CHEMICAL PHYSICS RESEARCH
Mohamad Al-Sheikhly-Laboratory for Radiation and Polymer Science

1. Irradiation of UHMWPE for Hip Replacement

2. Effects of Ionizing Radiation on Polymeric Cable Insulators in Nuclear Power Plants

3. Functionalization of Polvinylpyrrolidone nanogel for drug delivery systems

4. Critical Hydrogen Concentration Determination in Alpha Particle Irradiated Water

5. Long Term Stability of Ultra High Molecular Weight Polyethylene Fibers as Soft Ballistic Inserts

6. Fabrication of Polymer Electrolyte Membranes for Fuel Cells using Radiation Grafting

7. Biocompatible Nanomaterials for Drug Delivery & Magnetic Nanocomposites for Imaging

8. Polymerization reactions of 2-Ethylhexyl Acrylate
Quantum Materials: Magnetism, Superconductivity, Topology

Materials Synthesis

Quantum + Topological Physics

Extreme Environments, Big Experiments

Cu$_2$OSeO$_3$

"Lazarus" extreme high field reentrant superconductor (UTe$_2$)

UTe$_2$

Chiral surface states in a topological superconductor (UTe$_2$)

USb$_2$

Topological Interface Network under pressure (MoTe$_2$)

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

Visit: https://sites.google.com/site/npbutch for more info

Nicholas Butch
NIST & Physics
The group currently has 8 members, including one PhD student from CPHH

Aerospace Engineering
- Ultra-low phase noise optoelectronic oscillators
- Kerr optical frequency comb generation
- Navigation and sensing

Photonic Neuromorphic Computing
- Fundamental principles
- Application to ultrafast classification tasks

Telecommunication Engineering
- Optical chaos communication
- Wavelength division multiplexing using Kerr combs

Nonlinear and Quantum Photonics
- Laser-based all-optical signal processing using ultra-high-\( Q \) cavities
- Quantum communications

UMD CPHH Virtual Open House
October 2021

https://chembolab.umd.edu/
Prof. Russ Dickerson, AOSC

**Topics:** Atmospheric Chemistry and Physics, Air Quality, Climate, and Environmental Justice

**Methods:** In situ and remote measurements, Numerical simulations

**Support:** NOAA, NASA, NIST, DOE, MDEs

Canadian wildfires generated the worst air quality in decades: impacts on health and climate
Topological photonics
(higher-order phases, high dimensions, quantum Hall effects, phase transitions)

Nonlinear photonics
(frequency combs, spectroscopy, metrology)

Quantum nanophotonics
(entangled/squeezed light generation, quantum frequency conversion)

- For studying novel emergent phases of light and matter
- For applications in ultrafast, resource-efficient devices for (quantum-enhanced) communications, computing and sensing

A. Dutt et al., Science (2020); Nat. Comm. (2019);
Wang*, Dutt* et al., Science (2021)

Quantum sensing using squeezed light
Featured on

Most research projects involve three or more aspects ∈ {theory, simulation, design, nanofabrication, experiments}
Proteins in motion: dynamics as the bridge between structure and function

Elucidating motions inside a protein

Representing multi-domain proteins as dynamic conformational ensembles

Mechanisms of cellular signaling by poly-Ubiquitin chains and how to modulate them

We combine experiments (NMR, X-ray, SAXS/SANS) and computer modeling to determine the structure, dynamics, and function of proteins and to address the challenge of painting an adequate portrait of a protein as a dynamic ensemble of multiple structures.
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

Contact Info.: Ashwani K. Gupta, Distinguished University Professor
E-mail: akgupta@umd.edu ; Tel.: 301-405-5276, FAX: 314-9477
Website: http://www.enme.umd.edu/combustion/
Ultrafast charge migration probed with femto and attosecond pulses
Phys Rev A 97, 031407

Nonlinear quantum electrodynamics (QED)
induced at extreme intensities:

Exploiting ultracold degenerate atomic ensembles to explore fundamental processes
Phys. Rev. A 93, 063619
Theory and Computation in the Jarzynski group

Thermodynamics at the nanoscale

\[ \left\langle e^{-W/k_B T} \right\rangle = e^{-\Delta G/k_B T} \]

Physics of information processing

Quantum dynamics and thermodynamics

Biophysics out of equilibrium

Computational thermodynamics

Chris Jarzynski

cjarzyns@umd.edu

(301) 405-4439
Research in levitated nanomaterials at the Laboratory for Physical Sciences (LPS)

Dr. Bruce Kane, LPS, UMD, JQI

bekane@umd.edu

Levitation of sub-µm materials in an electric quadrupole ion trap

Thermal, mechanical, and chemical properties of levitated samples determined from optical scattering

Preparation of samples in LPS clean room
Nonlinear/Quantum Optics

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

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

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

Living Neural Networks – Multimodal Dynamics

Mechano-chemical Waves as Primary Sensors of the Physical Environment

Information in Shapes, Dynamics and Rhythms

Yang et al PNAS (2023)

Herr et al, CommsPhys (2022)

Recruiting one biophysics PhD student per year with interest in microscopy, cell biophysics, or data analytics/machine learning

Wolfgang Losert losertlab.umd.edu
Biomolecular Modeling: **Self-assembly processes**

**Peptide folding and aggregation in complex environments**
- Membrane induced peptide folding
- Peptide aggregation in lipid bilayers
- Peptide aggregation in extracellular matrix mimetics

**Protein allostery/evolution and stability**
- Biotin Protein ligases
- Protein stability in non-conventional solvents

**Biophysical properties of lipid bilayers**
- Lipid domain formation

**Mechanical properties of hydrogels**
- Polysaccharides/surfactants Hydrogels

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Probing and Controlling Nanoscale Chemical and Physical Processes

