Center for Soft Matter and Biological Physics Department of Physics, Virginia Tech Annual Report – Fiscal Year 2023

The Center for Soft Matter and Biological Physics was chartered on February 12, 2016. This annual report covers the period July 1, 2022, through June 30, 2023.

I. Mission Statement of the Center for Soft Matter and Biological Physics

The mission of the Center for Soft Matter and Biological Physics is to advance the rapidly growing research areas of soft matter and biological physics, in alignment with the long-range plans of the Department of Physics, the College of Science, and Virginia Tech. Special attention will be extended to how these developments can address many of the most significant problems currently facing society, including effective drug design and delivery, next generation materials, programmable biology, and models for human disease.

Center members will enjoy the benefits of a formal unifying organizational structure that will focus their research projects, and both nucleate new and strengthen already existing cooperative interdisciplinary efforts in soft matter and biological physics across campus. The Center structure will enhance its members' opportunities to attract external research funding, and to propose large collaborative center grants. In addition, the Center will increase its members' visibility both within Virginia Tech and externally and facilitate the establishment of a vibrant Center scientific seminar series.

The objectives of the Center for Soft Matter and Biological Physics are to

- serve as a formal unifying and trans-disciplinary organizational structure that supports the science program in soft matter and biological physics at Virginia Tech.
- increase the number of joint external grants from member investigators of the Center.
- develop collaborative Center proposals that focus on research and education in the areas of soft matter and biological physics and seek expanded external funding from government and foundational sources.
- establish a vibrant scientific seminar series on soft matter and biological physics and support the weekly Physics Department Condensed Matter Seminar with (mostly) external speakers.
- establish an annual symposium and/or summer school within the Center to promote both research and education in the areas of soft matter and biological physics.
- participate in the organization of local, national, and international conferences and workshops that include the Virginia Soft Matter Workshop series (an annual workshop rotating among major Virginia institutions); and to attract national and international conferences to Virginia Tech.
- develop an educational module in collaboration with other Virginia Tech Institutes such as the Macromolecules Innovation Institute (MII) to provide instruction and training to Virginia Tech students who are interested in or need an exposure to soft matter and biological physics.

II. Classification of Center and Organizational Structure

1. Organization

The Center for Soft Matter and Biological Physics is a department center administered by the Department of Physics in the College of Science.

Department Chair and Center Administrator:

• Dr. Mark Pitt, Professor, Department of Physics, College of Science

Center Director and Contact Person:

• Dr. Shengfeng Cheng, Associate Professor, Department of Physics, College of Science

Center Steering Committee:

- Dr. Justin Barone, Professor, Department of Biological Systems Engineering, College of Agriculture and Life Science and College of Engineering
- Dr. Jonathan Boreyko, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Daniel Capelluto, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Uwe Täuber, Professor, Department of Physics, College of Science
- Dr. Rana Ashkar, Assistant Professor, Department of Physics, College of Science

Center Website: https://csmb.phys.vt.edu

2. List of Faculty Affiliated with the Center

Regular faculty members (41) as of June 1, 2023:

- Dr. Rana Ashkar, Assistant Professor, Department of Physics, College of Science
- Dr. Justin Barone, Professor, Department of Biological Systems Engineering, College of Engineering
- Dr. Michael Bartlett, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Bahareh Behkam, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Jonathan Boreyko, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Yang Cao, Associate Professor, Department of Computer Science, College of Engineering
- Dr. Daniel Capelluto, Associate Professor, Department of Biological Sciences, College of Science

- Dr. Jing Chen, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Jiangtao Cheng, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Shengfeng Cheng, Associate Professor, Department of Physics, College of Science
- Dr. Sanket Deshmukh, Associate Professor, Department of Chemical Engineering, College of Engineering
- Dr. David Dillard, The Adhesive & Sealant Science Professor, Department of Biomedical Engineering and Mechanics, College of Engineering
- Dr. William Ducker, Professor, Department of Chemical Engineering, College of Engineering
- Dr. Alan Esker, Professor, Department of Chemistry, College of Science
- Dr. Silke Hauf, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Jean Heremans, Professor, Department of Physics, College of Science
- Dr. Sohan Kale, Assistant Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Nadir Kaplan, Assistant Professor, Department of Physics, College of Science
- Dr. Giti Khodaparast, Professor, Department of Physics, College of Science
- Dr. Oleg Kim, Assistant Professor, Department of Biomedical Engineering and Mechanics, College of Engineering
- Dr. Shihoko Kojima, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Arina Korneva, Assistant Professor, Department of Biomedical Engineering and Mechanics, College of Engineering
- Dr. Guoliang (Greg) Liu, Associate Professor, Department of Chemistry, College of Science
- Dr. Louis Madsen, Professor, Department of Chemistry, College of Science
- Dr. James McClure, Research Assistant Professor, National Security Institute
- Dr. Steve Melville, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Djordje Minic, Professor, Department of Physics, College of Science
- Dr. Amrinder Nain, Associate Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Vinh Nguyen, Associate Professor, Department of Physics, College of Science
- Dr. Alexey Onufriev, Professor, Department of Computer Science, College of Engineering
- Dr. Mark Paul, Professor, Department of Mechanical Engineering, College of Engineering
- Dr. John Phillips, Professor, Department of Biological Sciences, College of Science
- Dr. Michel Pleimling, Professor, Department of Physics and Associate Dean for Undergraduate Programs, College of Science
- Dr. David Popham, Professor, Department of Biological Sciences, College of Science
- Dr. Rui Qiao, Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Hans Robinson, Associate Professor, Department of Physics, College of Science
- Dr. Vicki Soghomonian, Associate Professor, Department of Physics, College of Science

- Dr. Carolina Tallon, Associate Professor, Department of Materials Science and Engineering, College of Engineering
- Dr. Uwe Täuber, Professor, Department of Physics, College of Science, Faculty of Health Sciences
- Dr. Zhenhua Tian, Assistant Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Layne Watson, Professor, Department of Computer Science, College of Engineering

