CURRICULUM VITAE

MEENAKSHI DUTT

Department of Chemical and Biochemical Engineering
Rutgers University, 98 Brett Road, Engineering Building, Room C-229, Piscataway, NJ 08854
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Email: meenakshi.dutt@rutgers.edu **Group Website:** http://dutt-lab.rutgers.edu/

EDUCATION
Ph.D. 2002   Physics, Duke University, USA
M.A. 1999   Physics, Duke University, USA
M.Sc. 1996   Physics, Indian Institute of Technology, India
B.Sc. 1994   Physics, Delhi University, India

PROFESSIONAL EXPERIENCE
2017-   Associate Professor, Department of Chemical and Biochemical Engineering, Rutgers, The State University of New Jersey, Piscataway, USA.
2011-17   Assistant Professor, Department of Chemical and Biochemical Engineering, Rutgers, The State University of New Jersey, Piscataway, USA.
2009-11   Postdoctoral Research Associate, Department of Chemical and Petroleum Engineering, University of Pittsburgh, USA (Adviser: *Prof. Anna C. Balazs*)
2007-09   Postdoctoral Research Associate, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, USA (Adviser: *Prof. Erik Luijten*)
2002-07   Postdoctoral Research Associate, Materials Science and Engineering, University of Cambridge, UK (Adviser: *Prof. James A. Elliott*)
1998-02   Research Assistant, Duke University, USA. (PhD Adviser: *Prof. Robert P. Behringer*)

ADJUNCT APPOINTMENTS
2023-   Editorial Board member, Frontiers in Soft Matter
2022-   Co-Director of REU site: Advanced Materials at Rutgers Engineering
2021-23   Busch Advisory Committee Member, Rutgers, The State University of New Jersey, Piscataway, USA.
2016-   Editorial Board member, Materials Research Society Advances
2005-07   Undergraduate College Supervisor, Fitzwilliam College, University of Cambridge, UK.
2004-07   M. Phil Supervisor, Department of Materials Science and Metallurgy, University of Cambridge, UK.
1996-98   Teaching Assistant, Duke University, USA.

HONORS & AWARDS
2017   NSF CAREER Award
2015   ACS COMP OpenEye Outstanding Junior Faculty Award

PEER-REVIEWED RESEARCH PUBLICATIONS
(supervised [a]Doctoral, [b]Masters (with thesis), [c]undergraduate students, [d] joint co-corresponding authors, **publicity or by invitation)

(A) 2012 - PRESENT

1. S. Mushnoori,[a] E. Zang,[c] A. Banerjee,[a] M. Hooten,[a] A. Merzky, M. Turilli, S. Jha and **M. Dutt**, Pipeline for Automating Compliance-based Elimination and Extension (PACE[2]): A Systematic Framework for High-throughput Biomolecular Simulation Workflows, Journal of Physics: Materials (2023), DOI: 10.1088/2515-7639/ad08d0.
2. M. Hooten,[a] A. Banerjee[a] and **M. Dutt**, Multiscale, Multiresolution Coarse-grained Model via a Hybrid Approach: Solvation, Structure and Self-assembly of Aromatic Tripeptides, Journal of Chemical Theory and Computation (2023), DOI: 10.1021/acs.jctc.3c00458.

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3. S. Mushnoori,[a] C. Y. Lu,[b] K. Schmidt[b] and **M. Dutt**, A Coarse-grained Molecular Dynamics Study of Phase Behavior in Co-assembled Lipomimetic Oligopeptides, Journal of Molecular Graphics and Modeling, Journal of Molecular Graphics and Modelling (2023), DOI: 10.1016/jmgm.2023.108624.

4. A. Banerjee[a] and **M. Dutt**, A Hybrid Approach for Coarse-graining Helical Peptoids: Solvation, Secondary Structure and Assembly, Journal of Chemical Physics (2023), DOI: 10.1063/5.0138510.

5. A. Banerjee[a] and **M. Dutt**, Impact of pH on the Formation and Stability of Dendronized Vesicles, Langmuir (2023), DOI: 10.1021/acs.langmuir.2c03386.

