#### Center for Soft Matter and Biological Physics Department of Physics, Virginia Tech Annual Report – Fiscal Year 2024

The Center for Soft Matter and Biological Physics was chartered on February 12, 2016. This annual report covers the period July 1, 2023, through June 30, 2024.

## 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 that rotates 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 and Interfaces 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, 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: <u>https://csmb.phys.vt.edu</u>

# 2. List of Faculty Affiliated with the Center

## Regular faculty members (41) as of June 1, 2024:

- 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, Assistant 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 Associate Professor, Virginia Tech 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. Vinh Nguyen, Associate Professor, Department of Physics, College of Science
- Dr. Amrinder Nain, Associate Professor, Department of Mechanical Engineering, College of Engineering
- 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, Assistant 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. Igor Tolokh, NIH R01 GM144596
- Dr. Suryabrahmam Buti, since June 2023, NSF 480672
- Dr. Wenya Shu, September 2020 January 2024, SU-235741

## Graduate research assistants:

- Narguess Alizade, Physics, since May 2024, SU-235741
- Maxwell T. Bessey, Physics, since May 2024, SU-235741
- Kenneth Distefano, Physics, ½ GRA fall 2023, GRA. Spring and summer 2024, NSF 480724
- Luke Elder, Computer Science, since June 2023, NIH R01 GM144596
- Kalani H. Ellepola, Physics, GRA summer 2024, NASA 426753
- Fatemeh Ghafouri, GBCB, since September 2022, NIH R01 GM144596
- Xi Hao, Macromolecular Science and Engineering, GRA summer 2023 and 2024 NSF 480341
- Dinidu Hathnagoda, Physics, ½ GRA summer 2024, SU 235371
- Lesle Howe, Physics, GRA summer 2023 and 2024, NASA 426733
- Chinmay Katke, Physics, since January 2021, SU 235741
- Mohamed M. Khattab, Physics, since May 2023, SU 235741
- Egor Kolesnikov, Physics, since September 2023, NIH R01 GM144596
- Teshani Kumarage, Physics, GRA summer II 2023 and summer 2024, SU 235371
- Bingham Liu, Physics, GRA summer 2023and 2024, NSF 480341
- Tharindu D. Rajapaksha, Physics, GRA summer 2024, NASA 426733

- Fahim Bin Selim, Physics, since April 2024, SU 235741
- Mohamed Swailem, Physics, ½ GRA fall 2023 and spring 2024, NSF 480724; Ph.D. defense 15 May 2024
- Junwen Wang, Mechanical Engineering, GRA summer 2023 and 2024, NSF 480341
- Fangzhou Yu, Physics, GRA summer 2023 and 2024, NSF 480341

#### Undergraduate research students:

- Zachary Aycock, Nanoscience, summer 2023, Hamlett Undergrad Research
- Grant Davis, Physics, summer 2023 and 2024, NSF 480341
- Luke Dinicola, Physics, spring 2024, Physics 4316
- Ethan Dolin, Physics, August 2023-December 2023, SU-235741 (Physics 4316)
- Lingji Jiang, Physics, summer and fall 2023, NSF 480341
- Julianna "Jules" Kelley, Physics, summer 2023, fall 2023 and spring 2024, HHMI grant
- Kinley Koch, Nanoscience, summer 2024, Hamlett Undergrad Research
- Nicholas Morris, Physics, summer 2023 through May 2024, SU 235371
- Marlo Pinto, Nanoscience, summer 2023, Hamlett Undergraduate Research
- Nathan Peters, Nanoscience, summer 2024, Hamlett Undergraduate Research
- Brannon Semp, Physics, summer 2023 through May 2024, SU 235371
- Mason Whittington, Nanoscience, summer 2024, Hamlett Undergraduate Research
- Canon Zeidan, Physics, fall 2023, NSF 48072

## 4. Classified Staff

• Katrina Lockhart Elfeky, Program Support Technician, funded through A-21 program. During her sixth year, Ms. Lockhart Elfeky' 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

N/A.

## 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 2023-2024

# New grants:

• U. S. National Science Foundation (NSF 481376), Division of Materials Research (DMR), *Emergent Dynamics and Scaling Laws in Bioinspired Lipid Membranes*, PI Rana Ashkar (Physics, 100%), September 1, 2024 – August 31, 2027, total volume \$ 530,376 for three years.

