# Center for Soft Matter and Biological Physics Department of Physics, Virginia Tech Annual Report – Fiscal Year 2017

The Center for Soft Matter and Biological Physics was chartered on February 12, 2016. This annual report covers the period July 1, 2016 through June 30, 2017.

#### 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, until May 15, 2017.

Center Website: http://www.phys.vt.edu/CSMBP/index.html

#### 2. List of Faculty Affiliated with the Center

Regular faculty members (33) as of June 30, 2017:

- Dr. Justin Barone, Associate Professor, Department of Biological Systems Engineering, College of Agriculture and Life Science and 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, 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. Silke Hauf, Assistant Professor, Department of Biological Sciences, College of Science
- 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. Steve Melville, Associate Professor, Department of Biological Sciences, College of Science
- Dr. Djordje Minic, Professor, Department of Physics, College of Science
- Dr. Reza Mirzaeifar, Assistant Professor, Department of Mechanical Engineering, College of Engineering
- Dr. Vinh Nguyen, Assistant Professor, Department of Physics, College of Science
- Dr. Alexey Onufriey, 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

#### 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; GRA summer 2017, ARO 450484
- Bart L. Brown, GRA summer 2016 and summer 2017, ½ GRA fall 2016 and spring 2017, DOE 429262
- Jacob A. Carroll, partial GRA (two weeks) summer 2017, ARO 450484
- Harshwardhan N. Chaturvedi, GRA summer 2016 and summer 2017, ½ GRA fall 2016 and spring 2017, DOE 429262
- Chuanhui Chen, GRA summer 2016, ARO 450347
- Sheng Chen, GRA summer 2016, DOE 429262; GRA summer 2017, ARO 450484
- Anamul Haque, GRA spring and summer 2016, NSF 479036
- Weigang Liu, GRA summer 2016 and summer 2017, ½ GRA fall 2016 and spring 2017, DOE 429262
- Ruslan I. Mukhamadiarov, GRA fall 2016, DOE 429262; GRA summer 2017, ARO 450484
- Riya Nandi, GRA summer 2017, ARO 450484
- Shannon R. Serrao, GRA summer 2017, ARO 450484
- 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 and fall 2016, spring and summer 2017, 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; summer 2017, ARO 450484
- Austin "Ada" Warren, physics, summer 2017, ARO 450484
- Nicholas V. Wilson, physics, fall 2016, spring and summer 2017, DOE 429262

#### 4. Classified Staff

Katrina Loan, Program Support Technician, funded through A-21 program, since July 1, 2016
 During her second year, Ms. Loan's salary will be provided by the Office of the Vice President for Research (80 %) and the Center for Soft Matter and Biological Physics (20 %).

#### Department fiscal staff:

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

#### **III.** Amendments to the Center Charter

The quorum requirement of 50 % of the Center's regular faculty members for official votes at Center meetings was lowered to 30 %; in addition, the presence of a simple majority (50 %) of the Center's Steering Committee will be required.

#### 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 2016-2017

#### New grants:

- 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.
- National Aeronautics and Space Administration (NASA) support, *RBI Analytical Modeling with the MCRT Environment Support (STARSS III)*, *SSAI/NASA*. PI Bob Mahan (Department of Mechanical Engineering, 50 %), co-PI Vinh Nguyen, (Department of Physics, 10 %), co-PI Brian Vick (Department of Mechanical Engineering, 40 %): December 1, 2016 September 30, 2017; total volume \$ 370,399.
- 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): April 15, 2017 April 14, 2021; total volume \$ 1,400,000 for four years.
- U.S. National Science Foundation (NSF 479739), 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 %): June 1, 2017 – May 31, 2019; total volume \$ 290,000 for two years.

#### Continuing grants:

- 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.

#### 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.
- U.S. National Science Foundation (NSF), Division of Chemistry CHE, Structure, Dynamics and Mechanisms B, *Unraveling Connections Among Biomolecular Structure, Interfacial Solvent Dynamics, and Conformational Dynamics*; PI Katie Mitchell-Koch (Wichita State University, 50%), co-PI Vinh Nguyen (Physics, 50%); August 01, 2017 July 31, 2020; total volume \$ 368,000 for three years.
- National Aeronautics and Space Administration (NASA) support, RBI Analytical Modeling with the MCRT Environment, SSAI/NASA. PI Bob Mahan (Department of Mechanical Engineering, 40 %), Co-PI Vinh Nguyen, (Department of Physics, 30 %), co-PI Brian Vick (Department of Mechanical Engineering, 30 %): October 01, 2017 September 30, 2018; total volume \$ 351,669.
- National Aeronautics and Space Administration (NASA) support, *Clouds and the Earth's Radiant Energy System (CERES) Analytical Modeling with the MCRT Environment, SSAI/NASA*. PI Bob Mahan (Department of Mechanical Engineering, 60 %), co-PI Vinh Nguyen, (Department of Physics, 40 %): October 01, 2017 September 30, 2018; total volume of \$158,332.
- National Aeronautics and Space Administration (NASA) support, engineering long-wavelength infrared photo-detectors based on two-dimensional Materials, PI Vinh Nguyen, (Department of Physics, 100 %): October 15, 2017 October 14, 2020; total volume \$ 599,445 for three years.
- National Aeronautics and Space Administration (NASA): Advanced Component Technology support, *Plasmonic Enhanced Long-Wavelength Photodetectors for Earth Radiation Budget Instruments*, PI Vinh Nguyen, (Department of Physics, 100 %): October 01, 2017 September 30, 2020; total volume \$ 605,000 for three 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.

