

Center for Soft Matter and Biological Physics
Department of Physics, Virginia Tech
Annual Report – Fiscal Year 2016

The Center for Soft Matter and Biological Physics was chartered on February 12, 2016. This annual report consequently only covers a period of five months, until June 30, 2016.

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 considerably 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. Patrick Huber, Professor, Department of Physics, College of Science, until August 10, 2016
- Dr. Mark Pitt, Professor, Department of Physics, College of Science, since August 10, 2016

Center Director and Contact Person:

- Dr. Uwe C. Täuber, Professor, Department of Physics, College of Science

Center Steering Committee:

- Dr. Daniel Capelluto, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Shengfeng Cheng, Assistant Professor, Department of Physics, College of Science
- Dr. William Ducker, Professor, Department of Chemical Engineering, College of Engineering
- Dr. Will Mather, Assistant Professor, Departments of Physics and Biological Sciences, College of Science

Center Website: <http://www.phys.vt.edu/CSMBP/about.html>

2. List of Faculty Affiliated with the Center

Regular faculty members (31) as of June 30, 2016:

- Dr. Justin Barone, Associate Professor, Department of Biological Systems Engineering, College of Engineering
- Dr. Daniel Capelluto, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Jing Chen, Assistant Professor, Department of Biological Sciences, College of Science
- Dr. Shengfeng Cheng, Assistant Professor, Department of Physics, College of Science
- 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. James Hanna, Assistant Professor, Department of Biomedical Engineering and Mechanics, College of Engineering
- Dr. Jean Heremans, Professor, Department of Physics, College of Science
- Dr. Sunny Jung, Associate Professor, Department of Biomedical Engineering and Mechanics, College of Engineering
- Dr. Giti Khodaparast, Associate Professor, Department of Physics, College of Science
- Dr. Shihoko Kojima, Assistant Professor, Department of Biological Sciences, College of Science
- Dr. Tim Long, Professor, Department of Chemistry and Director, Macromolecules and Interfaces Institute, College of Science
- Dr. Louis Madsen, Associate Professor, Department of Chemistry, College of Science
- Dr. Herve Marand, Professor and Associate Chair, Department of Chemistry, College of Science

- Dr. Will Mather, Assistant Professor, Departments of Physics and Biological Sciences, College of Science
- 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, Assistant Professor, Department of Physics, College of Science
- Dr. Alexey Onufriev, Associate 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 Director, Academy of Integrated Science, College of Science
- Dr. David Popham, Professor, Department of Biological Sciences, College of Science
- 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. Chenggang Tao, Assistant Professor, Department of Physics, College of Science
- Dr. Uwe Täuber, Professor, Department of Physics, College of Science
- Dr. John Tyson, University Distinguished Professor, Department of Biological Sciences, College of Science
- Dr. Layne Watson, Professor, Department of Computer Science, College of Engineering

Three more prospective regular faculty members are expected to be officially admitted at the Center faculty meeting on October 21, 2016:

- Dr. Yang Cao, Associate Professor, Department of Computer Science, College of Engineering
- Dr. Silke Hauf, Assistant Professor, Department of Biological Sciences, College of Science
- Dr. Reza Mirzaeifar, Assistant Professor, Department of Mechanical Engineering, College of Engineering

Affiliated emeriti faculty members:

- Dr. Jimmy Ritter, Associate Professor emeritus, Department of Physics, 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 Students Supported by Center Administered Funds

Graduate research assistants:

- Ahmadreza Azizi, ½ GRA summer 2016, DOE 429262
- Bart L. Brown, ½ GRA spring 2016, GRA summer 2016, DOE 429262
- Harshwardhan N. Chaturvedi, GRA summer 2016, DOE 429262
- Chuanhui Chen, GRA summer 2016, ARO 450347
- Sheng Chen, GRA summer 2016, DOE 429262
- Anamul Haque, GRA spring and summer 2016, NSF 479036
- Weigang Liu, GRA summer 2016, DOE 429262

- Shannon R. Serrao, ½ GRA summer 2016, 429262
- Xiangwen Wang, ½ GRA summer 2016, NSF 478819
- Husong Zheng, GRA summer 2016, ARO 450347

Undergraduate research students:

- Christopher Dobson, physics, summer 2016, Jeffress 443421
- Nathan W. Galliher, physics, summer 2016, DOE 429262
- Jason Gray, physics, spring 2016, NSF 478819
- Christopher Ryan Grosenick, physics, summer 2016, Jeffress 443421
- Peter F. Morrissey, physics, summer 2016, DOE 429262
- Maximilian D. Shafer, physics, summer 2016, DOE 429262
- Isaac Shoultz, physics, summer 2016, NSF 479036
- James Stidham, physics, summer 2016, NSF 478819

4. Classified Staff

- Katrina Loan, Program Support Technician, funded through A-21 program, since July 1, 2016

We had no classified staff working for the Center in Fiscal Year 2016. On our behalf, Will Mather wrote an application for a staff position through the A-21 program in March 2016. We received approval for this position in May, and subsequently hired Katrina Loan as our Program Support Technician, with starting date July 1, 2016. During her first year, her salary will be provided by the Office of the Vice President for Research (90 %) and the Center for Soft Matter and Biological Physics Overhead Return Fund (10 %).

Department fiscal staff:

- Jacqueline Woodyard, Business Manager, Department of Physics
- Sherri Collins, Assistant Business Manager, Department of Physics

III. Amendments to the Center Charter

Not applicable

IV. Stakeholder Committee

The Center does not currently have a Stakeholder Committee established. We propose as its members:

- Dr. Mark Pitt, Professor and Chair, Department of Physics
- Dr. Randy Heflin, Professor, Department of Physics, and Associate Dean for Research and Graduate Studies, College of Science
- Dr. Srinath Ekkad, Rolls Royce Professor, Department of Mechanical Engineering, and Associate Vice President for Research Programs, Office of the Vice President for Research and Innovation

V. Major Grants Received in 2015-2016

- Thomas F. and Kate Miller Jeffress Memorial Trust (Jeffress 443421), Jeffress Trust Awards Program in Interdisciplinary Research, *A computational model to study the self-assembly of microtubules*; PI Shengfeng Cheng (Physics, 100%): September 30, 2015 – September 29, 2016; total volume \$ 100,000 for one year.
- American Chemical Society (ACS 443428), Petroleum Research Fund (PRF), *Computational modeling of ionic polymers: from solution interpolyelectrolyte complexes to solid-state membranes*; PI Shengfeng Cheng (Physics, 100 %): September 1, 2016 – August 31, 2018; total volume \$ 110,000 for two years.
- U.S. Army Research Office (ARO 450347), Engineering Science Directorate, Materials Science Division grant *W911NF-15-1-0414, Fundamental investigation of dynamic phenomena in atomically thin layered materials*, PI Chenggang Tao (Physics, 100 %): August 1, 2015 - July 31, 2018; total volume \$ 389,187 for three years.
- U.S. Department of Energy (DOE 429262), Office of Basic Energy Sciences (BES) grant *DE-FG02-09ER46613, Non-equilibrium relaxation and aging scaling of driven topological defects in condensed matter*; PI Uwe C. Täuber (Physics, 50 %), co-PI Michel Pleimling (Physics, 50 %): August 15, 2015 – August 14, 2018; total volume \$ 450,000 for three years.
- U.S. National Science Foundation (NSF 417942), Division of Materials Research (DMR) grant *DMR-1507371, Non-equilibrium statistical mechanics of co-evolving complex systems*; PI Kevin E. Bassler (Physics, University of Houston, 50 %), co-PI Royce K.P. Zia (Physics, 50 %): January 16, 2016 – December 31, 2018; total volume: \$ 324,000 for three years; expected subcontract to Virginia Tech: \$ 11,270.

Continuing grants:

- U.S. National Science Foundation (NSF 479036), Division of Molecular and Cellular Biosciences (MCB) grant *MCB-1330180, A queueing framework for synthetic circuits in E. coli*; PI William H. Mather (Physics, 90 %), co-PI Kristy Collins (VBI, 10 %): September 1, 2013 – August 31, 2016; total volume \$ 961,252 for three years.
- U.S. National Science Foundation (NSF 478819), Division of Materials Research (DMR), Condensed Matter and Materials Theory grant *DMR-1205309, Transient and steady-state properties far from equilibrium*; PI Michel Pleimling (Physics, 100 %): September 1, 2012 - August 31, 2016 (one year no cost extension); total volume \$ 300,000 for three years.

