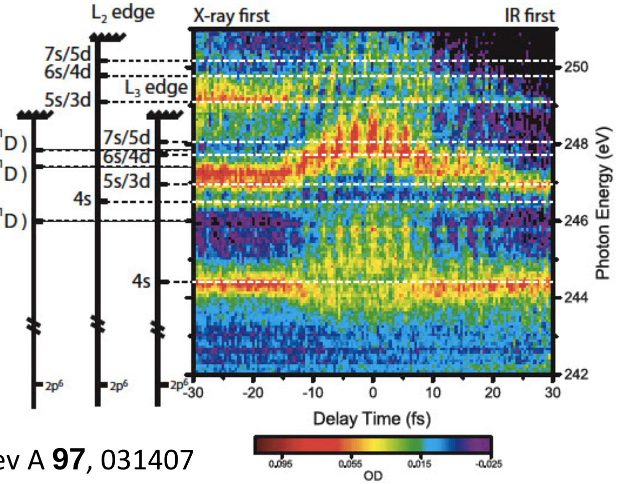
ireap.umd.edu/losertlab



Wendell Hill's AMO Lab

Quantum dynamics under extreme conditions

Fig. 2



Phys Rev A **97**, 031407

Ultrafast: Photoinduced charge separation in molecules is the first step in many chemical processes and central to our understanding of electron correlation and the energy exchange between electronic and nuclear motion. Catalysis, photosynthesis, photovoltaics and radiation damage in biomolecules all depend on this dynamics. We study these processes with femtosecond and attosecond pulses. Figures 1 and 2 are examples near the Ar L-edge, i.e., the displacing of 2p electrons.

Fig. 1

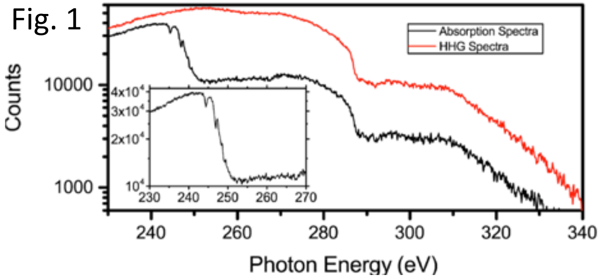
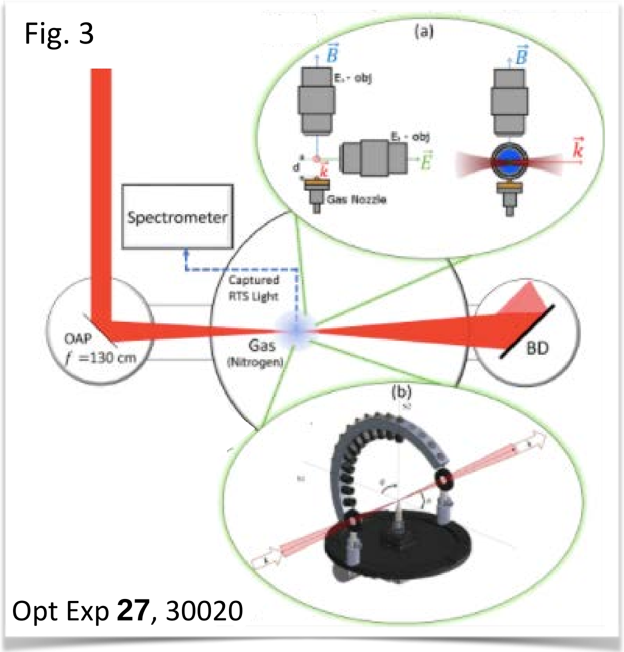