#### VII. Significant Accomplishments in 2017

#### 1. Faculty Search in Soft Matter and Biological Physics

The Physics Department advertised a tenure-track faculty position in soft matter and biological physics in the fall 2016. The search committee comprised Center faculty Justin Barone, Daniel Capelluto, Shengfeng Cheng, Alexey Onufriev, Vicki Soghomonian, and Uwe C. Tauber (chair). Five candidates were interviewed in January / February 2017. Our top choice Dr. Rana Ashkar (Oak Ridge National Laboratory, TN) accepted our offer; she will join the Physics Department and Center in January 2018.

#### 2. 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 p.m.), organized by Vinh Nguyen in collaboration with Ed Barnes (all Department of Physics). In the fall term 2016 and spring semester 2017, the Center has organized and financially supported the following seminars:

http://www1.phys.vt.edu/CSMBP/softmatter/Fall2016.shtml, http://www.phys.vt.edu/CSMBP/softmatter/Spring2017.shtml.

- August 29, 2016: Dr. Ting Ge, University of North Carolina at Chapel Hill, *Nanoparticle motion in entangled melts of linear and non-concatenated ring polymers.*
- September 5, 2016: Prof. Hans Werner Diehl, University Duisburg-Essen (Germany), Fluctuation-induced forces in confined He and ideal and imperfect Bose gases.
- October 24, 2016: Prof. David Odde, University of Minnesota, Mechanisms of microtubule kinetic stabilization by the anticancer drugs paclitaxel and vinblastine.
- November 14, 2016: Prof. Nicholas J. Mayhall, Virginia Tech, Using simple ab initio methods to construct even simpler Hamiltonians: applying spinflip methods for strong correlation and excited states.
- November 28, 2016: Prof. Jing Chen, Virginia Tech, *Mathematical modeling of myxobacterial motility*.
- December 5, 2016: Prof. Dmitry Matyushov, Arizona State University, Electrostatic soup of biology: Production of biological energy by the fluctuating protein-water interface.
- January 20, 2017: Dr. Rana Ashkar, Oak Ridge National Lab, Towards switchable topography and tunable fluctuations in biomimetic lipid bilayers.
- January 27, 2017: Dr. Liheng Cai, Harvard University, Soft matter approaches to biology: A tale of mucus hydrogel in human lung defense.
- February 6, 2017: Dr. Jejoong Yoo, University of Illinois Urbana-Champaign, *The physics of chromosomes: from DNA loops to nucleus-scale structure.*
- February 13, 2017: Dr. Maxim Lavrentovich, University of Pennsylvania, *Putting patterns on spheres: pollen grains and cholesteric liquid crystal shells.*
- February 20, 2017: Dr. Edward Banigan, Northwestern University, *Emergent length scales of the cell nucleus*.
- March 20, 2017: Prof. Christian Ray, University of Kansas, Regulation of bacterial growth in discrete steps and structured lineages.
- March 27, 2017: Prof. Katie Mitchell-Koch, Dept. of Chemistry, Wichita State University, *How do bio-molecular surfaces influence small molecule dynamics?*

- April 3, 2017: Prof. Ting Lu, University of Illinois at Urbana-Champaign, *Bottom-up assembly of microbial communities: modeling, analysis and engineering.*
- April 10, 2017: Prof. Jiadong Zang, University of New Hampshire, *Skyrmions in helimagnets*.
- June 2, 2017: Prof. P.S. Krishnaprasad, University of Maryland, *Sub-Riemannian geometry and finite time thermodynamics*.

The Center also provided financial support (\$ 400) for the Second Molecular Biophysics Symposium held at Virginia Tech on April 20, 2017, <a href="https://www.bi.vt.edu/molecular-biophysics-symposium">https://www.bi.vt.edu/molecular-biophysics-symposium</a>.

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

The Center held its second annual symposium on May 17 and 18, 2017, organized by Justin Barone (Department of Biological Systems Engineering) and Vinh Nguyen (Department of Physics), featuring two invited external keynote speakers on May 17:

- Prof. Jennifer Curtis, Physics, Georgia Tech,
   Fabricated and synthetic hyaluronan polymer brushes for tissue regulation and
   biomaterials.
- Prof. Sergei Sheiko, Chemistry, University of North Carolina Chapel Hill, Polymer genome for strategic design of tissue-like materials.