VI. Major Proposals Submitted or Pending

- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), Condensed Matter and Materials Theory, *CAREER: Self-organization of microtubules as model dynamic materials*; PI Shengfeng Cheng (Physics, 100%); total volume \$ 582,050 for five years.
- National Institutes of Health (NIH), National Institute of General Medical Sciences (NIGMS), *Accurate and efficient solvent models for molecular simulations: methods and biological applications*, PI Alexey Onufriev (Computer Science, 100%), volume \$ 2,866,433 for five years.

- U.S. National Science Foundation (NSF), Division of Materials Research (DMR), Condensed Matter and Materials Theory, *Systems far from equilibrium: relaxation processes and steady-state properties*; PI Michel Pleimling (Physics, 100%); total volume \$ 444,282 for three years.
- U.S. Army Research Office (ARO), 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); total volume \$ 1,485,501 for four years.

VII. Significant Accomplishments in 2016

1. Center for Soft Matter and Biological Physics Seminar Series

The Center runs a regular seminar series in conjunction with the Physics Department's Condensed Matter Seminars (Mondays, 4.00 – 5.00 pm), organized by Vinh Nguyen and Will Mather in collaboration with Ed Barnes (all Department of Physics): <http://www.phys.vt.edu/CSMBP/softmatter/Fall2016.shtml>.

In the spring semester 2016, the Center has organized and financially supported the following seminars:

- March 4, 2016: Curtis Ogle, Department of Physics, Virginia Tech, *Proteolytically coordinated activation of toxin-antitoxin modules*.
- March 21, 2016: Professor Dr. Nuno A. M. Araújo, Departamento de Física, Faculdade de Ciências, and Centro de Física Teórica e Computacional, Universidade de Lisboa, Portugal, *Self-organization of colloids under non-equilibrium conditions*.
- April 25, 2016: Professor Dr. A. Joshua Wand, University of Pennsylvania, *Internal motion and conformational entropy in protein function*.

2. Center for Soft Matter and Biological Physics Symposium

The Center held its first annual full-day symposium on May 19, 2016, organized by Sunny Jung (Department of Biomedical Engineering and Mechanics) and Vinh Nguyen (Department of Physics): <http://www.phys.vt.edu/CSMBP/workshops/flyers/Symposium2016.pdf>.

Michele Strauss (Department of Physics) provided staff support. In this context our Center was featured in VT News on May 18, 2016: <https://vtnews.vt.edu/articles/2016/05/science-softmatterlab.html>.

3. Center for Soft Matter and Biological Physics Summer Meetings

Through the summer months (Mondays 1.30 – 2.30 pm), the Center held informal meetings, organized by Vinh Nguyen and Will Mather (both Department of Physics), to promote scientific exchange and incite possible research collaborations: <http://www.phys.vt.edu/CSMBP/softmatter/Summer2016.shtml>.

- May 23, 2016: Ali Charkhesht and Vinh Nguyen, Department of Physics, Virginia Tech, *Protein hydration and dynamics*.

- June 6, 2016: Steve Melville, Department of Biological Sciences, Virginia Tech, *How do you pull a hydrophobic protein out of a membrane and put it in a fiber 1,000 times per second?*
- June 13, 2016: Will Mather, Department of Physics, Virginia Tech, *Whither noise? A discussion concerning the utility of stochastic modeling for cellular networks.*
- June 20, 2016: David Popham, Department of Biological Sciences, Virginia Tech, *Water and solutes in bacterial spores: Effects on protein and lipid mobility.*
- June 27, 2016: Alexey Onufriev, Department of Computer Science, Virginia Tech, *Existing water models for atomistic modeling: the bad and the ugly.*

4. Research Publications with Center Affiliation

- Sheng Chen and Uwe C. Täuber, *Non-equilibrium relaxation in a stochastic lattice Lotka-Volterra model*, *Physical Biology* **13**, 025005 – 1-11 (19 April 2016) [<http://arxiv.org/abs/1511.05114>].
- Linjun Li and Michel Pleimling, *Three-dimensional nonequilibrium Potts systems with magnetic friction*, *The Physical Review E* **93**, 042122 – 1-7 (20 April 2016) [<http://arxiv.org/abs/1604.02209>].
- Shengfeng Cheng and Gary S. Grest, *Dispersing nanoparticles in a polymer film via solvent evaporation*, *ACS Macro Letters* **5**, 694-698 (19 May 2016) [<http://arxiv.org/abs/1605.06408>].