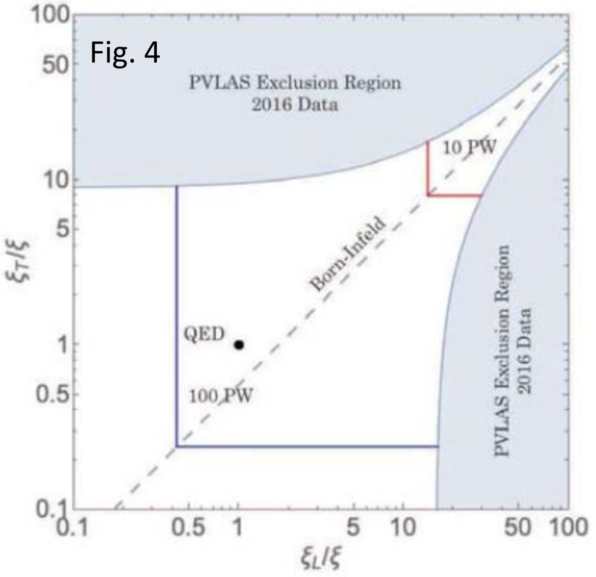
Fig. 3



Opt Exp **27**, 30020

Ultraintense: Petawatt-class lasers have placed us at the threshold of a new era where novel experiments of nonlinear aspects of electrodynamics -- quantum electrodynamics (QED) -- will be possible. We are developing technology to study virtual electron-positron pairs, the birefringence of the quantum vacuum and testing QED from the photon side. Figure 3 shows a potential technology for measuring extreme intensities while Fig. 4 indicates the predicted strength of the birefringence of the quantum vacuum.

Fig. 4



J Phys: Conf. Series **869**, 012015

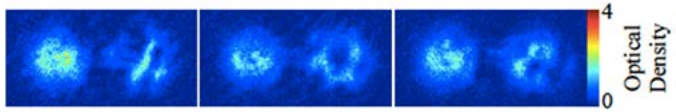


Fig. 5. Phys Rev A **93**, 063619

Ultracold: Ultracold atoms have revolutionized how some key questions in physics and chemistry are being addressed by providing a platform to study longstanding problems that are difficult, if not impossible to study otherwise. We are interested in exploiting these degenerate ensembles of gases (see for example, Fig. 5) to study fundamental questions related to the time-scale for tunneling.

Two-Dimensional Quantum Materials & Devices Innovation

Cheng Gong Dept. ECE cgong.weebly.com

Physical dimension of quantum materials: **sub-nanometer**

- **~ $\frac{1}{100{,}000}$ of the diameter of human hair.**
- **Quantum mechanics** dominates the material properties in such tiny space.
- Unprecedented platforms for **disruptive, miniaturized quantum devices**.

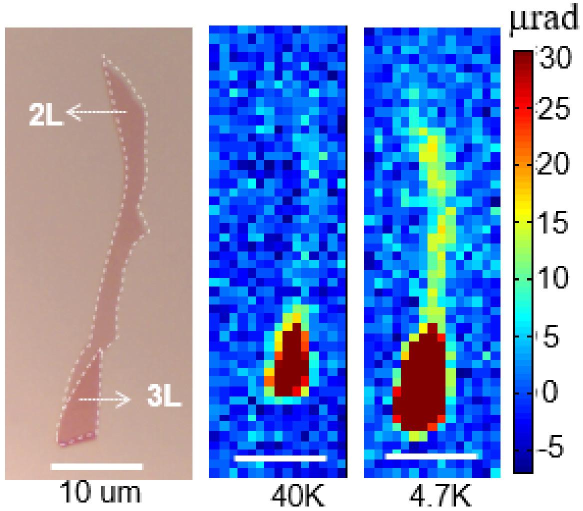
Nature *546*, 265 (2017).

Science *363*, eaav4450 (2019).

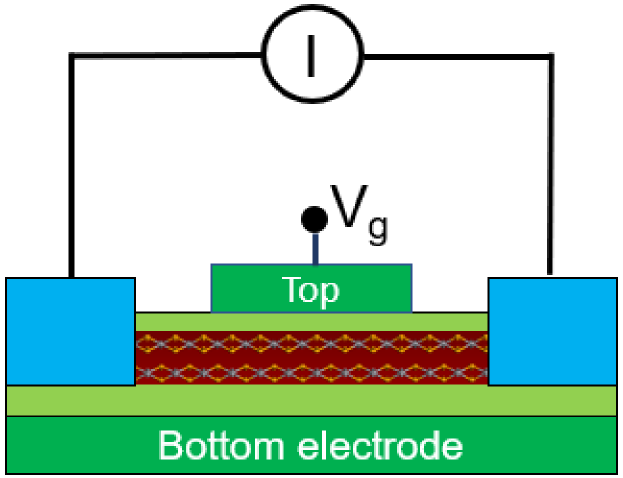
Nat. Commun. *10*, 2657 (2019).

PNAS. *115*, 8511 (2018).

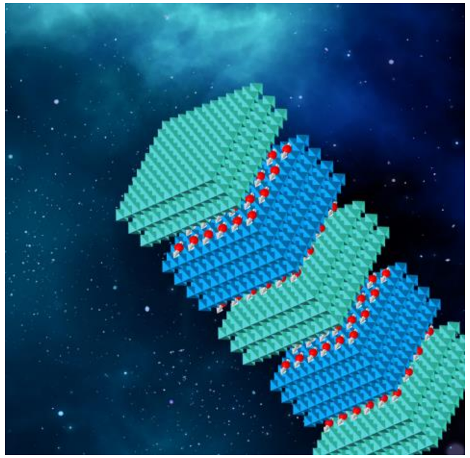
Nano Lett. *20*, 7230 (2020).