Affiliated Emeriti Faculty Members (5):

- Dr. Herve Marand, Professor emeritus, Department of Chemistry, College of Science
- Dr. Jimmy Ritter, Associate Professor emeritus, Department of Physics, College of Science
- Dr. John Tyson, University Distinguished Professor emeritus, Department of Biological Sciences, College of Science
- Dr. Dick Zallen, Professor emeritus, Department of Physics, College of Science
- Dr. Royce Zia, Professor emeritus, Department of Physics, College of Science

3. List of Postdocs and Students Supported by Center Administered Funds

Postdoctoral research associates:

- Dr. Suryabrahmam Buti, since June 2023-present, NSF 480672
- Dr. Vinh Ho, since May 2020 to January 2023, NASA 426703 and NASA 419463
- Dr. Wenya Shu, Physics, since September 2020, SU 235741
- Dr. Reda Tiani, Physics, since December 2021-April 2023, funded through a Belgian American Educational Foundational (B.A.E.F.) grant and postdoctoral fellowship from the Free University of Brussels, Belgium

Graduate research assistants:

- Chi Chen, physics, ½ GRA summer 2022, SU 235371
- Jiarong Cui, GRA summer 2023 (NASA 426733)
- Kenneth Distefano, physics, ½ GRA fall 2022, GRA summer 2023, NSF 480724
- Eugenia Datsomor, Biological Sciences, GRA summer 2022, 100% Capelluto grant, GTA summer 2022, 50% DEI department fellowship and 50% Biological Sciences
- Kalani Ellepola, physics, GRA ½ summer 2022, CeZAP 179965
- Xi Hao, MACR, GRA summer 2023, NSF 480341
- Lesle Howe, GRA summer 2022 (NASA 426703) and 2023 (NASA 426733)
- Yisheng Huang, physics, GRA summer 2023, NSF 480341
- Chinmay Katke, physics, since January 2021, SU 235741
- Mohamed M. Khattab, physics, since May 2023, SU 235741

- Teshani Kumarage, physics, GRA Summer 2022 Jeffress 453107, GRA Fall 2022
 CeZAP 179965, NSF 480672, Spring 2023 MII Interdisciplinary Collaborative Seed
 Program, Summer 2023, MII Interdisciplinary Collaborative Seed Program, SU 235371
- Binghas Liu, physics, GRA summer 2022 and 2023, NSF 480341
- Ayoyinka Okedigba, Chemistry, GTA summer 2022, 100% Chemistry, GRA summer 2022, 50% Capelluto grant, 50% Biological Sciences
- Hadi Rahmaninejad, physics, ½ GRA summer 2022, NSF 480672
- Tiffany Roach, Biological Sciences, GRA summer 2022, 50% IMSD, 50% MAOP
- Mohamed Swailem, physics, ½ GRA fall 2022 and spring 2023, GRA summer 2023, NSF 480724
- Junwen Wang, physics, GRA summer 2022 and 2023, NSF 480341
- Fangzhou Yu, GRA summer 2022 and 2023, NS 480341

Undergraduate research students:

- Zachary Aycock, nanoscience, summer 2022, Hamlett Undergrad Research
- John Caudill, chemical engineering, summer 2022, Jeffress 453107
- Grant Davis, physics, summer 2023, NSF 480341
- Xander Fry, summer 2023, NSF 480724
- Alex Habibi, nanomedicine and biological sciences, summer and fall 2022, Jeffress 453107, spring 2023, SU 235371
- Mason Hill, physics, summer 2023, NSF 480341
- Andrew Johnson, physics, summer 2022, NSF 480672
- Jesse McGovern, Physics, Summer 2023, SU 235741
- John McLaughlan, physics, summer 2022, NSF 480341
- Nick Morris, physics, summer 2022 and summer 2023, SU 235371
- Nathan Peters, nanoscience, summer 2023, Hamlett Undergraduate Research
- Marlo Pinto, nanoscience, summer 2023, Hamlett Undergraduate Research
- Marty Prattis, nanoscience, summer 2022, Hamlett Undergrad Research
- Ellee Pyle, nanoscience, summer 2022, Hamlett Undergrad Research
- Brannon Semp, physics, summer 2023, SU 235371
- Brady Talbert, physics, summer and fall 2022, SU 235741
- Canon Zeidan, physics, summer 2023, NSF 480724
- Maria Ziu, physics, summer and fall 2022, Jeffress 453107; spring and summer 2023, SU 235371
- Eleni Ziu, nanoscience, summer and fall 2022, Jeffress 453107; spring 2023, SU 235371

4. Classified Staff

• Katrina Loan, Program Support Technician, funded through A-21 program. During her sixth year, Ms. Loan's salary will be provided by the Office of the Vice President for Research (10%) and the Center for Soft Matter and Biological Physics (90%).

5. Department fiscal staff

- Jacqueline Woodyard, Director of Business Operations, Department of Physics
- Sherri Collins, Grant Coordinator, Department of Physics

III. Amendments to the Center Charter

The following amendments to the Center Charter was approved with a majority vote by the Center affiliated faculty in February, 2023.

<u>Original Statement</u>: The Center's Steering Committee will consist of four additional regular faculty members.

<u>Updated Statement</u>: The Center's Steering Committee will consist of four to six additional regular faculty members.

Original Statement: Four additional regular Center faculty members will be elected by simple majority vote by their peers to form the Center Steering Committee. The Steering Committee will meet regularly with the Director and serve in a supporting and advisory role. Certain executive tasks may be delegated by the Director to members of the Steering Committee. Updated Statement: Four to six additional regular Center faculty members will be elected by simple majority vote, with the standard quorum (30%), by their peers to form the Center Steering Committee that will serve for a term of two years. The Steering Committee will meet regularly with the Director and serve in a supporting and advisory role. Certain executive tasks may be delegated by the Director to members of the Steering Committee. During the term of the current Steering Committee, additional Committee members can be elected via special elections by simple majority vote, with the standard quorum (30%), by the current Center faculty members as long as the total number of Steering Committee members does not exceed six. The added Committee members will serve the remaining term of the current Steering Committee.