6. J. A. Logan, S. Mushnoori,[a] **M. Dutt** and A. V. Tkachenko, Symmetry-specific orientational order parameters for complex structures, Journal of Chemical Physics (2022), DOI: 10.1063/5.0076915.

7. **S. Mushnoori,[a] J. A. Logan, A. V. Tkachenko[d] and **M. Dutt**,[d] Controlling morphology in hybrid isotropic/patchy particle assemblies, Journal of Chemical Physics (2021), DOI: 10.1063/5.0076914. (*Editor's Pick*).

8. A. Banerjee,[a] C. Y. Lu[b] and **M. Dutt**, A Hybrid Coarse-Graining Model for Structure, Solvation and Assembly of Lipid-like Peptides, Physical Chemistry Chemical Physics (2021), DOI: 10.1039/D1CP04205J.

9. A. Banerjee,[a] A. Tam[c] and **M. Dutt**, Dendronized Vesicles: Formation, Self-organization of dendron-grafted Amphiphiles and Stability, Nanoscale Advances (2021), 3, 725 – 737. DOI: 10.1039/D0NA00773K.

10. ** S. Mushnoori, K. Schmidt, C.Y. Lu, E. Zang and **M. Dutt**, Peptide-based Vesicles and Droplets: A Review, Journal of Physics Condensed Matter (2020), 33, 053002.

11. A. Banerjee,[a] Z. Finkel[c] and **M. Dutt**, Self-Organization of Alpha Helical Proteins in Bioinspired Membranes and Vesicles, ChemRxiv (2020), DOI: 10.26434/chemrxiv.12746609.v1.

12. X. Yu[a] and **M. Dutt**, Implementation of Dynamic Coupling in Hybrid Molecular Dynamics-Lattice Boltzmann Approach: Modeling Aggregation of Amphiphiles, Computer Physics Communications (2020). DOI:10.1016/j.cpc.2020.107287.

13. S. Mushnoori,[a] L. Chong[a] and **M. Dutt**, Organization and Dynamics of Water on Titania Surfaces, MRS Advances (2019). DOI10.1557/adv.2019.384.

14. ** F. Aydin,[a] X. Chu[b] and **M. Dutt**, Computational Methods to Study Nanocomposites and Nanosuspensions for Heat Transfer Applications, Thermal Behavior and Applications in Carbon-based Materials, Elsevier, Eds. D. Papavassiliou, H. Duong and F. Gong (2019). (*Book Chapter, ISBN: 9780128176825)*

15. ** T.A. Deaton, F. Aydin,[a] N. Li, X. Chu,[b] **M. Dutt** and Y. Yingling, Dissipative Particle Dynamics Approaches to Modeling the Self-Assembly and Morphology of Neutral and Ionic Block Copolymers in Solution, Molecular Modeling and Simulation, Applications and Perspectives, Springer, Ed. E. Maginn (2019). (*Book Chapter, ISSN: 2364-5083*)

16. Z. Yang, **M. Dutt** and Y. Chiew, Structure and Phase Transitions of Two-Dimensional Core-Softened Colloidal Dumbbells: A Molecular Dynamics Study, Materials Research Express (2019), 6, 075076.

17. X. Yu[a] and **M. Dutt**, Harnessing the Hybrid Molecular Dynamics-Lattice Boltzmann Method to Study Molecular Characteristics of Biologically Inspired Vesicles, Molecular Systems Design & Engineering (2018), DOI: 10.1039/C8ME00029H. *(Featured as artwork for front cover of journal issue)*

18. J. Li,[b] K. Jin,[c] S. Mushnoori[a] and **M. Dutt**, Designing Antifouling Substrates: Interactions Between DPPC Membranes and PAMAM Dendron-grafted Surfaces, RSC Advances (2018), 8, 24982 – 24992.

19. F. Aydin,[a] X. Chu,[b] J. Greenstein[c] and **M. Dutt**, A Review on Phospholipid Vesicles Flowing Through Channels, MRS Communications (2018), DOI: 10.1557/mrc.2018.118. *(Invited Review)*

20. S. Mushnoori,[a] Kassandra Schmidt,[b] Vikas Nanda and **M. Dutt**, Designing Phenylalanine-based Hybrid Biological Materials: Controlling Morphology via Molecular Composition, Organic and Biomolecular Chemistry (2018), 16, 2499.