The other speakers on May 17 were:

- Dr. Rana Ashkar, Biology and Soft Matter, Oak Ridge National Laboratory, *Response of membrane fluctuations to protein binding and insertion.*
- Prof. Yang Cao, Computer Science, Virginia Tech,
   Multiscale stochastic simulation and the budding yeast cell cycle model.
- Prof. Jing Chen, Biological Sciences, Virginia Tech,
   Spatiotemporal model for pattern formation in phage-bacteria system.
- Prof. James Hanna, Biomedical Engineering and Mechanics, Virginia Tech, *Flexible structures*.
- Prof. Lou Madsen, Chemistry, Virginia Tech, Combining a Kevlar-like polymer with ionic liquids to enable safer and higher density batteries.
- Prof. Chenggang Tao, Physics, Virginia Tech, *Interfaces and defects in atomically thin materials.*

During the poster session on May 17, the best poster prize of \$ 110.00 was awarded to: Andrew Korovich, Curt Zanelotti, Rui Zhang, Xiuli Li, Lam Thieu, Deyang Yu, and Louis A. Madsen: *Understanding molecular transport and dynamics in soft materials: Ion conductors, polymeric micelles, and structured liquids.* 

The May 18 Graduate Student Workshop featured our keynote speakers:

- Prof. Jennifer Curtis, Mechanics of phagocytosis: Role of actin dynamics and curvature.
- Prof. Sergei Sheiko, Molecular mechanichemistry: from making to breaking complex architectures.

Katrina Loan provided staff support. More details are listed in our symposium program flyer: <a href="http://www.phys.vt.edu/CSMBP/workshops/flyers/CSMBP\_Symposium\_2017\_Program.pdf">http://www.phys.vt.edu/CSMBP/workshops/flyers/CSMBP\_Symposium\_2017\_Program.pdf</a>.

#### 4. Center for Soft Matter and Biological Physics Meetings

Through the semester (Fridays 4.00 - 5.00 p.m.) as well as summer months (Mondays 1.30 - 2.30 p.m.), 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://www1.phys.vt.edu/CSMBP/softmatter/Summer2016.shtml,

http://www1.phys.vt.edu/CSMBP/softmatter/Fall2016\_meetings.shtml,

http://www1.phys.vt.edu/CSMBP/softmatter/Spring2017 meetings.shtml,

http://www1.phys.vt.edu/CSMBP/softmatter/Summer2017.shtml.

- July 25, 2016: Prof. Justin Barone, Department of Biological Systems Engineering, Virginia Tech, *Protein amyloid self-assembly*.
- August 1, 2016: Prof. Shihoko Kojima, Department of Biological Sciences, Virginia Tech, *Oscillators from nature circadian clocks*.
- August 8, 2016: Prof. William Mather, Department of Physics, Virginia Tech, *Machine learning, with image analysis in Fiji as an example.*
- September 9, 2016: Udaya Sree Datla, Department of Biological Sciences, Virginia Tech, Evolutionary dynamics in synthetic predator-prey ecologies.
- September 23, 2016: Prudvi Gaddam, Department of Chemical Engineering, Virginia Tech, *A liquid state thermal diode*.
- September 30, 2016: Prof. William Mather, Department of Physics, Virginia Tech, *Modeling gene networks*.
- October 28, 2016: Harshwardhan Chaturvedi, Department of Physics, Virginia Tech, Flux lines in superconductors: planar defects and beyond.
- November 4, 2016: Dr. Chola Regmi, Department of Physics, Virginia Tech, *Tubulin binding energies from all-atom molecular dynamics simulations*.
- December 2, 2016: Bart Brown, Department of Physics, Virginia Tech, *Noncyclic interactions: games within games*.
- March 24, 2017: Sheng Chen, Department of Physics, Virginia Tech, Computational study of biodiversity with evolution and natural selection.

- March 31, 2017: Heather Deter, Department of Physics, Virginia Tech, Big data analysis of differential production within toxin-antitoxin systems.
- April 14, 2017: William Ducker, Department of Chemical Engineering, Virginia Tech, *Micrometer-sized spheres driven into crystalline array by simple rubbing.*
- June 9, 2017: Wen Xiong, Department of Biological Sciences, Virginia Tech, Structural and functional basis of alternative endosomal ESCRT-0 protein complexes.
- June 16, 2017: Udaya Sree Datla and Sheng Chen, Department of Physics, Virginia Tech, The spatiotemporal network dynamics of acquired resistance in engineered microecological systems.
- June 23, 2017: Chuanhui Chen, Department of Physics, Virginia Tech, Scanning probe microscopy study of molecular nanostructures on 2D materials.
- June 30, 2017: Wei Song, Department of Biological Sciences, Virginia Tech, Design of a disabled-2-derived peptide to impair platelet-mediated cancer cell extravasation.