# **Continuing grants:**

- Luther and Alice Hamlett Undergrad Research (444364), PI Vinh Nguyen (Physics, 100 %): September 10, 2017 June 30, 2025; total volume \$ 84,500 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, 480342), Division of Materials Research (DMR), *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.
- U. S. National Science Foundation (NSF 480576, 450575), 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.
- National Aeronautics and Space Administration (NASA 426733), *Smart Polyimide Expandable Collector to enable Investigations for Earth Science (SPECIES)*, PI Vinh Nguyen (Physics, 100%), August 1, 2021 July 31, 2025; total volume \$ 210,421 for three years.
- National Aeronautics and Space Administration (NASA 426753), *Array of depLoyable dIffractivE Neoteric opticS (ALIENS)*, PI Vinh Nguyen (Physics, 100%), September 01, 2022 July 31, 2025; total volume \$65,067 for three years.

- U.S. National Science Foundation (NSF 480672), Division of Molecular and Cellular Biosciences (MCB), *EAGER: Topographically induced lateral organization in biomimetic lipid membranes*, PI Rana Ashkar (Physics, 100%): August 1, 2021 – July 31, 2024; 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), *EPSRC EP/V014439/1 & NSF-DMS-2128587, Eco-evolutionary dynamics of fluctuating populations,* PIs: Mauro Mobilia and Alastair Rucklidge (University of Leeds, U.K.), £ 443,468. PI Uwe C. Täuber (Physics, 50 %) and co-PI Michel Pleimling (Physics, 50 %): August 15, 2021 July 31, 2024; total volume \$ 300,000 for three years.
- U. S. National Science Foundation (NSF 480972, 480971), Major Research Instrumentation Program (MRI), *Development of an Optical Super-resolution Instrument for Measuring Concentration Profiles and Diffusion Dynamics in Thin Films*, PI William A. Ducker (Chemical Engineering, 50%), co-PI Hans Robinson (Physics, 50%): September 1, 2022 – August 31, 2025, total volume \$ 530,376 for three years.

## VI. Major Proposals Submitted or Pending

- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), Research Experience for Undergraduates (REU) Program, *REU Site: Training Highschoolers and Undergraduates in Methods across Biology and Soft-matter -- a Unified Perspective (THUMBS-UP)*. PI: Rana Ashkar (Physics, 50%), co-PI: Shengfeng Cheng (Physics, 50%). July 1, 2024 – June 30, 2027; total volume \$358,784 for three years.
- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), CAREER Program, *CAREER: Multiscale Design and Control of Fast Deforming Hydrogels.* PI: C. Nadir Kaplan (Physics, 100%): February 1, 2025 – January 31, 2030; total volume \$471,845 for five years.

## VII. Significant Accomplishments in 2023-2024

## 1. Center for Soft Matter and Biological Physics Symposium

*The 2024 Annual Symposium of the Center for Soft Matter and Biological Physics* was organized by Profs. Rana Ashkar, Nadir Kaplan, and Shengfeng Cheng, and was held on August 31, 2024, though the organizing efforts were made during the period of this Annual Report. The details of this Symposium will be included in the Annual Report in FY 2025.

#### 2. International Symposium on Non-Equilibrium Dynamics of Complex Systems

The Center held an international symposium on Non-Equilibrium Dynamics of Complex Systems which was held on September 15 and 16, 2023, organized by Ulrich Dobramysl, Ruslan Mukhamadiarov, Riya Nandi, Mohamed Swailem, Louie Hong Yao, Shengfeng Cheng, Karin Tauber, and Katrina Lockhart-Elfeky. The symposium featured multiple international and domestic speakers, which presented combining expertise on both strong theoretical approaches and computational methods. It debated current results and the medium and long-term evolution of non-equilibrium statistical physics and its relevance to complex systems research in connected areas departments. During this symposium a celebration of the contribution achievements of Prof. Uwe Tauber (Physics, Virginia Tech) was acknowledged.

International Speakers:

- Andrea Gambassi, SISSA, Italy Centenarian but Still Surprising: The Ising Model and its (Quantum) Interface Dynamics
- Malte Henkel, University de Lorraine Nancy, France Thoughts on Dynamical Symmetries in Phase-Ordering Kinetics
- Erwin Frey, Ludwig-Maximilians-University Germany, Anomalous Collective Dynamics of Auto-Chemotactic Populations
- Mauro Mobilia, University of Leeds, UK, Eco-Evolutionary Dynamics of Microbial Populations: The Role of Fluctuations
- Sebastian Diehl, University of Cologne, Germany, Measurement Induced Phase Transitions: New Applications for Non-Equilibrium Statistical Mechanics?
- Pasquale Calabrese, SISSA, Italy, *The quantum Mpemba Effect*
- Riya Nandi, University of Geneva, Switzerland, Cell Cycle Synchronization and Cell Size Regulation in Drosophila Histoblast
- Ben Vollmayr-Lee, Bucknell University *Time Reversal in Doi-Peliti Field Theory*
- Ling Miao/Dirk Jan Bukman, American Physical Society, For Physicists and By Physicists: The Physical Review Journals and Uwe (joint talk)
- Nuno-Araujo, Universidade de Lisboa, Portugal, Self-Folding Kirigami at the Microscale
- Ruslan Mukhamadiarov, Ludwig-Maximilians-University, Germany *Clonal Dynamics of Surface-Drive Growing Tissues*