IV. Stakeholder Committee

The Center does not have an established Stakeholder Committee. We propose as members:

- Dr. Mark Pitt, Professor and Chair, Department of Physics
- Dr. John Morris, Professor, Department of Chemistry and Associate Dean for Research and Graduate Studies, College of Science
- Dr. Daniel Sui, Professor, Vice President for Research, and Innovation

V. Major Grants Received in 2022-2023

New grants:

- National Aeronautics and Space Administration, Langley Research Center (NASA 426753), Array of depLoyable dIffractivE Neoteric opticS (ALIENS), PI Vinh Nguyen (Physics, 100%), September 01, 2022 July 31, 2024; total volume \$65,067 for two years.
- MII Interdisciplinary Collaborative Seed Program, Innovative design and synthesis of dextran-conjugated cholesterol, PI Rana Ashkar (Physics, 50%), co-PI Kevin Edgar (Sustainable Biomaterials, 50%), Jan. 1, 2023 June 29, 2023 (1/2 CY support for 2 graduate students).
- National Science Foundation, ADVANCING KnowlEDGE -- Engineering Deans' Gender Equity -- Initiative: Aligning Systems to Ensure Inclusion and Equity in Advancement of Diverse Women Engineering Faculty (09-01-2022 -- 08-31-2027) PI: Jackie El-Sayed, co-PI: Rana Ashkar, Sarah Rajala, Gretal Leibnitz, Ershela Sims; Maximum Award Amount: \$ 999,967 (This grant does not come with research funds but it is an ADVANCE grant for increasing equity and inclusion in the advancement of women faculty in engineering. The program closely adapts the design for climate site visits that Prof. Rana Ashkar led during her tenure as the chair of the APS climate site visits program).

Continuing grants:

- U.S. Army Research Office (ARO 450484), Engineering Sciences Directorate, Mechanical Sciences Division, Control of universal scaling, noise strength, and pattern formation in critical dynamics, PI Uwe C. Täuber (Physics, 50 %), co-PI Michel Pleimling (Physics, 50 %), with subcontract to P. S. Krishnaprasad (Electrical and Computer Engineering, University of Maryland): April 15, 2017 – August 14, 2022; total volume \$ 1,654,294 for four years.
- U. S. National Science Foundation (NSF 480575), Division of Materials Research (DMR), *Tapered Bottlebrush Block Copolymers: Synthesis, Solution Self-Assembly, and Simulations*, PI John Matson (Chemistry, 85%), co-PI Rana Ashkar (Physics, 15%), June 1, 2021 May 31, 2024, total volume \$ 441,459 for three years.
- The Thomas F. and Kate Miller Jeffress Memorial Trust, *Reversing pathology through informed molecular regulation of lipid rafts*; PI Rana Ashkar (Physics, 70 %), co-PI Sanket Deshmukh (Chemical Engineering, 30 %); July 1, 2021 June 30, 2022; total volume \$ 100,000 for one year.
- U.S. Department of Defense, Air Force Office of Scientific Research (AFOSR 450618), FA9550-18-1-0263, Impact of Hydration and Collective Dynamics on Protein Functions, PI Vinh Nguyen (Physics, 100 %), July 01, 2018 June 30, 2023; total volume \$ 488,779 for five years.

- Luther and Alice Hamlett Undergrad Research (444364), PI Vinh Nguyen (Physics, 100 %): September 10, 2017 June 30, 2025; total volume \$ 74,500 for eight years.
- U.S. National Science Foundation (NSF 480222), Division of Materials Research (DMR), *Lithography on a nanosphere-an optical approach to arbitrarily patterned patchy particles*, PI Hans Robinson (Physics, 70%), co-PI Webster Santos (Chemistry, 30%): August 26, 2019 August 31, 2024; total volume \$ 286,821 for three years.
- U.S. National Science Foundation (NSF 480341), Division of Materials Research (DMR), Condensed Matter and Materials Theory, *CAREER: Nonequilibrium physics in drying soft matter solutions*; PI Shengfeng Cheng (Physics, 100%): June 1, 2020 May 31, 2025; total volume \$ 514,786 for five years.
- National Aeronautics and Space Administration (NASA 426733), Advanced Component Technology, *Smart Polyimide Expandable Collector to enable Investigations for Earth Science (SPECIES)*, PI Vinh Nguyen (Physics, 100%), August 1, 2021 July 31, 2024; total volume \$ 210,421 for three years.
- U.S. National Science Foundation (NSF 480672), Division of Molecular and Cellular Biosciences (MCB), Molecular Biophysics: *EAGER: Topographically induced lateral organization in biomimetic lipid membranes;* PI Rana Ashkar (Physics, 100%): August 1, 2021 July 31, 2023; total volume \$ 297,204 for two years.
- Joint U.K. Engineering and Physical Sciences Research Council (EPSRC) / U.S. National Science Foundation (NSF 480724) – Division of Mathematical Sciences (DMS) grant EPSRC EP/V014439/1 & NSF-DMS-2128587,

Eco-evolutionary dynamics of fluctuating populations.

PIs: Mauro Mobilia and Alastair Rucklidge (Department of Applied Mathematics, University of Leeds, U.K.), £ 443,468.

PI Uwe C. Täuber (Physics, 50 %), co-PI Michel Pleimling (Physics, 50 %), August 15, 2021 – August 14, 2024; total volume \$ 300,000 for three years.