21. A. Moretti, B. Zhang,[b] B. Lee, **M. Dutt** and K.E. Uhrich, Degree of unsaturation and backbone orientation of amphiphilic macromolecules influence local lipid properties in large unimalellar vesicles, Langmuir (2017), 33 (51), 14663 - 14673.

22. X. Chu,[b] X. Yu,[a] J. Greenstein,[c] F. Aydin,[a] G. Uppaladadium[b] and **M. Dutt**, Flow-induced Shape Reconfiguration, Phase Separation and Rupture of Bio-inspired Vesicles, ACS Nano (2017), 11 (7), 6661 – 6671.

23. **M. Dutt**, L. Chong,[a] V. Karra[b] and S. Libring,[c] Self-Assembly of Virus Capsids Decorated with Block Copolymers: A Simulation Study, Journal of Materials Research 2017, DOI: 10.1557/jmr.2016.427.

24. X. Chu,[b] F. Aydin[a] and **M. Dutt**, Modeling Interactions between Multicomponent Vesicles and Anti-Microbial Peptide Mimetic Nanoparticles, ACS Nano 2016, DOI: 10.1021/acsnano.5b08133.

25. F. Aydin[a] and **M. Dutt**, Surface Reconfiguration of Binary Lipid Vesicles Via Electrostatically-induced Nanoparticle Adsorption, Journal of Physical Chemistry B 2016, DOI: 10.1021/acs.jpcb.6b02334.

26. F. Aydin,[a] X. Chu,[b] G. Uppaladadium,[b] D. Devore, R. Goyal, S. Murthy, Z. Zhang, J. Kohn and **M. Dutt**, Self-Assembly and Critical Aggregation Concentration Measurements of ABA Triblock Copolymers with Varying B Block Types: Model Development, Prediction and Validation, Journal of Physical Chemistry B 2016, DOI: 10.1021/acs.jpcb.5b12594.

27. F. Aydin,[a] G. Uppaladadium[b] and **M. Dutt**, Harnessing Steric Hindrance to Control Interfacial Adsorption of Patchy Nanoparticles onto Hairy Vesicles, Biointerfaces 2016. DOI: 10.1016/j.colsurfb.2016.01.061. (*Featured as artwork for front cover of journal issue*).

28. L. Chong,[a] F. Aydin[a] and **M. Dutt**, Implicit Solvent Coarse-Grained Model of Polyamidoamine Dendrimers: Role of Generation and pH, J. Comp. Chem. 2015, DOI: 10.1002/jcc.24277.

29. M. Sebastiano,[c] X. Chu,[b] F. Aydin,[a] L. Chong[a] and **M. Dutt**, Interactions of Bio-inspired Membranes with Peptides and Peptide-mimetic Nanoparticles, AIMS Materials Science (2015). DOI: 10.3934/matersci.2015.3.303.

30. S. Mushnoori,[b] L. Chong[a] and **M. Dutt**, Molecular Dynamics of Study Water over Pt/TiO$_2$ Surfaces, Materials Today: Proceedings, 2016, 3, 513 – 517.

31. F. Aydin,[a] G, Uppaladadium[b] and **M. Dutt**, Harnessing Nanoscale Confinement to Design Sterically Stable Vesicles of Specific Shapes via Self-Assembly, J. Phys. Chem. B 2015 DOI: 10.1021/acs.jpcb.5b02239.

32. L. Chong[a] and **M. Dutt**, Design of PAMAM-COO Dendron-Grafted Surfaces to Promote Pb(II) Ion Adsorption, Physical Chemistry Chemical Physics 2015, DOI: 10.1039/C5CP00309A.

33. F. Aydin,[a] G. Uppaladadium[b] and **M. Dutt**, The Design of Shape-Tunable Hairy Vesicles, Colloids and Surfaces B: Biointerfaces 2015, DOI: 10.1016/j.colsurfb.2015.01.049.