Domestic Speakers:

- Tim Halpin-Healy, Barnard College, Columbia University *The Dynamics of Conformity vs. Dissent*
- Royce Zia, Virginia Tech Detecting Detailed Balance Violation in NESS

- Alexander Wagner, North Dakota State University Coarse graining from Discrete Particles to Continuum Descriptions: What we can Learn from Alternate Mapping Procedures with Examples for the Lattice Boltzmann Method
- Michel Pleimling, Virginia Tech Non-Equilibrium Properties of Interacting Skyrmion Systems
- Randy Kamien, University of Pennsylvania, *Conic Sections, Liquid Crystals, and all That*
- David Nelson, Harvard University Defect Emission and Absorption for Liquid Crystals on Cones
- Lauren Childs, Virginia Tech Infection Induced Impacts on Population Dynamics in Epidemiology: When Greater Disease Grows the Population

# 3. Center for Soft Matter and Biological Physics Seminar Series

The Center held seminars through the fall 2023 and the spring 2024 semesters (Mondays 4.00 – 5.00 p.m.), hosted by different center members, to promote scientific exchange and incite possible research collaborations (<u>https://csmb.phys.vt.edu/events/Seminar.html</u>):

- September 25, 2023: Prof. John Franck, Syracuse University, New York Confinement and Interfaces make Water Weird: Observations with Ultra-Sensitive Magnetic Resonance Cross-Relaxation
- November 11, 2023: Nick Smith, Virginia Tech, Blacksburg, Virginia Probe of Multifunctionality in BaTiO<sub>3</sub>-BiFeO<sub>3</sub> Films and Nanorod Arrays
- December 7, 2023: Dr. Joseph Spenser, Naval Research Laboratory, Washington, DC Research in Physics Resulted in NRL Internship/Employment at NRL/ Overview Ga2O3/NiO
- January 8, 2024: Dr. Dhritiman Bhattacharya, Georgetown University, Washington, DC Nano-magnetism for Next-Generation Computing
- February 26, 2024: Dr. David Hoogerheide, NIST, Gaithersburg, Maryland New Frontiers in Fast Neutron Reflectometry for Soft Matter Systems
- March 4, 2024: Dr. Jorge Puebla, RIKEN, Japan Resonant Absorption of Surface Acoustic Waves in Magnetic Thin Films
- March 18, 2024: Prof. Marija Vucelja, University of Virginia Anomalous Thermal Relaxations of Physical Systems
- March 25, 2024: Prof. Elham Ghadiri, Wake Forest University, Virginia Advanced Ultrafast Laser Microscopy and Spectroscopy for Photochemical Analysis at Nanoscale
- March 26, 2024: Prof. Jing Yan, Yale University, New Haven, Connecticut Bacterial Biofilms as Self-shaping Growing Nematics
- April 1, 2024: Leslie Howe, Virginia Tech, Blacksburg, Virginia Photogating Effect in Low Dimensional Structures for Photodetection and Biosensing
- April 8, 2024: Dr. Yijian Zou, Perimeter Institute Exploring Defect and Boundary Criticality on the Fuzzy Sphere

- May 6, 2024: Dr. Hunter King, Rutgers University-Camden *Transport Phenomena Wielded by 2 Insects*
- May 7, 2024: Prof. Michel Calame, EMPA Zurich-Switzerland *Transport Phenomena Wielded by 2 Insects*