VI. Major Proposals Submitted or Pending

- U.S. National Science Foundation (NSF), *REU Site: Training Highschoolers and Undergraduates in Methods across Biology and Soft Matter a Unified Perspective (THUMBS-UP)*, declined (\$358,784 3 years, PI: Rana Ashkar 50%, co-PI: Shengfeng Cheng 50%), pending.
- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), DMREF Program, *Collaborative Research: DMREF: Biological Formation and Organization Rules for Mineralized Structures (BIO-FORMS)*. PI: Ling Li (Mechanical Engineering, 40%) Co-PI: Sohan Kale (Mechanical Engineering, 30%) Cihan Nadir

Kaplan (Physics, 30%): September 1, 2023 – August 31, 2027; total volume \$1,449,657 for four years (June 2023).

- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), DMREF Program, *DMREF: Machine Learning and Computational Modeling Empowered Design of Ionic Polyetherimides*. PI: Guoliang Liu (Chemistry, 40%) Co-PI: Shengfeng Cheng (Physics, 30%), Xi Chen (Industrial Systems and Engineering, 30%): September 25, 2023 September 24, 2027; total volume \$2,000,000 for four years (June 2023), declined.
- U.S. National Science Foundation (NSF), *The Role of Molecular Forces in Emergent Dynamics of Lipid Self-Assemblies*, declined (\$708,336 3 years, PI: Rana Ashkar 55%, co-PI: Michael Brown 45%, Alex Sodt 0%).
- U.S. National Science Foundation (NSF), *REU Site: Training Highschoolers and Undergraduates in Methods bridging Biology and Soft Matter a Unified Perspective (THUMBS-UP)*, declined (\$350,875 3 years, PI: Shengfeng Cheng 50%, co-PI: Rana Ashkar 50%)
- U.S. National Institute of Health (NIH), R21, *Principles of How a Peripheral Protein Binds and Curves Membranes*, declined (\$100,000 2 years, PI: Daniel Capelluto 80%, co-PI: Rana Ashkar 20%).
- Keck Foundation, *Towards Artificial Cell Technology with Molecularly Tunable Functionality*, Phase I proposal, declined (\$1M 3 years, PI: Rana Ashkar 60%, co-PI: Alex Sodt 20%, Michael Brown 20%) one of only 2 proposals invited from VT for Phase I submission.

VII. Significant Accomplishments in 2022-2023

1. Center for Soft Matter and Biological Physics Symposium

The Center held its annual symposium this year jointly with Oak Ridge National Lab (ORNL) as the VT-ORNL Joint Symposium on Soft Matter and Biological Physics on May 17 and 18, 2023. The symposium was co-organized by Rana Ashkar and Shengfeng Cheng from Virginia Tech and John Katsaras from ORNL. The symposium featured 3 external keynote speakers, 3 invited external speakers, and 12 internal Virginia Tech presenters from different departments. On May 17, a poster session was held. Awards were announced at the end of the symposium on May 18.

Keynote External Speakers:

 Mark Dadmun, Oak Ridge National Laboratory and University of Tennessee Correlating Structure of Functional Polymeric Systems to Performance with Neutron Scattering

- Flora Meilleur, Oak Ridge National Laboratory and North Carolina State University *Activation of Molecular Dioxygen by Lytic Polysaccharide Monooxygenases*
- Benjamin Doughty, Oak Ridge National Laboratory Soft Matter Interfaces At and Away from Equilibrium

Invited External Speakers:

- Jan-Michael Carrillo, Oak Ridge National Laboratory

 Beyond Implicit Solvents: Advancing Soft Matter Simulations with Explicit Solvent

 Molecular Dynamics
- John Katsaras, Oak Ridge National Laboratory
 Lipid Bilayers as Platforms for Understanding the Brain and for the Development of
 Neuromorphic Computing
- Yangyang Wang, Oak Ridge National Laboratory Spatial Correlations of Polymer Dynamics

12 Internal Speakers:

- Justin Barone, Biological Systems Engineering, Virginia Tech Dynamics of Viscoelasticity-Driven shape change
- Michael Bartlett, Mechanical Engineering, Virginia Tech Multifunctional Soft Materials for Electronics, Robots, and Adhesives
- Bahareh Behkam, Mechanical Engineering, Virginia Tech
 Bacteria-mediated Mechanobiological Solutions for Combating Cancer and Implant
 Infection
- Jonathan Boreyko, Mechanical Engineering, Virginia Tech *Ice Dynamics: Boiling, Ratcheting, Pulsating, and Jumping*
- Jiangtao Cheng, Mechanical Engineering, Virginia Tech Manipulating droplet jumping behaviors on hot microstructure surfaces: from vibration to explosion
- Greg Liu, Chemistry, Virginia Tech Engineering of Polymers and 2D Materials for Energy and Environmental Sciences
- Louis Madsen, Chemistry, Virginia Tech Effects of Nanoconfinement on Ions and Small Molecules in Soft Matter
- James McClure, National Security Institute, Virginia Tech Digital Twins from Microscope Image Data
- Vinh Nguyen, Physics, Virginia Tech Impact of Water-Protein Interactions on Protein Dynamics
- Ayoyinka Okedigba, Chemistry, Virginia Tech
 Thermodynamic Analysis of Soybean Meal Bowman-Birk and Kunitz Trypsin
 Inhibitors Interactions with Animal Serine Proteases
- Wenya Shu, Physics, Virginia Tech Multiscale Theory for Cell Migration in Complex Biological Microenvironments
- Mohamed Swailem, Physics, Virginia Tech

 Computing Macroscopic Reaction Rates in Reaction-Diffusion Systems using MonteCarlo Lattice Simulation

During the poster session on May 17, the poster prize of \$100.00 each was awarded to:

- Zacary Croft, Chemistry, Virginia Tech Oxidation of Graphene-on-Copper with Polymer Thin-films
- Leslie Howe, Physics, Virginia Tech Diffractive Optic Elements on Plastic Membranes
- Teshani Kumarage, Physics, Virginia Tech Liposomal Design for Drug Delivery Applications Using Sterol-Conjugated Lipids
- Tiffany Roach, Biological Sciences, Virginia Tech
 Phosphoinositide Mediated Auto-Regulation of TOM1's Commitment to Cargo
 Trafficking

On May 18, the Graduate Student Workshop featured tutorials by 3 keynote speakers:

- Prof. Mark Dadmun, ORNL and University of Tennessee Tailor Made polymeric Feedstocks for Additive Manufacturing Using Polymer Science Principles.
- Dr. Benjamin Doughty, Oak Ridge National Laboratory

 An Introduction to Probing Surfaces with Nonlinear Optics
- Prof. Flora Meilleur, ORNL & North Carolina State University Neutron Crystallography to Model Hydrogen Atoms in Protein Structures

In the afternoon of May 18, 2023, a roundtable was held between VT faculty and ORNL scientists to discuss the future of collaborating on research, developing joint proposals, and training STEM workforce. It was agreed that such joint VT-ORNL annual symposium would be held regularly in the future.