#### 5. Research Publications 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 (1 August 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].
- Brato Chakrabarti and James A. Hanna, Catenaries in viscous fluid, Journal of Fluids and Structures 66, 490-516 (9 September 2016) [http://arxiv.org/abs/1509.01282].

• Deepu K. George, Ali Charkhesh, A. Hull, A. 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,

*The Journal of Physical Chemistry B* **120**, 10757-10767 (23 September 2016).

• Julia M. Selfridge, Tetsuya Gotoh, Samuel Schiffhauer, Jingjing Liu, Phillip E. Stauffer, Andrew Li, Daniel G.S. Capelluto, and Carla V. Finkielstein, *Chronotherapy: intuitive, sound, founded... but not broadly applied, Drugs* **76**, 1507–1521 (3 October 2016).

• Weigang Liu and Uwe C. Täuber,

Critical initial-slip scaling for the noisy complex Ginzburg-Landau equation, *Journal of Physics A: Mathematical and Theoretical* **49**, 434001 – 1-17 (3 October 2016) [http://arxiv.org/abs/1606.08263].

• Saeed Izadi, Ramu Anandakrishnan, and Alexey V. Onufriev, Implicit solvent model for million-atom atomistic simulations: insights into the organization of 30-nm chromatin fiber, Journal of Chemical Theory and Computation 12, 5946-5959 (17 October 2016).

• Nguyen Q. Vinh

*Probe conformational dynamics of proteins in aqueous solutions by terahertz spectroscopy, Proceedings of SPIE* **9934**, 9934-26V-2 (26 October 2016).

- Nick Argibay, Michael Chandross, Shengfeng Cheng, and Joe R. Michael, Linking microstructural evolution and macro-scale friction behavior in metals, J. Mater. Science **52**, 2780-2799 (21 November 2016).
- Hiba Assi, Harshwardhan Chaturvedi, Michel Pleimling, and Uwe C. Täuber, Structural relaxation and aging scaling in the Coulomb and Bose glass models, European Physical Journal B 89, 252 – 1-15 (21 November 2016) [http://arxiv.org/abs/1606.02971].
- Jingyi Wang, Husong Zheng, Guanchen Xu, Lifei Sun, Dake Hu, Zhixing Lu, Lina Liu, Chenggang Tao, and Liying Jiao,

  Controlled synthesis of two-dimensional 1T-TiSe2 with charge density wave transition by chemical vapor transport,

  Journal of the American Chemical Society (JACS) 138, 16216-16219 (29 November 2016).
- Jacob Carroll, Matthew Raum, Kimberly Forsten-Williams, and Uwe C. Täuber, Ligand-receptor binding kinetics in surface plasmon resonance cells: a Monte Carlo analysis, Physical Biology 13, 066010 – 1-12 (5 December 2016) [http://arxiv.org/abs/1606.08294].
- Ekaterina V. Katkova, Alexey V. Onufriev, Boris Aguilar, and Vladimir B. Sulimov, Accuracy comparison of several common implicit solvent models and their implementations in the context of protein-ligand binding,

  Journal of Molecular Graphics and Modelling 72, 70-80 (21 December 2016).

• Andrew Mellor, Mauro Mobilia, and R. K. P. Zia, Heterogeneous out-of-equilibrium nonlinear q-voter model with zealotry, The Physical Review E 95, 012104 – 1-15 (4 January 2017).

• Vinh X. Ho, T. V. Dao, Hongxing X. Jiang, Jingyu Y. Lin, John M. Zavada, Steve A. McGill, and Nguyen Q. Vinh,

Photoluminescence quantum efficiency of Er optical centers in GaN epilayers, Scientific Reports 7, 39997 (5 January 2017).

• Vinh X. Ho, Steve. P. Dail, T. V. Dao, Hongxing X. Jiang, Jingyu Y. Lin, John M. Zavada, and Nguyen Q. Vinh,

Temperature dependence studies of Er optical centers in GaN epilayers grown by MOCVD, MRS Advances: Electronics, Magnetics and Photonics 2, 135-140 (16 January 2017).

• Uwe C. Täuber,

Phase transitions and scaling in systems far from equilibrium, Annual Reviews of Condensed Matter Physics **8**, 14 – 1-26 (19 January 2017) [http://arxiv.org/abs/1604.04487].

• Tuo-Xian Tang, Ami Jo, Jingren Deng, Jeffrey F. Ellena, Iulia M. Lazar, Richey M. Davis, and Daniel G.S. Capelluto,

Structural, thermodynamic, and phosphatidylinositol 3-phosphate binding properties of Phafin2, Protein Science 23, 814-823 (13 February 2017).