### 4. Research Publications with Center Affiliation

- Egor S. Kolesnikov, Yeyue Xiong, and Alexey V. Onufriev *Implicit Solvent with Explicit Ions Generalized Born Model in Molecular Dynamics: Application to DNA*  Journal of Chemical Theory and Computation (published 16 September 2024) <u>https://doi.org/10.1021/acs.jetc.4c00833</u>
- Anthony Morciglio and Royce K. P. Zia Understanding the Oscillations of an Epidemic Due to Vaccine Hesitancy Mathematical Biosciences and Engineering 8(21), 6829-6846 (published 9 August 2024) https://www.aimspress.com/article/id/66b5f99bba35de127fcb7799
- Mohamed Swailem and Uwe C. Täuber *Computing macroscopic reaction rates in reaction-diffusion systems using Monte Carlo simulations* Physical Review E 110(7), 014124 (published 17 July 2024) <u>https://journals.aps.org/pre/abstract/10.1103/PhysRevE.110.014124</u>
- Leslie Howe, Tharindu D. Rajapaksha, Kalani H. Ellepola, Vinh X. Ho, Zachary Aycock, Minh L. P. Nguyen, John P. Leckey, Dave G. MacDonnell, Hyun Jung Kim, and Nguyen Q. Vinh *High-Efficiency Multilevel Phase Lenses with Nanostructures on Polyimide Membranes* Advanced Optical Materials 12, 2400847 (published 16 July 2024) [https://doi.org/10.1002/adom.202400847]
- Royce K P Zia Signals of Detailed Balance Violation in Nonequilibrium Stationary States: Subtle, Manifest, Extraordinary Journal of Physics A 28(57), 285003 (published 2 July 2024) <u>https://iopscience.iop.org/article/10.1088/1751-8121/ad5ac8</u>
- Igor S. Tolokh, Dan E. Folescu, and Alexey V. Onufriev Inclusion of Water Multipoles into the Implicit Solvation Framework Leads to Accuracy Gains Journal of Physics Chemistry B 128(24), 5855-5873 (published 11 June 2024) <u>https://doi.org/10.1021/acs.jpcb.4c00254</u>
- H.L. Scott, V. Burns- Casamayor, A.C. Dixson, R.F. Standaert, C.B. Stanley, L.-R. Stingaciu, J.-M.Y. Carrillo, B.G. Sumpter, J. Katsaras, W. Qiang, F.A. Heberle, B. Mertz, R. Ashkar, and F.N. Barrera

Neutron spin echo shows pHLIP is capable of retarding membrane thickness fluctuations Biochim. Biophys. Acta (BBA) - Biomembranes **1866**(7), 184349 (published 28 May 2024)

https://doi.org/10.1016/j.bbamem.2024.184349

- Chinmay Katke, Peter A. Korevaar, and C. Nadir Kaplan *Diffusiophoretic fast swelling of chemically responsive hydrogels*  Physical Review Letters 132, 208201 (published 15 May 2024) <u>https://doi.org/10.1103/PhysRevLett.132.208201</u>
- Daniel L. Barton, Yow-Ren Chang, William Ducker, and Jure Dobnikar Data-driven modelling makes quantitative predictions regarding bacteria surface motility PLoS Computational Biology 20(5): e1012063 (published 14 May 2024) <u>https://doi.org/10.1371/journal.pcbi.1012063</u>
- Jianpeng Wu, Chengbing Yang, Wenya Shu, Yuxin Wang, and Liyong Wang Research on self-healing characteristic and state prediction method of the copper based powder metallurgy materials on friction interface Surf. Topogr.: Metrol. Prop. 12, 025017 (published 9 May 2024) <u>https://doi.org/10.1088/2051-672X/ad44b7</u>
- Alexander Y Afanasyev, Yoonjin Kim, Igor S Tolokh, Igor V Sharakhov, and Alexey V Onufriev The Probability of Chromatin to be at the Nuclear Lamina has no Systematic Effect on its Transcription Level in Fruit Flies BMC Epigenetics & Chromatin 17(13), 1756-8935 (published 06 May 2024) https://doi.org/10.1186/s13072-024-00528-8
- Jianpeng Wu, Jian Yang, Wenya Shu, Jiahao Cui, and Liyong Wang *Coupling mechanism and data-driven approaches for Hydro-viscous Drive torque characteristics under impact condition* Tribology International 195, 109600 (published 28 March 2024) <u>https://doi.org/10.1016/j.triboint.2024.109600</u>
- Wenya Shu, C. Nadir Kaplan, and Justin R. Barone Dynamic, viscoelasticity-driven shape change of elastomer bilayers ACS Applied Polymer Materials 6(6), 3160-3169, (published 01 March 2024) <u>https://doi.org/10.1021/acsapm.3c02898</u>
- Medha Sawhney, Bhas Karmarkar, Eric J. Leaman, Arka Daw, Anuj Karpatne, and Bahareh Behkam Motion Enhanced Multi-Level Tracker (MEMTrack): A Deep Learning-Based Approach to Microrobot Tracking in Dense and Low-Contrast Environments Advanced Intelligent Systems 6, 2300590 (published 15 February 2024) https://doi.org/10.1002/aisy.202300590