5. Submitted Papers with Center Affiliation

- Alexander Drozdetski, Igor S. Tolokh, Lois Pollack, Nathan Baker, and Alexey V. Onufriev, *Opposing effects of multivalent ions on the flexibility of DNA and RNA*, *Physical Review Letters* **117**, 028101 – 1-5 (6 July 2016).
- Shengfeng Cheng and Mark O. Robbins, *Nanocapillary adhesion between parallel plates*, *Langmuir* **32**, 7788-7795 (14 July 2016) [<http://arxiv.org/abs/1608.00436>].
- Saeed Izadi and Alexey V. Onufriev, *Accuracy limit of rigid 3-point water models*, *The Journal of Chemical Physics* **145**, 074501 – 1-10 (15 August 2016).
- Harshwardhan Chaturvedi, Hiba Assi, Ulrich Dobramysl, Michel Pleimling, and Uwe C. Täuber, *Flux line relaxation kinetics following current quenches in disordered type-II superconductors*, *Journal of Statistical Mechanics: Theory and Experiment* **2016**, 083301 – 1-16 (19 August 2016) [<http://arxiv.org/abs/1606.06100>].
- Ahmed Roman, Debanjan Dasgupta, and Michel Pleimling, *A theoretical approach to understand spatial organization in complex ecologies*, *Journal of Theoretical Biology* **403**, 10-16 (21 August 2016) [<http://arxiv.org/abs/1605.02028>].

- Nguyen Q. Vinh,
Probe conformational dynamics of proteins in aqueous solutions by terahertz spectroscopy,
to appear in: *Proceedings of SPIE* Vol. **9934**, 9934-26V-2 (September 2016).
- Weigang Liu and Uwe C. Täuber,
Critical initial-slip scaling for the noisy complex Ginzburg-Landau equation, to appear in:
Journal of Physics A: Mathematical and Theoretical (2016) [<http://arxiv.org/abs/1606.08263>].
- Brato Chakrabarti and James A. Hanna,
Catenaries in viscous fluid, to appear in:
Journal of Fluids and Structures (2016) [<https://arxiv.org/abs/1509.01282>].
- Uwe C. Täuber,
Phase transitions and scaling in systems far from equilibrium, to appear in:
Annual Reviews of Condensed Matter Physics **8** (March 2017) [<http://arxiv.org/abs/1604.04487>].
- Julia M. Selfridge, Tetsuya Gotoh, Samuel Schiffhauer, Jingjing Liu, Phillip Stauffer, Andrew Li,
Daniel G.S. Capelluto, and Carla V. Finkelstein,
Chronotherapy: intuitive, sound, founded... but not broadly applied,
to appear in: *Drugs* (2016).
- Jeffrey F. Ellena, Wen Xiong, Xiaolin Zhao, Narasimhamurthy Shanaiah, and Daniel G.S.
Capelluto,
Backbone 1H , ^{15}N , and ^{13}C resonance assignments of the TomI VHS domain,
to appear in: *Biomolecular NMR Assignments* (2017).
- Tuo-Xian Tang, Wen Xiong, Carla V. Finkelstein, and Daniel G. S. Capelluto,
Identification of ligand-binding modulators using the protein-lipid overlay assay,
to appear in: *Methods in Molecular Biology* (2017).
- Hiba Assi, Harshwardhan Chaturvedi, Michel Pleimling, and Uwe C. Täuber,
Structural relaxation and aging scaling in the Coulomb and Bose glass models,
submitted to: *European Physical Journal B* (2016) [<http://arxiv.org/abs/1606.02971>].
- Jacob Carroll, Matthew Raum, Kimberly Forsten-Williams, and Uwe C. Täuber,
Ligand-receptor binding kinetics in surface plasmon resonance cells: a Monte Carlo analysis,
submitted to: *Physical Biology* (2016) [<http://arxiv.org/abs/1606.08294>].
- Diego F. Cortes, Tuo-Xian Tang, Daniel G. S. Capelluto, and Iulia M. Lazar,
Nanoflow valve for the removal of trapped air in microfluidic structures,
submitted to: *Sensors & Actuators B: Chemical* (2016).
- Deepu K. George, Ali Charkhesht, Olivia A. Hull, Archana Mishra, Daniel G.S. Capelluto,
Katie R. Mitchell-Koch, and Nguyen Q. Vinh,
*New insights into the dynamics of zwitterionic micelles and their hydration waters by gigahertz-
to-terahertz dielectric spectroscopy*,
submitted to: *The Journal of Physical Chemistry* (2016).
- Nick Argibay, Michael Chandross, Shengfeng Cheng, and Joe R. Michael,
Linking microstructural evolution and macro-scale friction behavior in metals,
submitted to: *Acta Materialia* (2016).