2. Center for Soft Matter and Biological Physics Seminar Series

The Center held seminars through the fall 2022 and the spring 2023 semesters (Mondays 4.00 – 5.00 p.m.), hosted by different center members, to promote scientific exchange and incite possible research collaborations (https://csmb.phys.vt.edu/events/Seminar.html):

- July 18, 2022: Dr. Tom Burkart, Ludwig-Maximilians University, München, Germany *Probing the Impact of Temporally Varying Environments on Population Coexistence*
- October 24, 2022: Dr. Tom Burkart, Ludwig-Maximilians University, München, Germany
 - Light, Proteins, and Shape: Exploiting Protein Pattern Formation for Light-Controlled Oocyte Deformations
- November 14, 2022: Prof. Uwe Täuber & Prof. Rana Ashkar, Physics, Virginia Tech *Interactive Discussion of Postdoc and Faculty Application Process*

- December 5, 2022: Hong Yao, Physics, Virginia Tech Critical Dynamics of the Antiferromagnetic O(3) Nonlinear Sigma Model with Conserved Magnetization
- January 23, 2023: Dr. Gabriele Perfetto, University of Tubingen, Germany *Quantum Reaction-Diffusion Dynamics*
- May 23, 2022: Prof. Alastair Rucklidge, University of Leeds
 Cycling Behavior and Spatial Structure in a Hetero-clinic Network model of Rock-Paper-Scissors-Spock-Lizard

3. Research Publications with Center Affiliation

• Louie Hong Yao and Uwe C. Täuber,

Critical dynamics of the antiferromagnetic O(3) nonlinear sigma model with conserved magnetization,

Physical Review E, 105(6), 064128 (published 27 June 2022).

[https://doi:10.1103/PhysRevE.105.064128]

• Laura E. Hanzly, Natasha Chauhan, and Justin R. Barone

Mechanically cycling gelatin bilayers

Smart Materials and Structures, 31(8), 085005 (published 30 June 2022).

[https://doi.org/10.1088/1361-665X/ac798e]

• Mahmudul Hasan and Daniel G. S. Capelluto

The PH Domain and C-Terminal polyD Motif of Phafin2 Exhibit a Unique Concurrence in Animals

Membranes **12**(7), 696 (published 7 July 2022)

[https://doi.org/10.3390/membranes12070696]

• Changwoo Do, Rana Ashkar, et al.

EXPANSE - A Time-of-Flight EXPanded Angle Neutron Spin Echo Spectrometer at the Second Target Station of the Spallation Neutron Source,

Review of Scientific Instruments 93, 075107(published 11 July 2022)

[https://doi.org/10.1063/5.0089349]

• Yang Liu, Keturah Bethel, Manjot Singh, Junru Zhang, Rana Ashkar, Eric Davis, and Blake Johnson,

Comparison of Bulk- vs. Layer-by-layer-cured Stimuli-responsive PNIPAM-Alginate Hydrogel Dynamic Viscoelastic Property Response via Embedded Sensors,

ACS Applied Polymer Materials 4, 5596 (Published 17 July 2022).

[https://doi.org/10.1021/acsapm.2c00634]

• Dan E. Folescu and Alexey V. Onufriev

A Closed-Form, Analytical Approximation for Apparent Surface Charge and Electric Field of Molecules

ACS Omega 7(30), 26123-26136 (published 19 July 2022)

- Abhishek K. Singh, Luan C. Doan, Djamila Lou, Chengyuan Wen, and Nguyen Q. Vinh *Interfacial layers between ion and water detected by terahertz spectroscopy* J. Chem. Phys. 157, 054501 (published 03 August 2022)
 [https://doi.org/10.1063/5.0095932]
- Henry J. Lessen, Kayla C. Sapp, Andrew H. Beaven, Rana Ashkar, and Alexander J. Sodt Molecular Mechanisms of Spontaneous Curvature and Softening in Complex Lipid Bilayer Mixtures,

Biophys. J. **121**(17), 3188-3199 (published 4 August 2022) [https://doi.org/10.1016/j.bpj.2022.07.036]

• Vinh X. Ho, Yifei Wang, Leslie Howe, Michael P. Cooney, and Nguyen Q. Vinh Shallow Impurity States in Doped Silicon Substrates Enabling High Responsivity for Graphene Mid-Infrared Photodetectors,

ACS Appl. Nano Mater. **5**(9), 12477-12486 (published 15 August 2022) [https://doi.org/10.1021/acsanm.2c02011]

- Zechen Zhang, Jared R. Arkfeld, and William A. Ducker Proximity-induced Surfactant Aggregation,
 Colloid and Interface Science Communications 50, 100657 (published 9 September 2022).
 [https://doi.org/10.1016/j.colcom.2022.100657]
- James E. McClure, Ming Fan, Steffen Berg, Ryan T. Armstrong, Carl Fredrik Berg, Zhe Li, and Thomas Ramstad

Relative permeability as a stationary process: Energy fluctuations in immiscible displacement,

Physics of Fluids **34**, 092011 (published 20 September 2022). [https://doi.org/10.1063/5.0107149]

• Ruslan I. Mukhamadiarov and Uwe C. Täuber,

Effects of lattice dilution on the nonequilibrium phase transition in the stochastic susceptible-infectious-recovered model,