Light-matter interaction

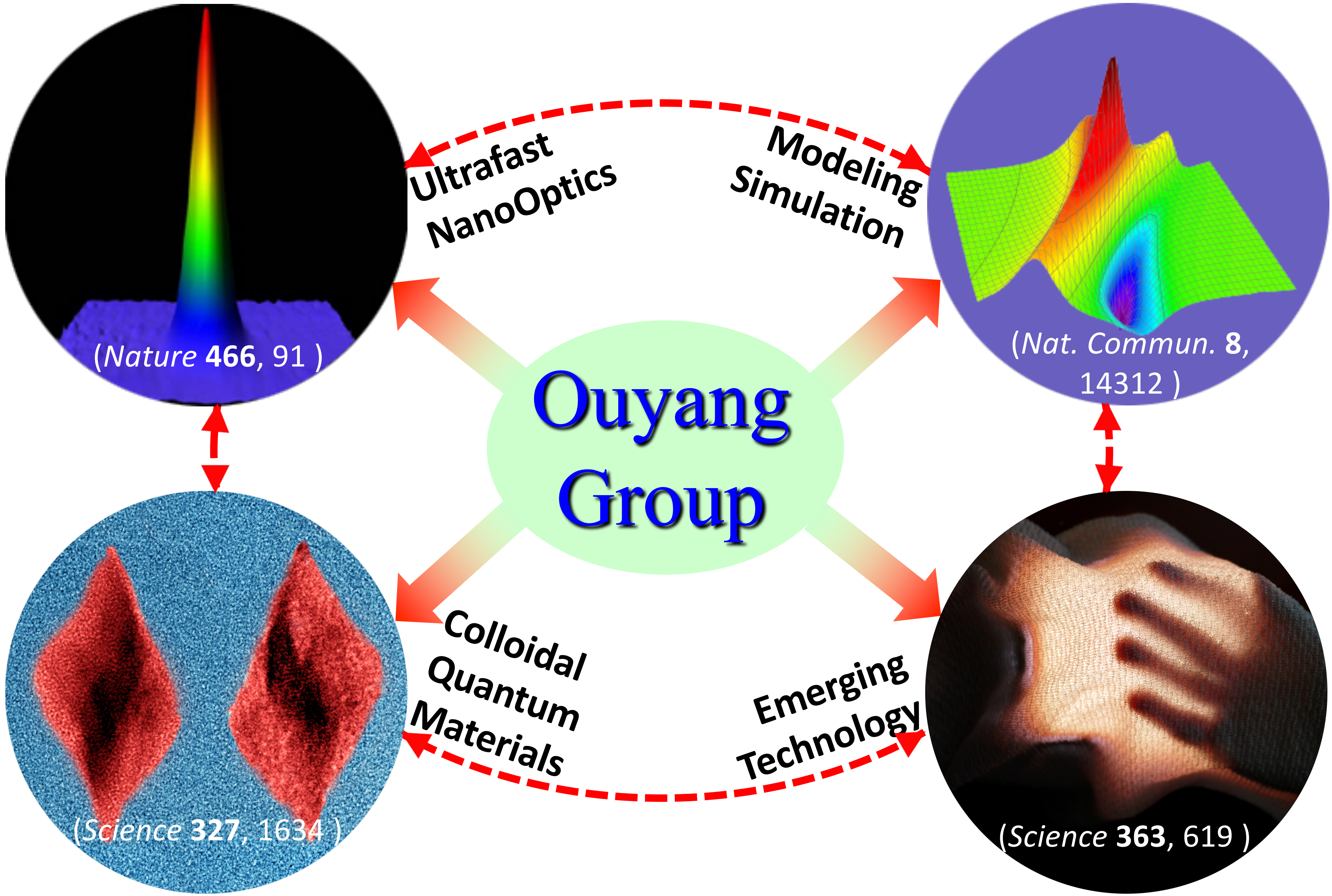


Spintronic devices



Material simulation

Probing and Controlling Nanoscale Chemical and Physical Processes



mouyang@umd.edu

Experimental Neutron Interferometry at the NIST Center for Neutron Research

Generation and detection of spin-orbit coupled neutron beams

Dusan Sarenac[a,1], Connor Kapahi[a,b], Wangchun Chen[c,d], Charles W. Clark[e], David G. Cory[a,f,g,h], Michael G. Huber[i], Ivar Taminiau[a], Kirill Zhernenkov[a,j,k], and Dmitry A. Pushin[a,b]