• Xiaolin Zhao, Wen Xiong, S. Xiao, Tuo-Xian Tang, Jeffery F. Ellena, G. Armstrong, Carla V. Finkielstein and Daniel G.S. Capelluto,

Membrane targeting of TIRAP is negatively regulated by phosphorylation in its phosphoinositidebinding motif,

Scientific Reports 7, 43043 (22 February 2017).

 Emmanuel Virot, Grace Ma, Christophe Clanet, and Sunghwan Jung, *Physics of chewing in terrestrial mammals*, *Scientific Reports* 7, 43967 (7 March 2017).

• Xiangwen Wang and Michel Pleimling,

Foraging patterns in online searches,

Physical Review E 95, 032145 (29 March 2017) [http://arxiv.org/abs/1703.03901].

• Harmeet Singh and James. A. Hanna,

Pick-up and impact of flexible bodies,

Journal of the Mechanics and Physics of Solids 106, 46-59 (22 May 2017)

[http://arxiv.org/abs/1611.03332].

## 6. Submitted Papers with Center Affiliation

• Heather S. Deter, Roderick V. Jensen, William H. Mather, and Nicholas C. Butzin. *Mechanisms for differential protein production in toxin-antitoxin systems*, *Toxins* **2017**, 9 (4 July 2017).

- Barton L. Brown and Michel Pleimling, Coarsening with nontrivial in-domain dynamics: Correlations and interface fluctuations, Physical Review E **96**, 012147 (24 July 2017) [http://arxiv.org/abs/1707.03447].
- Shadisadat Esmaeili, Darka Labavić, Michel Pleimling, and Hildegard Meyer-Ortmanns, *Breaking of time-translation invariance in Kuramoto dynamics with multiple time scales*, *EPL (Europhysics Letters)* **118**, 40006 1-6 (27 July 2017).
- Shannon R. Serrao and Uwe C. Täuber, A stochastic analysis of the spatially extended May-Leonard model, to appear in: Journal of Physics A: Mathematical and Theoretical (2017) [http://arxiv.org/abs/1706.00309].
- Bassel Heiba, Sheng Chen, and Uwe C. Täuber, Boundary effects on population dynamics in stochastic lattice Lotka-Volterra models, submitted to: Physica A (2017) [http://arxiv.org/abs/1706.02567].
- Harmeet Singh and James A. Hanna, *On the planar elastica, stress, and material stress*, submitted to: *Proceedings of the Royal Society A* (2017) [http://arxiv.org/abs/1706.03047].
- Nicholas C. Butzin and William H. Mather Engineered orthogonal degradation pathways in Escherichia coli, to appear in: ACS Synthetic Biology (2016).
- Arin D. Nelson, Jeffrey B. Weiss, Baylor Fox-Kemper, Royce K.P. Zia, and Fabienne Gaillard, An ensemble observing system simulation experiment of global ocean heat content variability, submitted to: Ocean Science (2016).
- Jeffrey B. Weiss, Baylor Fox-Kemper, Dibyendu Mandal, Arin D. Nelson, and Royce K. P. Zia, *Nonequilibrium oscillations, probability angular momentum, and the climate system*, submitted to: *Dynamics and Statistics of the Climate System* (2016).
- Kevin E. Bassler and Royce K. P. Zia, Emergence of a spectral gap in a class of random matrices, submitted to: Journal of Physics A: Mathematical and Theoretical (2017).
- 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* (2017).
- Udaya Sree Datla, William H. Mather, Sheng Chen, Isaac W. Shoultz, Uwe C. Täuber, Caroline N. Jones, and Nicholas C. Butzin,

  The spatiotemporal network dynamics of acquired resistance in an engineered microecology, submitted to: Scientific Reports (2017).
- Aubrey M. Davis, Laura E. Hanzly, Barbara L. DeButts, and Justin R. Barone, Characterization of dimensional stability in flax fiber reinforced polypropylene composites, submitted to: Polymer Composites (2017).