- Yirui Chen, Elias J. Topo, Beiyan Nan, and Jing Chen Mathematical Modeling of Mechanosensitive Reversal Control in Myxococcus Xanthus Frontiers in Microbiology 14, 1294631 (published 08 January 2024). <u>https://doi.org/10.3389/fmicb.2023.1294631</u>
- Mohsen Hosseini, Jinge Huang, Myra D. Williams, Gerardo Alexander Gonzalez, Xiuping Jiang, Joseph O. Falkinham III, and William A. Ducker *Robust and Transparent Silver Oxide Coating Fabricated at Room Temperature Kills Clostridioides difficile Spores, MRSA, and Pseudomonas aeruginosa* Microorganisms 12(1), 83 (published 31 December 2023) <u>https://doi.org/10.3390/microorganisms12010083</u>
- Lewis Bass, Luke H. Elder, Dan E. Folescu, Negin Forouzech, Igor S. Tolokh, Anuj Karpatne, and Alexey V. Onufriev
   *Improving the Accuracy of Physics-Based Hydration-Free Energy Predictions by Machine Learning the Remaining Error Relative to the Experiment* Journal of Chemical Theory and Computation 20(1), 396-410 (published 27 December 2023).
   https://doi.org/10.1021/acs.jctc.3c00981
- Hui Zhang, Yufei Ma, Wenya Shu, Yijie Wang, Chunyu Cao, Wanting Wan, Nianyuan Shi, Zhao Wei, Dandan Pei, Ang Li, and Feng Xu Cellular-Scale Matrix Stiffness Gradient at Soft-Hard Tissue Interfaces Regulates Immunophenotype of Mesenchymal Stem Cells Advanced Functional Materials 34, 2309676 (published 21 December 2023) https://doi.org/10.1002/adfm.202309676
- Wenya Shu and C. Nadir Kaplan. *A multiscale theory for spreading and migration of adhesion-reinforced mesenchymal cells*  J.R. Soc. Interface 209(20), 1742-5662 (published 13 December 2023). <u>https://royalsocietypublishing.org/doi/10.1098/rsif.2023.0317</u>
- Jianpeng Wu, Jiahao Cui, Wenya Shu, Liyong Wang, and Heyan Li *Coupling mechanism and data-driven approaches for high power wet clutch torque modeling and analysis*  Tribology International 191, 109166 (published 4 December 2023) <u>https://doi.org/10.1016/j.triboint.2023.109166</u>
- T. Kumarage, N.B. Morris, and R. Ashkar *The Effects of Molecular and Nanoscopic Additives on Phospholipid Membranes* Front. Phys. 11, 1251146 (published 19 November 2023) <u>https://doi.org/10.3389/fphy.2023.1251146</u>

- H. Rahmaninejad, A.J. Parnell, W.-L. Chen, N. Duzen, T. Sexton, G. Dunderdale, 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* ACS Applied Materials & Interfaces 15(47), 54942–54951 (published 16 November 2023) <u>https://doi.org/10.1021/acsami.3c12744</u>
- R. Muheim and J. B. Phillips *Effects of low-level RF fields reveal complex pattern of magnetic input to the avian magnetic compass*  Scientific Reports 13(1), 19970 (published 15 November 2023). <u>https://doi.org/10.1038/s41598-023-46547-5</u>
- Binghan Liu, Gary S. Grest, and Shengfeng Cheng Inducing stratification of colloidal mixtures with a mixed binary solvent Soft Matter 19, 9195-9205 (published 14 November 2023) <u>https://doi.org/10.1039/D3SM01192E</u>
- M. Alaboalirat, S. J. Scannelli, H. Rahmaninejad, J.-M. Carrillo. C. Do, J.B. Matson, and R. Ashkar Solution Structure and Scaling Laws of Cylindrical and Tapered Bottlebrush Polymers Macromolecules 56(22), 9264-9276 (published 9 November 2023) <u>https://doi.org/10.1021/acs.macromol.3c01412</u>
- Nicholas F. Pietra, Andrew G. Korovich, Priyanka M. Ketkar, Thomas H. Epps III, and Louis A. Madsen *Role of Intradomain Heterogeneity on Ion and Polymer Dynamics in Block Polymer Electrolytes: Investigating Interfacial Mobility and Ion-Specific Dynamics and Transport* Macromolecules 56(21), 8393-8403 (published 30 October 2023) <u>https://doi.org/10.1021/acs.macromol.3c00925</u>
- Priyanka M. Ketkar, Nicholas F. Pietra, Andrew G. Korovich, Louis A. Madsen, and Thomas H. Epps III *Role of Intra-Domain Heterogeneity on Ion and Polymer Dynamics in Block Polymer Electrolytes: An Approach for Spatially Resolving Dynamics and Ion Transport* Macromolecules 56(21), 8404-8416 (published 30 October 2023) <u>https://doi.org/10.1021/acs.macromol.3c00926</u>
- Reda Tiani and Uwe C. Täuber Stochastic Analysis of chemical Reactions in Multi-component interacting systems at criticality Europhysics Letters 144(1), 11005-1-7 (published 16 October 2023) <u>https://iopscience.iop.org/article/10.1209/0295-5075/acff15</u>
- Egor S. Kolesnikov, Ivan Yu. Gushchin, Petr A. Zhilyaev, and Alexey V. Onufriev