Physical Review E, **106**(3), 034132, 1-8 (published 23 September 2022). [https://doi:10.1103/PhysRevE.106.034132]

- Yanfei Tang, John E. McLaughlan, Gary S. Grest, and Shengfeng Cheng
 Modeling solution drying by moving a liquid-vapor interface: Method and applications,
 Polymers 14(19), 3996 (published 23 September 2022).
 [https://doi.org/10.3390/polym14193996]
- Yeyue Xiong, Saeed Izadi, Alexey V. Onufriev
 Fast Polarizable Water Model for Atomistic Simulations,
 J. Chem. Theory Comput. 18(10), 6324-6333 (published 3 October 2022)
 [https://doi.org/10.1021/acs.jctc.2c00378]

Fathima T. Doole, Teshani Kumarage, Rana Ashkar, and Michael F. Brown *Cholesterol Stiffening of Lipid Membranes*,
 J. Membrane Biology 255, 385 (published 11 October 2022) [https://doi.org/10.1007/s00232-022-00263-9]

Saeed Behzadinasab, Mohsen Hosseini, Myra D. Williams, H. M. Ivester, I. C. Allen, Joseph O. Falkinham III and William A. Ducker
 Antimicrobial Activity of Cuprous, Oxid-coated and Cupric Oxide-coated Surfaces, Journal of Hospital Infection 129, 58-64 (published 10 November 2022)
 [https://doi.org/10.1016/j.jhin.2022.07.022]

 Zachary Benmamoun, Trent Wyhopen, You Li and William A. Ducker Mechanism and Efficacy of Cu₂O-Treated Fabric.
 Antibiotics 11(11), 1633 (published 16 November 2022) [https://doi.org/10.3390/antibiotics11111633]

• Daniel G. S. Capelluto

The repertoire of protein-sulfatide interactions reveal distinct modes of sulfatide recognition

Front. Mol. Biosci. **9** (published 30 November 2022) [https://doi.org/10.3389/fmolb.2022.1080161]

- Milka Doktorova, George Khelashvili, Rana Ashkar, and Michael F. Brown *Molecular simulations and NMR reveal how lipid fluctuations affect membrane mechanics*, Biophys. J. **122**, 984 (published 5 December 2022) [https://doi.org/10.1016/j.bpj.2022.12.007]
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• Fathima T. Doole, Sudipta Gupta, Teshani Kumarage, Rana Ashkar, and Michael F. Brown

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 Elastohydrodynamic lubrication model and failure test for micro-contact thermodynamic
 characteristics of friction interface
 Tribology International 185, 108499 (published 11 April 2023)
 [https://doi.org/10.1016/j.triboint.2023.108499]

• Alexey V. Onufriev

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 ACS Nano 17(12), 11362-11373 (published 8 May 2023).
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- Louie Hong Yao, Mohamed Swailem, Ulrich Dobramysl, and Uwe C. Täuber, *Perturbative field-theoretical analysis of three-species cyclic predator-prey models*, Journal of Physics A: Mathematical and Theoretical 56(22), 225001, 1-42 (published 10 May 2023). [https://doi.org/10.1088/1751-8121/acd0e4]
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Antibiotics **12**(5), 920 (published 17 May 2023).
[https://doi.org/10.3390/antibiotics12050920]

Hadi Rahmaninejad and Rana Ashkar
 Neutron scattering studies of nanoscale polymer-based coatings,
 Polymer-Based Nanoscale Materials for Surface Coatings, pp 349-381 (book chapter, published 19 May 2023)
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 Evidence for two liquid forms,
 J. Chem. Phys. 158, 204507 (published 28 May 2023)

J. Chem. Phys. **158**, 204507 (published 28 May 2023 [https://doi.org/10.1063/5.0142818]

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- Mohamed Swailem and Uwe C. Täuber *Lotka-Volterra predator-prey model with periodically varying carrying capacity*, Physical Review E, **107**(6), 064144 (published 30 June 2023). [https://doi:10.1103/PhysRevE.107.064144].

4. Submitted Papers with Center Affiliation

Soeren Brandt, Ida Pavlichenko, Anna V. Shneidman, Haritosh Patel, Austin Tripp,
Timothy S. B. Wong, Sean Lazaro, Ethan Thompson, Aubrey Maltz, Thomas Storwick,
Holden Beggs, Katalin Szendrei-Temesi, Bettina Lotsch, C. Nadir Kaplan, Claas W.
Visser, Michael P. Brenner, Venkatesh N. Murthy, Joanna Aizenberg
Non-Equilibrium Sensing of Volatile Compounds Using Active and Passive Analyte
Delivery,

Proc. Natl. Acad. Sci. U.S.A. **120**, e2303928120 (published 26 July 2023). [https://doi.org/10.1073/pnas.2303928120]

- Nina Hong, Jiarong R. Cui, Hyun Jung Kim, Ross G. Shaffer, and Nguyen Q. Vinh,
 New Insights into Refractive Indices and Birefringence of Undoped and MgO-Doped Lithium Niobate Crystals at High Temperatures Optical Materials 145, 114365 (published 24 September 2023)
 [https://doi.org/10.1016/j.optmat.2023.114365]
- Reda Tiani and Uwe C. Täuber, Stochastic analysis of chemical reactions in multi-component interacting systems at criticality, submitted to Europhysics Letters (submitted on 28 May 2023). [arXiv:2305.17726].

• Wenya Shu and C. Nadir Kaplan.

A multiscale theory for spreading and migration of adhesion-reinforced mesenchymal cells

submitted to J. R. Soc. Interface (submitted on 2 June 2023). [https://doi.org/10.1101/2023.05.03.539193].