- Barbara L. DeButts, Laura E. Hanzly, and Justin R. Barone, *Protein-rubber nanocomposites*, submitted to: *Journal of Applied Polymer Science* (2017).
- Barbara L. DeButts, Cara R. Spivey, and Justin R. Barone, Protein aggregates as the nanofiller in polymer nanocomposites, submitted to: Composites Part A (2017).
- Jeffrey F. Ellena, Wen Xiong, Xiaolin Zhao, Narasimhamurthy Shanaiah, and Daniel G.S. Capelluto, Backbone <sup>1</sup>H, <sup>15</sup>N, and <sup>13</sup>C resonance assignments of the Tom1 VHS domain, to appear in: Biomolecular NMR Assignments (2017).
- Laura E. Hanzly, Barbara L. DeButts, Danielle Shell, and Justin R. Barone, Early stage protein 'pompons' are realized in vitro in viscous polymer solutions submitted to: Biomacromolecules (2017).
- Vinh X. Ho, T. M. Al Tahtamouni, Hongxing X. Jiang, Jingyu Y. Lin, John M. Zavada, Tom Gregorkiewicz, and Nguyen Q. Vinh, *Room-temperature lasing action in GaN quantum wells in the infrared 1.5 µm region*, submitted to: *Physical Review Letters* (2017).
- Yanlong Li, Chuanhui Chena, John Burton, Kyungwha Park, Randy Heflin, and Chenggang Tao, Self-assembled PCBM bilayer on graphene and HOPG examined by AFM and STM, submitted to: Nanotechnology (2017).
- J. R. Mahan, N. Q. Vinh, N. B. Munir, and V. X. Ho, Monte Carlo ray-trace diffraction based on the Huygens-Fresnel principle, submitted to: Applied Optics (2017).
- Deepam Maurya, Ali Charkhesht, Sanjeev K. Nayak, Fu-Chang Sun, Deepu George, Abhijit Pramanick, Min-Gyu Kang, Hyun-Cheol Song, Marshall M. Alexander, Djamila Lou, Giti A. Khodaparast, S. Pamir Alpay, N. Q. Vinh, and Shashank Priya, Soft phonon mode dynamics in Aurivillius type structures, submitted to: Physical Review Letters (2017).
- Tuo-Xian Tang, Wen Xiong, Carla V. Finkielstein, and Daniel G. S. Capelluto, *Identification of ligand-binding modulators using the protein-lipid overlay assay*, to appear in: *Methods in Molecular Biology* (2017).
- Husong Zheng, Salvador Valtierra, Nana Ofori-Opoku, Chuanhui Chen, Lifei Sun, Liying Jiao, Kirk H. Bevan, and Chenggang Tao, Electrical stressing induced monolayer vacancy island Growth on TiSe<sub>2</sub>, submitted to: Physical Review Applied (2017).

#### 7. Invited Presentations with Center Affiliation

• Uwe C. Täuber, Sebastian Diehl, Weigang Liu, George L. Daquila, and Sheng Chen, *Aging scaling in driven systems*,

STATPHYS 26 Statistical Physics Conference Satellite "Non-Equilibrium Dynamics in Classical and Quantum Systems: From Quenches to Slow Relaxations", Pont-à-Mousson, France, 13 July 2016.

#### • Daniel Capelluto,

Intrinsic disorder in adaptor proteins increases commitment to endosomal trafficking, Leloir Institute Foundation, Buenos Aires, Argentina, 14 July 2016.

• Michel Pleimling, Hiba Assi, Harshwardhan N. Chaturvedi, Ulrich Dobramysl, and Uwe C. Täuber, *Relaxation processes in interacting vortex matter*,

STATPHYS 26 Statistical Physics Conference Satellite "Non-Equilibrium Dynamics in Classical and Quantum Systems: From Quenches to Slow Relaxations", Pont-à-Mousson, France, 15 July 2016.

#### • Alexey V. Onufriev,

Electrostatics of DNA and RNA: small differences and their large consequences, 2016 Protein Electrostatics Conference, Berlin, Germany, July 2016.

#### • Alexey V. Onufriev,

Choice of water model matters,

American Chemistry Society National Meeting, Philadelphia, PA, August 2016.

#### • Nguyen Q. Vinh,

*Probe conformational dynamics of proteins in aqueous solutions by terahertz spectroscopy,* 2016 SPIE Optics + Photonics, San Diego, CA, 29 August 2016.

#### • Uwe C. Täuber,

Non-equilibrium relaxation and aging scaling in driven systems, Condensed Matter Seminar, Michigan State University, East Lansing, MI, 17 October 2016.

#### • Justin R. Barone.

Self-assembly of amyloid fibers and their use in composites, Fiber Science Department, Cornell University, Ithaca, NY, 20 October 2016.

#### • Uwe C. Täuber,

The 2016 Nobel Prize in Physics: Topological phase transitions and topological phases of matter, Physics Colloquium, Virginia Tech, Blacksburg, VA, 21 October 2016.

#### • James Hanna

Pick-up and impact of flexible objects,

*GEM 2016: Geometry and Materials Science Workshop*, Okinawa Institute of Science and Technology, Onna, Japan, October 2016.

#### • Nguyen Q. Vinh and J. B. Mahan,

IR detectors: Technology development,

NASA Trutinor: Mission concept for earth & atmosphere energy system, NASA Langley, Hampton, VA, 2 November 2016.

#### • Nguyen Q. Vinh,

*Microscopic structure of Er-optical centers in GaN epilayers by high magnetic fields,* 83<sup>nd</sup> Annual SESAPS Meeting, Charlottesville, VA, 10 November 2016.