Ouyang Group

Ultrafast NanoOptics

Modeling Simulation

Colloidal Quantum Materials

Emerging Technology

(Nature 466, 91)

(Nat. Commun. 8, 14312)

(Science 327, 1634)

(Science 363, 619)

mouyang@umd.edu
12 faculty
27 affiliate members
8 research scientists
30 postdocs
55 grad students
20 undergrads
4 tech/admin staff

Research Facilities:
- 15 shared labs
- bulk materials synthesis
- thin-film synthesis (PLD + MBE)
- physical properties (mK, 20T, Mbar)
- XRD facilities
- ion mill, sputtering, evaporation
- AFM, STM, surface probes
materials synthesis facilities

- Molten Flux Solvent
- Bridgman Gradient
- Czochralski Tetra-Arc
- Pulsed Laser Deposition
- Optical Floating Zone
- single-arc melters
- 1700C argon furnaces

Correlated KFe$_{2-x}$Co$_x$Se$_2$
Ferro-TI Sb$_{2-x}$V$_x$Te$_3$
Dirac semimetal RhSb$_3$
Heavy fermion YbAu$_3$
Kondo-FM CeAlGe
Quasi-1D Rb$_2$Cr$_3$As$_3$
Kondo-TI SmB$_6$

Molecular Modeling of the Cell

Chromatin

Entropy Production of the Cytoskeleton

Coarse-Graining

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...

microkelvin atoms suspended in vacuum
william.phillips@nist.gov wdp@umd.edu
Thermoelectric Materials for Energy & Space

Solid-state physics guided:

- Fabrication of materials & nanostructures
- Computer guided design
- Construction and testing of thermoelectric devices

Goals:

- Operation at extreme temperature
- Operation at extreme speeds
- Waste heat to electricity conversion
- Accurate measurements of heat fluxes

Hi-T Heat Flux Sensor
(MOST RECENT WORK)

Collaborative & Interdisciplinary
Materials-AERO-Fire Protection
UMD-Germany-Czech Rep
Polymers that Stop Bleeding

We have invented polymers that convert liquid blood into a gel via self-assembly.

A gel to stop bleeding based on it is available at CVS/Walgreens.

Cell-Like Microcapsules

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.

Smart Gels for Drug Delivery

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

https://complexfluids.umd.edu
Light-Matter Interactions in the Bio-University

Imaging through turbid media

- Edrei & Scarcelli, Optica (2016)

Soft-matter “lasers” to map forces


Bio - Optics

Photon-phonon probe to map stiffness


Edrei & Scarcelli, ACS photonics 2020
This group’s precision measurements fill the gap between space- and ground-based research activities of other groups on campus.

The AMS, ATIC, BESS, and CREAM instruments are based on particle detectors like those used at accelerators, but they are flown in space for cosmic ray measurements.

The instruments are for the most part built in-house by students and young scientists, many of them currently working in the on-campus laboratory.

The CREAM Science Operation Center at UMD remotely controls the instruments flying in Antarctica by sending commands and receiving data via satellite.
We fabricate atomically precise arrays of atoms to perform the analog quantum simulation of quantum systems such as the extended Fermi Hubbard model. These simulators are used to investigate quantum mechanical systems beyond the scope of classical computation.

\[ H_{\text{array}} = H_t + H_\mu + H_U + H_f \]

We use single electron transistors as charge sensors to measure the spin of individual electrons. These charge sensors, coupled to single or few atom structures, form the basis of electron spin qubits for applications in quantum computing.
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

MD simulations

\[ \mathcal{L} = I(x, x_{\Delta t}) - \gamma I(\chi, x) \]

Learn Information Bottleneck = RC

Training data from biased MD

Artificial Intelligence + Statistical Physics + Enhanced Sampling

Wang, Ribeiro, Tiwary *Nature Comm.* 2019

Tsai, Kuo, Tiwary *Nature Comm.* 2020

Tsai, Smith, Tiwary *J. Chem. Phys.* 2019

@tiwarylab
Mechanobiology of immune response and gene regulation

Immune receptor dynamics
Regulation of T & B cell signaling

Gene regulation
Imaging of transcription factor dynamics in live cell nuclei

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

Arpita Upadhyaya
arpitau@umd.edu

Cellular Force generation

Cytoskeletal dynamics

Biophys J. 2014, Nature Comm., 2020

Mol. Biol. Cell 2015, PNAS, 2018

Mol. Biol. Cell 2018
Quantum defects in diamond

Quantum Diamond Microscope

Nanoscale sensor of fields, temperature, forces + robust biocompatible material

Quantum sensing & imaging
=> Life & chemical sciences

Quantum Diamond Microscope

NMR of single cells & proteins => metabolomics

Single cell & biomarker detection

Live cell magnetic imaging

Single-neuron MEG in whole animals

C
magnetotactic bacteria

1 um

Ronald Walsworth
walsworth.umd.edu
Organic Color-Center Quantum Defects

• What happens when organic chemistry meets quantum physics?
• How does an exciton—electron-hole pair—in an atomic defect trap respond to local chemical perturbation?
• What if chemical information can be gathered, transformed, and transmitted at the Heisenberg limit of sensitivity and precision?

Recent papers on the subject
“Selective filling of n-hexane in a tight nanopore”
“Nanosensor-based monitoring of autophagy-associated lysosomal acidification in vivo.***
“Single Particle Imaging in Live Brain Slices at Ultra-Low Excitation Doses”
“Probing Trions at Chemically Tailored Trapping Defects”
“Single-defect spectroscopy in the shortwave infrared”
“organic colour-centre quantum defects” – a review
“Engineering Defects with DNA.”

Interested? Please contact:
Prof. YuHuang Wang (yhw@umd.edu)
http://www2.chem.umd.edu/groups/wang/