34. V. C. Muthukumar,[b] L. Chong[a] and **M. Dutt**, Designing Soft Nanomaterials via the Self- Assembly of Functionalized Icosahedral Viral Capsid Nanoparticles, J. Materials Research 2015, 30, 141 – 150.

35. L. Chong[a] and **M. Dutt**, Computer Simulations of Fluid Flow over Catalytic Surfaces for Water Splitting, Applied Surface Science 2014. DOI: 10.1016/j.apsusc.2014.08.172.

36. F. Aydin[a] and **M. Dutt**, Bioinspired Vesicles Encompassing Two-Tail Phospholipids: Self-Assembly and Phase Segregation via Implicit Solvent Coarse-Grained Molecular Dynamics, J. Phys. Chem. B, 2014, 118, 8614–8623.

37. F. Aydin,[a] P. Ludford[c] and **M. Dutt**, Phase Segregation in Bio-Inspired Multi-Component Vesicles Encompassing Double Tail Phospholipid Species, Soft Matter, 2014, 10, 6096-6108.

38. E. Koufos,[c] B. Muralidharan[b] and **M. Dutt**, Computational Design of Multi-Component Bio-inspired Bilayer Membranes, AIMS Material Science, 2014, 1, 103 – 120.

39. **M. Dutt** and J.A. Elliott, Granular Dynamics Simulations of the Effect of Grain Size Dispersity on Uniaxially Compacted Powder Blends, Granular Matter, DOI: 10.1007/s10035-013-0463-3.

40. **M. Dutt**, O. Kuksenok and A.C. Balazs, Nano-pipette directed transport of nanotube transmembrane channels and hybrid vesicles, Nanoscale 2013, 5(20), 9773. DOI: 10.1039/C3NR33991B.

41. Evan Koufos[c] and **M. Dutt**, Design of Nanostructured Hybrid Inorganic-biological Materials via Self-assembly, *Materials Research Society (MRS) Spring 2013 Conference Proceedings*.

42. P. Ludford,[c] F. Aydin[a] and **M. Dutt,** Design and Characterization of Nanostructured Biomaterials via the Self-assembly of Lipids. *MRS Fall 2012 Conference Proceedings*.

43. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs, Designing Tunable Bio-nanostructured Materials via Self-assembly of Amphiphilic Lipids and Functionalized Nanotubes. *MRS Spring 2012 Conference Proceedings*.

(B) Before 2012

44. **M. Dutt**, M.J. Nayhouse, O. Kuksenok, S.R. Little and A.C. Balazs, Interactions of End-functionalized Nanotubes with Lipid Vesicles: Spontaneous Insertion and Nanotube Self-Organization. Current Nanoscience, 2011, 7, 699-715.

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45. **M. Dutt**, O. Kuksenok, M.J. Nayhouse, S.R. Little and A.C. Balazs, Modeling of the Self-Assembly of Lipids and Nanotubes in Solution: Forming Vesicles and Bicelles with Transmembrane Nanotube Channels. ACS Nano, 2011, 5, p.4769-4782.

46. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs, Forming Transmembrane Channels using End-Functionalized Nanotubes. Nanoscale, 2011, 3, 240-250.

47. R.P. Behringer and **M. Dutt**, A Particle-Substrate Numerical Model for a quasi-2D Driven Dissipative Granular Gas, Powders and Grains 2009: Proceedings of the 6th International Conference on Micromechanics of Granular Media, 1145, 1112 (2009).

48. **M. Dutt** and J. Elliott, The Effect of Particle Size Dispersity in Dense Granular Packings on the Void Structure and the Interparticle Contact Frictional State, Powders and Grains 2009: Proceedings of the 6th International Conference on Micromechanics of Granular Media, 1145, 803 (2009).

49. **M. Dutt** and J. Elliott, Numerical Model for Ultra-fine Particles in the Absence and Presence of Gravity, Powders and Grains 2009: Proceedings of the 6th International Conference on Micromechanics of Granular Media, 1145, 101 (2009).

50. M. Benedict, **M. Dutt** and J.A. Elliott, Dynamically Tesselating Algorithm for Analysis of Pore Size Distribution in Particle Agglomerates. Physica A, 2007, 378, 465-474.