# • Hiba Assi, Bart Brown, Harshwardhan N. Chaturvedi, Ulrich Dobramysl, Michel Pleimling, and Uwe C. Täuber,

*Non-equilibrium relaxation of driven topological defects*, 83<sup>nd</sup> *Annual SESAPS Meeting*, Charlottesville, VA, 12 November 2016.

#### • Nguyen Q. Vinh,

Er doped GaN quantum well structures for photonic devices, 2016 MRS Fall Meeting, Boston, MA, 30 November 2016.

#### • Michel Pleimling

Virginia Tech's Academy of Integrated Science: Retooling science for the 21st century, College of Science Distinguished Speaker Series, Rochester Institute of Technology, Rochester, NY, 15 December 2016

#### • Uwe C. Täuber, Sebastian Diehl, Weigang Liu, and Sheng Chen,

Non-equilibrium relaxation and aging scaling in driven systems,

116th Statistical Mechanics Conference,

Rutgers University, New Brunswick, NJ, 18 December 2016.

#### • James Hanna.

(Some issues arising in) variational elasticity of thin plates,

Variational Models of Soft Matter Conference,

Pontifical Catholic University of Chile, Santiago, Chile, January 2017.

#### • Justin R. Barone.

Self-assembly of protein -sheets and their use in nanocomposites, Chemical and Life Sciences Engineering Department, Virginia Commonwealth University, Richmond, VA, 1 February 2017.

#### • Justin R. Barone,

High performance natural polymer materials,

*Macromolecular Science and Engineering Department*, Case Western Reserve University, Cleveland, OH, 16 February 2017.

#### Sunghwan Jung,

Drinking and diving,

Fluid Seminar, Brown University, Providence, RI, 1 March 2017.

#### • Justin R. Barone,

High performance natural polymer materials, Plastics Engineering Department, University of Massachusetts-Lowell, Lowell, MA, 6 March 2017.

#### • Justin R. Barone,

High performance natural polymer materials, School of Chemistry and Biochemistry, Georgia Tech, Atlanta, GA, 13 March 2017.

#### • James Hanna,

Surprises and open questions in mechanics of moving contacts, James Madison University, Harrisonburg, VA, March 2017.

#### • Justin R. Barone,

Amyloid reinforced rubber nanocomposites, 253<sup>rd</sup> National Meeting of the American Chemical Society, San Francisco, CA, 3 April 2017.

#### • Justin R. Barone,

*Amyloid reinforced polyvinyl alcohol nanocomposites,* 253<sup>rd</sup> *National Meeting of the American Chemical Society*, San Francisco, CA, 3 April 2017.

#### • Daniel Capelluto,

Mechanisms of modulation of adaptor protein binding to membrane phosphoinositides, Department of Chemistry & Biochemistry, University of Maryland, College Park, MD, 4 April 2017.

• Uwe C. Täuber, Sebastian Diehl, Weigang Liu, George L. Daquila, and Sheng Chen, Non-equilibrium relaxation and aging scaling in driven systems, Workshop "Nonequilibrium Dynamics: Diffusion, Populations and Aging", TIFR Centre for Interdisciplinary Sciences (TCIS), Hyderabad, India, 30 June 2017.

#### 8. Awards and Recognitions

### Faculty:

- Daniel Capelluto, Department of Biological Sciences,
   M. L. Andrews Cancer Research Award, Virginia Academy of Science,
   July 1, 2016 June 30, 2017, \$ 3000.
- Michel Pleimling, Department of Physics and Academy of Integrated Science, 2017 Dr. Carroll B. Shannon Excellence in Teaching Award of College of Science

#### Graduate students:

- Bart L. Brown,
   2017 William E. Hassinger Graduate Fellowship, Department of Physics
- Jacob A. Carroll,
   2017 Lubna R. Ijaz Scholarship, Department of Physics
   Best Oral Presentation Award, Second Molecular Biophysics Symposium, Virginia Tech (2017).

- Ali Charkhesht,
   2017 Graduate James A. Jacobs Memorial Scholarship, Department of Physics
- Chuanhui Chen, 2017 Physics Department Graduate Teaching Assistant Excellence Award
- Sheng Chen, 2017 Ray F. Tipsword Graduate Scholarship, Department of Physics
- Shadi Esmaeili, 2017 Ray F. Tipsword Graduate Scholarship, Department of Physics
- Shannon R. Serrao, 2017 Graduate Wan-Zia Scholarship, Department of Physics
- Tuo-Xian Tang, 2017 Robert and Marion Patterson Scholarship Award, Department of Biological Sciences 2017 Graduate School of Virginia Tech Fellowship
- Wen Xiong,
   Best Oral Presentation, Virginia Academy of Science (2016)
   2017 Noel Krieg Graduate Fellowship, Department of Biological Sciences
   Best Oral Presentation Award, Second Molecular Biophysics Symposium, Virginia Tech (2017)