- Emmanuel Viot, Grace Ma, Christophe Clanet, and Sunghwan Jung,
Physics of chewing,
submitted to: *Proceedings of the National Academy of Sciences of the USA* (2016).
- Philip Hochendoner, Nicholas C. Butzin, Curtis T. Ogle, and William H. Mather,
Entrainment of a bacterial synthetic gene oscillator through proteolytic queuing,
submitted to: *ACS Synthetic Biology* (2016).
- Xiangwen Wang and Michel Pleimling,
Foraging patterns in online searches,
submitted to: *The Physical Review E* (2016).

6. Invited Presentations with Center Affiliation

- Daniel Capelluto,
The leading role of lipids in protein signaling,
Northern Virginia Community College, 17 February 2016.
- Nguyen Q. Vinh,
Optical excitation of Er centers in GaN epilayers grown by MOCVD, SPIE Photonics West,
Optical Components and Materials XIII, San Francisco, CA, 17 February 2016.
- Shengfeng Cheng,
Evaporation-induced nanoparticle self-assembly in a polymer matrix,
American Physical Society March Meeting, Baltimore, MD, 16 March 2016.
- Uwe C. Täuber,
Control of universal scaling, noise strength, and pattern formation in critical dynamics,
U.S. Army Research Office Workshop *Statistical Physics of Stochastic Optimal Control and Learning*, Atlanta, GA, 14 June 2016.

7. Awards and Recognitions

- Daniel Capelluto,
M. L. Andrews Cancer Research Award, Virginia Academy of Science,
July 1, 2016 – June 30, 2017, \$ 3000.

VIII. Industrial Affiliates Program

Not applicable

IX. Report of Financial Condition

Center Financial Report Fiscal Year 2016		
Operations Account (171688)		
Starting Balance	\$	-
	Income	
Starts FY2017	\$	-
	Expenses	
Ending Balance	\$	-
Overhead Account (235052)		
Starting Balance	\$	-
	Income	
Overhead Earnings	\$	9,834.78
Symposium Support	\$	1,100.00
	Expenses	
Seminar	\$	(324.50)
Symposium	\$	(1,235.60)
Ending Balance	\$	9,374.68

Center Financial Projection Fiscal Year 2017		
Operations Account (171688)		
Starting Balance	\$	-
	Income	
A21 Award	\$	31,500
	Expenses	
90% Staff Salary (Katrina Loan)	\$	(31,500)
Ending Balance	\$	-
Overhead Account (235052)		
Starting Balance	\$	9,374.68
	Income	
Overhead Earnings	\$	12,000
Symposium Support	\$	1,000
	Expenses	
Seminar	\$	(3,000)
Symposium	\$	(6,000)
Sowers Symposium Speaker	\$	(2,000)
10% Staff Salary (Katrina Loan)	\$	(3,415)
Ending Balance	\$	7,959.68

X. Major Issues of the Center

The Center will maintain its successful seminar series and regular discussion meetings. We intend to organize a symposium with external speakers in May 2017. Our principal goal over the next year will be to generate new interdisciplinary research collaborations leading to several collaborative grant proposals.