Why Na+ has Higher Propensity than K+ to Condense DNA in a Crowded Environment, Journal of Chemical Physics **159**(14), 145103 (published 10 October 2023) <u>https://doi.org/10.1063/5.0159341</u>

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- 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 V. Lotsch, C. Nadir Kaplan, Claas W. Visser, Michael P. Brenner, Venkatesh N. Murthy, and Joanna Aizenberg *Nonequilibrium sensing of volatile compounds using active and passive analyte delivery* Proceedings of the National Academy of Sciences 120(31), e2303928120 (published 26 July 2023) https://doi.org/10.1073/pnas.2303928120
- Xiaochu Li, Mathew Bloomfield, Alexandra Bridgeland, Daniela Cimini, and Jing Chen

A Fine Balance among key Biophysical Factors in Required for Recovery of Bipolar Mitotic Spindle from Monopolar and Multipolar Abnormalities Molecular Biology of the Cell **9**(34), 10-0485 (published 24 July 2023) https://doi.org/10.1091/mbc.E22-10-0485

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### 5. Submitted Papers with Center Affiliation

- T. Kumarage, S. Gupta, N. B. Morris, F. T. Doole, H. L. Scott, L.-R. Stingaciu. S. V. Pingali, J. Katsaras, G. Khelashvili, M. Doktorova, M. F. Brown, R. Ashkar *Cholesterol Modulates Membrane Elasticity via Universal Biophysical Laws* Nature Common. (submitted on 20 August 2024)
- A. Eftaiha, S. Buti, N. B. Morris, A. Qaroush; K. Assaf, D. Foudeh, S. Hammad, R. Ashkar Langmuir (submitted on 4 August 2024)
- Uwe C. Täuber, Stochastic spatial Lotka-Volterra predator-prey models to appear in Order, disorder, and criticality. Advanced problems of phase transition theory and complex systems, Vol. VIII, Y. Holovatch (ed.), Chap. 2, 67-115 World Scientific Publ., Singapore (submitted on 08 May 2024) <u>https://doi.org/10.48550/arXiv.2405.05006</u>
- Leslie Howe, Yifei Wang, Kalani Ellepola, Vinh X. Ho, Rosalie L. Dohmen, Marlo Pinto, Wouter D. Hoff, Michael P. Cooney, and Nguyen Q. Vinh, *Interfacial Photogating Graphene Field-Effect Sensors for Detecting Photosensory Biomolecules* Advanced Electronic Materials (submitted)
- Leslie Howe, Kalani H. Ellepola, Nusrat Jahan, Brady Talbert, James Li, Michael P. Cooney, and Nguyen Q. Vinh, *Characterization and Modelling of Interfacial Photogating Effect in Graphene Field-Effect Transistor Photodetectors on Silicon* ACS Applied Electronics materials (submitted)

#### 6. Invited Presentations with Center Affiliation

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

• Shengfeng Cheng

Drying of Colloidal and Polymer Solutions Department of Physics Seminar, Southeast University, Nanjing, China (20 July 2023)

• Rana Ashkar

*Invited lecture on applications of neutron scattering in soft matter and biological physics* Neutron and X-ray Summer school jointly run by Oak Ridge National Lab and Argonne National Lab, Oak Ridge, TN (6 August 2023)