#### Undergraduate students:

- Nathan W. Galliher, 2017 College of Arts and Sciences Astronaut Scholarship
- Isaac W. Shoultz, 2017 Webster & Sara Schoene Richardson Memorial Scholarship, Department of Physics
- James Stidham III, 2017 H.Y. Loh Award, Department of Physics
- Austin "Ada" Warren,
   2017 Hugh D. Ussery Scholarship, Department of Physics

#### 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. Five student travel grants may be issued for each spring and fall semester per year, totaling up to \$ 4,000. The spring 2017 recipients were:

#### • Wen Xiong,

*Molecular basis of the endosomal adaptor protein Tom1 function*, Biophysical Society 61<sup>st</sup> Annual Meeting, New Orleans, LA, February 2017.

#### Jacob Carroll,

Ligand-receptor binding kinetics in surface plasmon resonance cells: a Monte Carlo analysis, 2017 American Physical Society March Meeting, New Orleans, LA, March 2017.

#### Shadi Esmaeili,

Response to an external field of a system of coupled Kuramoto oscillators, 2017 American Physical Society March Meeting, New Orleans, LA, March 2017.

#### • Shannon Serrao,

A field-theoretic approach to the May-Leonard cyclic population dynamics model, 2017 American Physical Society March Meeting, New Orleans, LA, March 2017.

#### • Yow-Ren Chang,

Effect of surface topography on bacterial surface motility, 254<sup>th</sup> American Chemical Society National Meeting, Washington, DC, August 2017.

#### 10. Student New Collaboration Incentive Awards

In January 2017, the Center established a grant for graduate students supporting new research collaborations related to the Center's mission, aiding planned or ongoing research involving students from different research groups. The students are to submit a brief application with a description of their planned research. If accepted they can be awarded up to \$400, possibly later supplemented with a student travel grant. Two grants may be issued in each spring and fall semester per year, totaling up to \$800.00. The spring 2017 recipients were:

- Wen Xiong (Biological Sciences) and Chuanhui Chen (Physics), Molecular basis of the endosomal adaptor protein Tom1 function.
- Sheng Chen (Physics) and Udaya Sree Datla (Biological Sciences),

  The spatiotemporal network dynamics of acquired resistance in engineered microecological systems.

#### VIII. Industrial Affiliates Program

Not applicable

# IX. Report of Financial Condition

		IX. Report of Fi	nancial Condition			
Center Financial Report Fiscal Year 2017			Center Financial Projection Fiscal Year 2018			
Operations Account (176188)			Operations Account (	176188)		
Starting Balance		\$ 38,904.91	Starting Balance		\$	849.28
In	come			Income		
Starts FY2017		\$ (38,055.63)	A21 Award		\$	28,702
Exp	enses			Expenses		
			80% Staff Salary (Katr	ina Loan)	\$	(28,702)
Ending Balance		\$ 849.28	Ending Balance		\$	849.28
Overhead Account (235052)			Overhead Account (235052)			
Starting Balance		\$ 9,374.68	Starting Balance		\$	27,744.95
	come			Income		
Overhead Earnings		\$ 34,742.34	Overhead Earnings		\$	20,000
Symposium Support		\$ 1,030.00				
Fue				Francisco		
Salary	enses	\$ (4,228.29)	Seminar	Expenses	\$	(6,000)
Seminar Travel		\$ (4,228.29)	Symposium		\$	(4,000)
Student Travel		\$ (4,976.63)	Sowers Symposium Speaker		\$	(2,000)
Center Symposium Travel		\$ (1,990.97)	Sowers Symposium S	peaker	Ş	(2,000)
Biophysics Symposium Suppo	art .	\$ (600.00)				
Supplies & Budget	,,,,	\$ (383.00)				
Center Symposium Supplies		\$ (446.44)				
Center Collabration Awards		\$ (800.00)				
Center Symposium Awards		\$ (210.00)				
Other Charges		\$ (2,162.72)				
outer drianges		7 (2,102.72)	20% Staff Salary (Katrina Loan)		\$	(7,176)
Ending Balance		\$ 27,744.95	Ending Balance		ċ	28,569.35

#### X. Major Issues of the Center

Owing to continuing as well as substantial new external grants, the Center's financial standing looks very solid. We especially appreciate Dr. Seong-Ki Mun's transfer of considerable overhead return funds to us.

I believe it is fair to say that the Center has reached all its initial goals during its first year of existence.

We appreciate the opportunity to hire Dr. Rana Ashkar (Oak Ridge National Lab, TN) as a new tenure-track assistant professor in the Department of Physics. Yet owing to Prof. Will Mather's resignation from Virginia Tech in May 2017, we will certainly require additional senior personnel hires in the near future.

The Center will maintain its successful seminar series and regular discussion meetings. We plan to continue to organize annual symposia with external speakers, and to support other related conferences.

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

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