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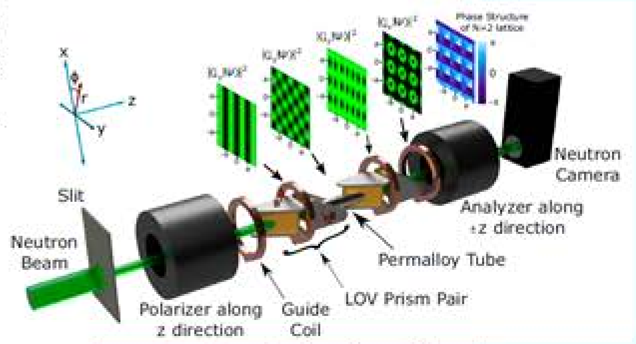
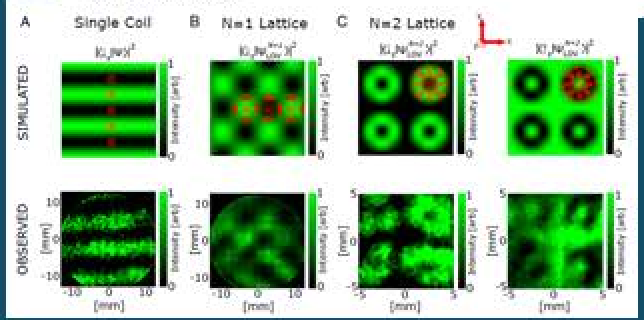
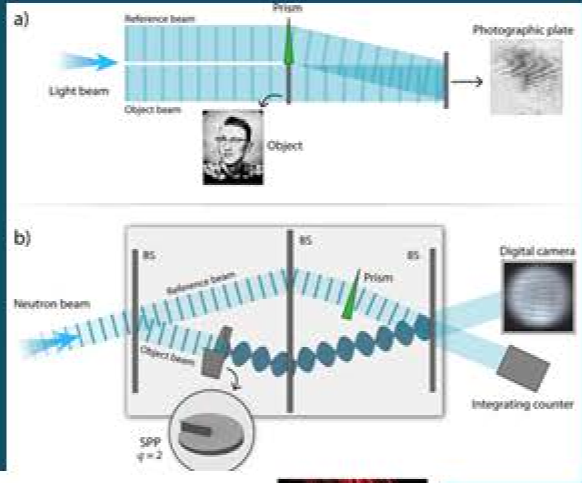
Science and Engineering, University of Maryland, College Park, MD 20742; ...
University of Maryland, College Park, MD 20742; [f]Department of Chemistry, ...
for Theoretical Physics, Waterloo, ON N2L 2Y5, Canada; [h]Canadian Institute ...
Measurement Laboratory, National Institute of Standards and Technology, G...
Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, 85748 Garching, ...
Research, 141980 Dubna, Moscow Region, Russia

Edited by Anton Zeilinger, University of Vienna, Vienna, Austria, and approv...

Spin-orbit coupling of light has come to the fore in nanooptics and plasmonics, and is a key ingredient of topological photonics and chiral quantum optics. We demonstrate a basic tool for incorporating analogous effects into neutron optics: the generation and detection of neutron beams with coupled spin and orbital angular momentum. The ^{3}He neutron spin filters are used in conjunction with specifically oriented triangular coils to prepare neutron beams with lattices of spin-orbit correlations, as demonstrated by their spin-dependent intensity profiles. These correlations can be tailored to particular applications, such as neutron studies of topological materials.







Holography with a neutron interferometer

Dusan Sarenac, Michael G. Huber, Benjamin Heacock, Muhammad Arif, Charles W. Clark, David G. Cory, Chandra B. Shahi, and Dmitry A. Pushin

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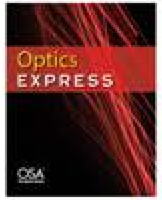