- Shannon R. Serrao and Uwe C. Täuber Spatially inhomogeneous stochastic cyclic competition models: Stabilizing vulnerable ecologies through immigration waves, XLIII Dynamics Days Europe 2023, Naples, Italy (05 September 2023)
- Royce K. P. Zia *Detecting Detailed Balance Violation in Nano-Equilibrium Steady States*  International Symposium on Non-Equilibrium Dynamics of Complex Systems, Blacksburg, VA (15-16 September 2023)
- Shengfeng Cheng Drying of Colloidal and Polymer Solutions
   Department of Macromolecular Science Seminar, Fudan University, Shanghai, China (20 September 2023)
- Shengfeng Cheng Drying of Colloidal and Polymer Solutions College of Engineering Seminar, Westlake University, Hangzhou, China (21 September 2023)
- Rana Ashkar *Membrane Fluctuations and Elasticity Probed by NSE*  Soft Materials Dynamics workshop, Oak Ridge National Lab, Oak Ridge, TN (September 2023)
- Shengfeng Cheng Drying of Colloidal and Polymer Solutions College of Chemistry Seminar, Jilin University, Changchun, China (19 October 2023)
- Shengfeng Cheng Drying of Colloidal and Polymer Solutions
   Polymer Science Lecture Series, CAS Changchun Institute of Applied Chemistry, Changchun, China (20 October 2023)

• Shengfeng Cheng

Drying of Colloidal and Polymer Solutions Center for Complex Flow and Soft Matter Research Seminar, Southern University of

Science and Technology, Shenzhen, China (7 November 2023)

• Shengfeng Cheng

Self-assembly of Chiral Cytoskeletal Filaments International Symposium on Soft Matter and Topology, Shenzhen, China (9 November 2023)

- Shengfeng Cheng Drying of Colloidal and Polymer Solutions School of Emergent Soft Matter Seminar, South China University of Technology, Guangzhou, China (13 November 2023)
- Rana Ashkar

*Predictive Laws of Membrane Elasticity: From Fundamental Principles to Practical Applications* 

Materials Science & Engineering Department Seminar, University of Illinois, Urbana-Champaign, IL (29 January 2024)

- Mohammed Swailem and Uwe C. Täuber, *Computing macroscopic reaction rates in reaction-diffusion systems using Monte Carlo simulations*, Postgraduate Research Student Seminar, Department of Applied Mathematics, University of Leeds, U.K. (22 January 2024)
- Kenneth Distefano and Uwe C. Täuber, *Spatially extending the predator-prey Lotka-Volterra model*, Postgraduate Research Student Seminar, Department of Applied Mathematics, University of Leeds, U.K. (22 January 2024)
- Uwe C. Täuber, Fluctuations and spatial correlations in chemical reaction kinetics, population dynamics, and epidemic spreading, 15th Conference on Dynamical Systems Applied to Biology and Natural Sciences (DSABNS), Caparica, Portugal (7 February 2024)
- Mohammed Swailem and Uwe C. Täuber, *Computing macroscopic reaction rates in reaction-diffusion systems using Monte Carlo simulations* 15th Conference on Dynamical Systems Applied to Biology and Natural Sciences (DSABNS), Caparica, Portugal (7 February 2024)
- Ruslan Mukhamadiarov and Uwe C. Täuber,

*Effects of lattice dilution on the nonequilibrium phase transition in the stochastic SIR model* 

15th Conference on Dynamical Systems Applied to Biology and Natural Sciences (DSABNS), Caparica, Portugal (7 February 2024)

- Shengfeng Cheng
   Molecular dynamics simulation of drying and self-assembly
   American Physics Society March Meeting, Minneapolis, MN (7 March, 2024)
- Alexey Onufriev *The nucleosome as the hydrogen atom of epigenetics* Erwin Schrödinger International Institute for Mathematics and Physics (ESI), Wien, Austria (11 March, 2024)
- C. Nadir Kaplan

*Controlled dynamics of shape-shifting soft matter* Physics & Astronomy Seminar, James Madison University, Harrisonburg, VA (21 March 2024)

• Uwe C. Täuber

*Fluctuation effects and pattern formation in chemical reactions, population dynamics, and epidemic spreading,* 

three lectures, Basque Centre for Applied Mathematics (BCAM) MME Course, Bilbao, Spain (31 May and 4 June, 2024)

 Rana Ashkar Membrane Elasticity and Phase Separation with Free and Bound Sterols Biological Membranes and Membrane Proteins Meeting, Santa Fe, NM (June 2024)

# • Shengfeng Cheng

*A polymer chain model based on an analytical rod-rod interaction potential* 14th International Symposium on Polymer Physics, Chongqing, China (11 June 2024)

• Shengfeng Cheng

Molecular dynamics modeling of dispersion drying and biofilament self-assembly 5th International Symposium on Soft Matter Science and Engineering (SMSE 2024), Guangzhou, China (18 June 2024)

## 7. Provisional Patents

N/A

## 8. 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 received the Alumni Award for Excellence in Graduate Academic Advising -- awarded to one faculty member at Virginia Tech who "serves advisees in exemplary ways".
- Rana Ashkar was elected chair of the APS Committee on the Status of Women in Physics.