• C. Chen, N. Morris, T. Kumarage, H. Rahmaninejad, M. Kane, L. Collins, R. Toomey, and R. Ashkar

Nanostructured PNIPAM Coatings with Topographically and Mechanically Tunable Properties

submitted to Soft Matter

• H. Rahmaninejad, A. J. Parnell, T. Sexton, G. Dunderdale, W.-L. Chen, J. F. Ankner, W. Bras, C. K. Ober, A. J. Ryan, and R. Ashkar

Synthesis and Characterization of Stimuli-Responsive Polymer Brushes in Nanofluidic Channels

submitted to ACS Appl. Mater. Interfaces

• M. Alaboalirat, H. Rahmaninejad, S. J. Scannelli, J.-M. Carrillo, C. Do, J. B. Matson, and R. Ashkar

Solution structure of traditional and tapered bottlebrush polymers using small-angle neutron scattering

under revision with Macromolecules

• S. Gupta, S. Chakraborty, H. J. Lessen, T. Kumarage, N. Morris, F. Heberle, A. J. Sodt, and R. Ashkar

Domain Induced Viscoelastic Effects in Phase-Separating Lipid Membranes under review with Phys. Rev. Lett.

• Binghan Liu, Gary S. Grest, and Shengfeng Cheng

Inducing stratification of colloidal mixtures with a mixed binary solvent. Under review with Soft Matter

5. Invited Presentations with Center Affiliation

• Shannon R. Serrao and Uwe C. Täuber

Spatially inhomogeneous stochastic cyclic competition models: Stabilizing vulnerable ecologies through immigration waves,

SIAM Conference on the Life Sciences (SIAM-LS22), Pittsburgh, PA (14 July 2022). Chinese Physical Society (CPS) Fall Meeting 2022, Symposium on Statistical Physics and Complex Systems (virtual 19/20 November 2022).

124th Statistical Mechanics Conference, Rutgers University, Piscataway, NJ (8 May 2023).

• R.K.P. Zia

Optimal launch angles: Novel perspectives of an ancient problem
Fall 2022 Semi-virtual Meeting of Chesapeake Section of the American Association of
Physics Teachers, Virginia Tech Northern Virginia Center, Falls Church, VA
(semi-virtual 22 October 2022).

• Uwe C. Täuber

Stochastic spatial Lotka-Volterra predator-prey models, Ising Lectures 2023, Lviv, Ukraine (virtual 11 May 2023).

• Rana Ashkar

Santa Fe Meeting on Biological Membranes and Membrane Proteins, Santa Fe, New Mexico (June 21, 2022)

• Rana Ashkar

Neutron and X-ray Summer school jointly run by Oak Ridge National Lab and Argonne National Lab (July 11, 2022)

• Rana Ashkar

Biological Physics/Physical Biology (BPPB) seminar series, virtual (Aug. 19, 2022)

• Rana Ashkar

89th Annual Meeting of the Southeastern Section of the American Physical Society (SESAPS), University of Mississippi (Nov. 5, 2022)

Rana Ashkar

International Conference on Frontiers in Science, virtual (Nov. 12, 2022)

• Rana Ashkar

Lehigh University (Physics Department), Bethlehem, PA (April 7, 2023)

Rana Ashkar

Virginia Soft Matter Workshop, Virginia Commonwealth University (April 22, 2023)

• Rana Ashkar

Telluride Workshop on "Complexity in the Chemistry and Physics of Lipid Membranes" (June 22, 2023)

• Shengfeng Cheng

Drying of Colloidal and Polymer Solutions
Polymers and Advanced Materials (PAM) Seminar, University of Akron, Akron, OH, USA (April 28, 2023)

• Shengfeng Cheng

Drying of Colloidal and Polymer Solutions

College of Chemistry and Molecular Engineering Seminar, Peking University, Beijing, China (June 21, 2023)

• Shengfeng Cheng

Drying of Colloidal and Polymer Solutions
Polymer Science Frontier Seminar, Institute of Chemistry at Chinese Academy of Sciences,
Beijing, China (June 26, 2023)

• Nguyen Q. Vinh

Graphene-Semiconductor Nanostructures Enabled Broadband Photodetection Materials Science and Engineering Seminar, Phenikaa University, Hanoi, Vietnam (July 27, 2022)

• Nguyen Q. Vinh

Impact of Water-Protein Interactions on Protein Dynamics
Telluride Workshop on Water Structure, Dynamics and Thermodynamics in Biology,
Telluride Science Innovation Center, Telluride, CO, USA (June 25 - 29, 2023)

6. Provisional Patents

Not applicable.

7. Awards and Recognitions

Faculty:

- Rana Ashkar was elected as a member of the advisory committee of the Quite Intense Kinetics Reflectometer (QIKR) and the Wide-Angel Spin Echo (EXPANSAE) instruments to be commissioned at the Second Target Station (STS) at Oak Ridge National Lab (2021-2024)
- Rana Ashkar was appointed as the next chair for the APS Committee on the Status of Women in Physics
- Rana Ashkar was nominated to the 2023 Graduate Alumni Advising Award.

Graduate students:

- Mohamed Swailem, Wan-Zia Scholarship in Physics, Department of Physics, 7 April 2023.
- Teshani Kumarage one of 7 graduate students nationwide to be selected to the 2023 Neutron Scattering Graduate Research Program at Oak Ridge National Lab (ORNL) – the program fully

supports a graduate student for a period of 4 to 6 months to conduct their research at ORNL (scheduled for Spring-Fall 2023).

- Teshani Kumarage
 Tipsword Graduate Fellowship, Department of Physics (Spring 2023)
- Teshani Kumarage
 MII Interdisciplinary Graduate Collaborative Fellow (for her participation in an MII funded grant to develop more stable, biocompatible vaccine nanocarriers).
- Teshani Kumarage
 Outstanding Oral Presentation Award at the Center for Soft Matter and Biological
 Physics Symposium (Summer 2022).
- Hadi Rahmani
 Outstanding Poster Award at the Center for Soft Matter and Biological Physics
 Symposium (Summer 2022).