LETTER

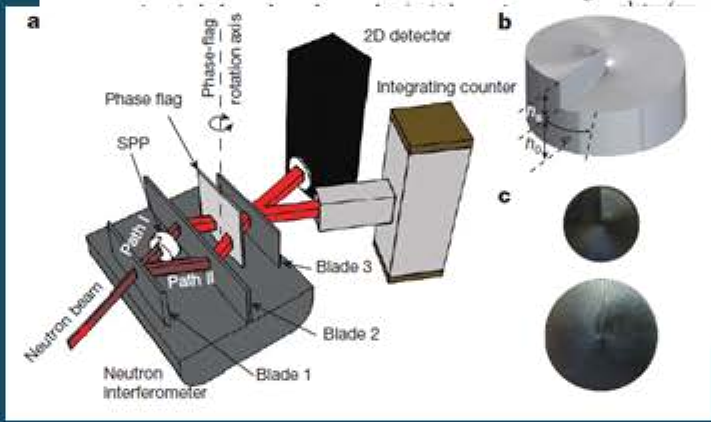
doi:10.1038/nature15265

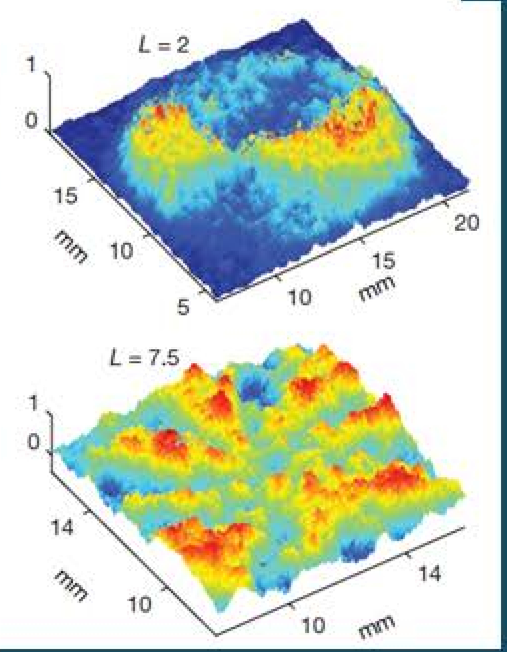
Controlling neutron orbital angular momentum

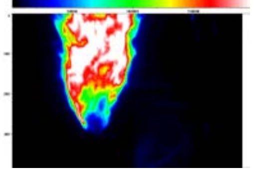
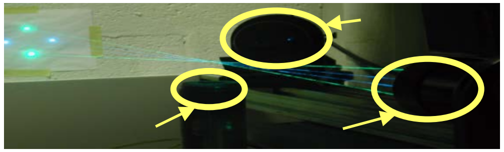
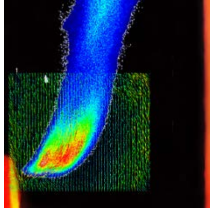
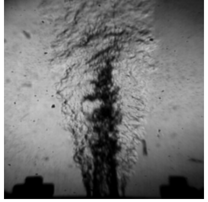
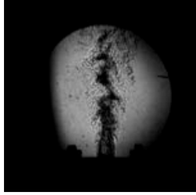
Charles W. Clark[1], Roman Barankov[2], Michael G. Huber[3], Muhammad Arif[3], David G. Cory[4,5,6,7] & Dmitry A. Pushin[6,8]

The quantized orbital angular momentum (OAM) of photons[1] offers an additional degree of freedom and topological protection from noise. Photonic OAM states have therefore been exploited in various applications[2,3] ranging from studies of quantum entanglement and quantum information science[4–7] to imaging[8–12]. The OAM states of electron beams[13–15] have been shown to be similarly useful, for example in rotating nanoparticles and determining the chirality of crystals[16–19]. However, although neutrons—as massive, penetrating and neutral particles—are important in materials characterization, quantum information and studies of the foundations of quantum mechanics, OAM control of neutrons has yet to be achieved. Here, we demonstrate OAM control of neutrons using

micrometre... beam profil... The inpu... states and i... the neutron... metry to de... any given ti... an SPP ch... function Ψ, ... the SPP, ... $\Psi \to \exp(i$... a schematic...





The Combustion Laboratory at UMD

State of the art Lab. with comprehensive Diagnostics & Experimental facilities

Theme: Clean and efficient combustion of fossil and future fuels

Sample Projects

- Gasification, pyrolysis and Waste to clean fuel conversion
- Colorless Green Distributed Combustion (CDC) for gas turbine application using High Temperature Air Combustion Technology (HiTAC)
- High speed combustion/Propulsion
- Micro-combustor with regeneration using gas and liquid fuels
- Sensors and diagnostics for combustion control in combustors and power plants
- Sulfur and energy recovery from acid gases
- Underwater propulsion and two phase mixing
- Mixing and ignition in rocket injectors

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Website: http://www.enme.umd.edu/combustion/