### Graduate students:

- Kenneth Distefano, *William E. Hassinger Graduate Fellowship*, Department of Physics, 5 April 2024.
- Sara Shabani, *Clayton Williams Graduate Fellowship*, Department of Physics, 5 April 2024.
- Teshani Kumarage one of 7 graduate students nationwide 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 (Spring-Fall 2023).

#### Undergraduate students:

- Jasmine Albert (URM) Graduate scholarship from the Physics program at the College of William & Mary (Spring 2024).
- Al Mercedes Casado (freshman, visiting REU student, URM) Best poster award at the VT Department of Physics REU poster session (summer 2023).
- Grant Davis Graduate scholarship from the Physics program at Georgetown University (Spring 2024).
- Brannon Semp Graduate scholarship from the Physics program at the University of Virginia (Spring 2024).

## 9. 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:

• Sara Shabani, *Tweets vs Pathogen Spread: A Case Study of COVID-19 in American States* American Physics Society March Meeting 2024 (6-8 March 2024)

## VIII. Industrial Affiliates Program

N/A

#### IX. Report of Financial Condition

				ix. Report	of Financial Condition			
Center Finan	cial Report	Fiscal Y	ear 20	)24	Center Financial Pro	ection Fiscal Yea	r 2025	
center mandar neport rived i tell 2027								
Operations Account	(176188)			14	Operations Account (176188)			
Starting Balance			\$	27,258.08	Starting Balance		\$	(45.35)
	Inco	me				Income		
Starts FY2024			\$(	27,303.43)	A21 Award			
	Expe	nses				Expenses		
	100				12.5% Staff Salary (Katrina Lock	nart-Elfeky)	\$	(6,300)
Ending Balance			\$	(45.35)	Ending Balance		\$	(6,345.35)
104				. 90				1280.329 SA
Overhead Account (2	235052)				Overhead Account (235052)			
Starting Balance			\$	465.26	Starting Balance		\$	4,681.94
	Inco	me				Income		
Overhead Earnings			\$	11,227.01	Overhead Earnings		\$	12,600
						Expenses		
	Expe	nses			Seminar	50 J	\$	(1,000)
Classified Salaries			\$	(823.59)	Symposium		\$	(2,500)
Seminar Travel			\$	(116.88)	Student Travel		\$	(1,000)
Faculty Travel			\$	(504.73)	Center's Awards/Grants		\$	(800)
Seminar Supplies an	d Meals		\$	2	Supplies & Budget		\$	(100)
Student Travel			\$		Faculty Travel		\$	(1,000)
Centers Symposium			\$	(5,565.13)	10175-822-01			
Supplies & Budget			\$				\$	<del>.</del> :
Other Charges			\$	¥.,				
Ending Balance			\$	4,681.94	Ending Balance		\$	10,881.94
					Dept. Contribution 87.5%		\$	(44,688)
Overhead Account (235552)					Overhead Account (235552)			
Starting Balance			Ś	218.86	Starting Balance		Ś	621.61
	Inco	me	Ť		0	Income	Ŧ	1.
	nses				Expenses			
Centers Symposium	and the second s	0.52330	\$	(840.47)	Center Symposium Travel	1750 (1876)	\$	(800)
Meeting Facilities Rentals			\$	-	Honorariums		\$	
Centers Symposium Awards			\$		Meeting Facilities Rentals		\$	(250)
Breakfast, Lunch and Dinners			\$	50	Centers Symposium Awards		\$	(400)
Food and Dietary supplies			\$	-	Breakfast, Lunch and Dinners		\$	-
Supplies & Budget			\$	Di	Food and Dietary supplies		\$	<u>04</u>
Centers Awards			\$	-	Supplies & Budget		\$	(50)
Continuous Charges Budget			\$		Continuous Charges Budget		\$	
Other Charges			\$	-	Other Charges			
Ending Balance			\$	(621.61)	Ending Balance		\$	(878.39)

#### X. Major Issues of the Center

In FY 2023 and FY2024, we have been recovering from the pandemic and reviving the annual symposia, seminars, discussion meetings, and social activities.

We shall continue to organize seminars and annual symposia with external speakers, and to support other related conferences.

Our principal task over the next few years remains to generate new interdisciplinary research collaborations leading to collaborative grant proposals.

The Center is currently working actively to apply for a Research Experience for Undergraduates (REU) grant from the U.S. National Science Foundation, which will enable us to house an 8-week REU summer program in the field of soft matter and biological physics.

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, 2024

S. Cheng

Dr. Shengfeng Cheng Associate Professor of Physics, Virginia Tech Director, Center for Soft Matter and Biological Physics