Undergraduate students:

• Eleni Ziu won the best award at the Conference for Undergraduate Women in Physics (CUWiP) held in Princeton (Jan 2023).

8. Student Travel Grants

In January 2017, the Center established a grant to support conference travel for graduate students whose advisers who are affiliated with the Center, but do not have current external funding available for this purpose. The students are requested to submit a brief application with presentation title, abstract, and conference description, all connected with research related to the Center's mission. The students can be awarded up to \$ 400 for conference travel. Four student travel grants may be issued for each spring and fall semester per year, totaling up to \$ 2,000. This year's recipients were:

- Seokgyun Ham, Mechanical Engineering, Virginia Tech
 Modulation of slippage at brine-oil interfaces by surfactants: The effects of surfactant density and tail length,
 96th ACS Colloid and Surface Science Symposium, Golden, Colorado, July 10 13,
 2022.
- Ndidi Eyegheleme, Mechanical Engineering, Virginia Tech
 Synthetic trees for renewable water harvesting,
 Micro Flow and interfacial Phenomena Conference, Evanston, Illinois June 18 21,
 2023.

VIII. Industrial Affiliates Program

Not applicable.

IX. Report of Financial Condition

		IX. Report	of Financial Condition			
Center Financi	Center Financial Report Fiscal Year 2023		Center Financial Proje	ction Fiscal Yea	r <mark>20</mark> 24	
Operations Account (176188)			Operations Account (176188)			
Starting Balance		\$ 31,049.87			7,022.38	
Starting balance	Income	\$ 51,045.67	Starting balance	Income	٠	1,022.30
Starts FY2023	meome	\$(24,027.49)	A21 Award	meome	Ś	9,450
	Expenses	V(=.//=-//	1,-2,11,31,3	Expenses	7	-7,155
			28% Staff Salary (Katrina Lockhart		\$	(12,550)
Ending Balance		\$ 7,022.38	Ending Balance	- 17	Ś	3,922.50
					Ť	,
Overhead Account (23	5052)		Overhead Account (235052)			
Starting Balance		\$ 11,716.25	Starting Balance		\$	465,26
and admired	Income			Income		010EE-09E
Overhead Earnings		\$ 20,862.22	Overhead Earnings		Ś	12,600
					1	
				Expenses		
	Expenses		Seminar		\$	(2,000)
Classified Salaries	•	\$(28,460.16)	Symposium		\$	(5,700)
Seminar Travel		\$ (1,308.00)	Student Travel		\$	(1,000)
Faculty Travel		\$ (1,608.22)	Center's Awards		\$	(1,000)
Seminar Supplies and	Meals	\$ (582.00)	Supplies & Budget		\$	(100)
Student Travel		\$ -	Faculty Travel		\$	(2,000)
Centers Symposium		\$ -				
Supplies & Budget		\$ (154.83)	42% Staff Salary (Katrina Lockhart	-Elfeky)	\$	(12,227)
Other Charges		\$ -				
Ending Balance		\$ 465.26	Ending Balance		\$ (10,961.71)
			Dept. Contribution 30%		\$	(13,446)
Overhead Account (23	5552)		Overhead Account (235552)			
Starting Balance		\$ -	Starting Balance		\$	218.86
	Income			Income		
	Expenses	0000 SANK SANKS		Expenses	92.	
Centers Symposium Ti		\$ (719.28)	Center Symposium Travel		\$	(2,000)
Meeting Facilities Ren			Honorariums		\$	(V), (C)
Centers Symposium Awards			Meeting Facilities Rentals		\$	(600)
Breakfast, Lunch and Dinners		\$ (1,481.17)	Centers Symposium Awards		\$	
Food and Dietary supplies		\$ 262.21	Breakfast, Lunch and Dinners		\$	(2,600)
Supplies & Budget		\$ (90.09)	Food and Dietary supplies		\$	
Centers Awards		\$ (800.00)	Supplies & Budget		\$	(50)
Continuous Charges Budget Other Charges		\$ 3,047.19	Continuous Charges Budget		\$	-
Other Charges		\$ -	Other Charges		×	/E 024 4 -1
Ending Balance		\$ 218.86	Ending Balance		\$	(5,031.14)

X. Major Issues of the Center

The Center's financial standing remains solid. Since March 2020, owing to the COVID-19 pandemic, expenses had been much reduced.

Until March 2020, the Center maintained a very lively and successful seminar series and discussion meetings. The COVID-19 pandemic naturally affected our regular events severely, forcing us to move our annual symposium, seminars, as well as summer discussion meetings to purely online mode. Our in person activities started to resume since 2022 but the process is slow and we have not recovered our full strength yet.

We were pleased to run our annual research symposium jointly with the Oak Ridge National Laboratory (ORNL), mostly in person with a virtual access option via Zoom, on May 17 and 18, 2023. The event featured 6 staff scientists from ORNL and a dozen of Virginia Tech research groups. We were delighted to give out various student awards during this event.

We shall continue to organize annual symposia with external speakers, and to support other related conferences including the Virginia Soft Matter Workshop series. We will invite more external speakers to visit Virginia Tech for the Soft Matter and Biological Physics Seminar series. We will also reinstate the weekly Friday Discussion Meeting platform for more internal discussions of research, collaboration, and student training/career development.

Our principal task over the next few years remains to generate new interdisciplinary research collaborations leading to collaborative grant proposals. The NSF REU proposal developed in 2022 and revised/resubmitted in 2023 is a good starting point for such efforts.

We intend to also explore further new course developments, ideally across departments and colleges, and to establish a summer school related to the Center's research mission.

September 29, 2023

Dr. Uwe C. Täuber

Professor of Physics, Faculty of Health Sciences, Virginia Tech

Director, Center for Soft Matter and Biological Physics (until 31 August 2022)

Lead Editor, Physical Review E

The C. Toute

Dr. Shengfeng Cheng

S. Cherg

Associate Professor of Physics, Virginia Tech

Director, Center for Soft Matter and Biological Physics (since 1 September 2022)