51. **M. Dutt** and R.P. Behringer, Effect of Surface Friction on a Two-Dimensional Granular System: Numerical Model for a Granular Collider Experiment. Phys. Rev. E, 2007, 75, 021305.

52. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott, Granular templating: effects of boundary structure on particle packings generated by simultaneous shear and compression, Europhysics Letters 77, 18001 (2007).

53. **M. Dutt** and J.A. Elliott, Microstructural Studies of Dense Granular Media and Their Importance to the Pharmaceutical Industry, International Congress of Industrial and Applied Mathematics 2007, Proceedings in Applied Mathematics and Mechanics.

54. J.A. Elliott, M. Benedict and **M. Dutt**, Applications of DL_POLY to Modeling of Mesoscopic Particulate Systems. Molecular Simulations, 2006, 32, 1113-1121.

55. X.W. Fu, **M. Dutt**, A.C. Bentham, B.C. Hancock, R.E. Cameron and J.A. Elliott, Investigation of Particle Packing in Model Pharmaceutical Powders Using X-ray Microtomography and Discrete Element Method. Pow. Tech., 2006, 167, 134-140.

56. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott, An Implementation of Granular Dynamics for Simulating Frictional Elastic Particles Based on the DL_POLY Code. Computer Physics Communications, 2005, 166, 26-44.

57. X.W. Fu, G.E. Milroy, **M. Dutt**, A.C. Bentham, B.C. Hancock and J.A. Elliott, Quantitative analysis of packed and compacted granular system by X-ray microtomography, Medical Imaging 2005: Image Processing, Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE) 5747 Pt. 1-3, 1955-1964 (2005).

58. R.P. Behringer and **M. Dutt**, The Granular Collider: Particle-Substrate Model and the Numerical Experiment, Powders and Grains 2005, ed. R. Garcia-Rojo, H.J. Herrmann and S. McNamara, Balkema, Rotterdam, 2005.

59. C. Bentham, **M. Dutt**, B. Hancock and J. Elliott, Effects of Size Polydispersity on Pharmaceutical Particle Packings, Powders and Grains 2005, ed. R. Garcia-Rojo, H.J. Herrmann and S. McNamara, Balkema, Rotterdam, 2005.

60. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott, Studies of Particle Packings in Mixtures of Pharmaceutical Excipients, Powders and Grains 2005, ed. R. Garcia-Rojo, H.J. Herrmann and S. McNamara, Balkema, Rotterdam, 2005.

61. B. Hancock, **M. Dutt**, C. Bentham and J. Elliott, Ordered Packing Induced by Simultaneous Shear and Compaction, Powders and Grains 2005, ed. R. Garcia-Rojo, H.J. Herrmann and S. McNamara, Balkema, Rotterdam, 2005.

62. M. Benedict, **M. Dutt** and J. Elliott, Porosity Determination in Mesoscale Simulations using Artificial Intelligence Technique, Proceedings of the Intelligent Processing and Manufacturing of Materials 2005.

63. **M. Dutt** and R.P. Behringer, Effects of Surface Friction on a Two Dimensional Granular System: Cooling Bound System, Phys. Rev. E 70, 061304 (2004).

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64. Benjamin Painter, **M. Dutt** and R.P. Behringer, Energy Dissipation and Clustering for a Cooling Granular Material on a Substrate, Physica D 175, 43 (2003).

OTHER PEER-REVIEWED RESEARCH PUBLICATIONS (UNDER PREPARATION, SUBMITTED, OR UNDER REVISION)
([a] supervised Doctoral students, [b] supervised Masters (with thesis) students, [c] supervised undergraduate students, [d] joint co-corresponding authors, ** publicity or by invitation)

1. ** A. Banerjee,[a] M. Hooten,[a] Nour Srouji, Rebecca Welch,[c] Joseph Shovlin[b] and **M. Dutt**, A Perspective on Coarse-graining Methodologies for Biomolecules: Resolving Self-assembly over Extended Spatiotemporal Scales, submitted.
2. M. Hooten,[a] S. Murthy and **M. Dutt**, Framework for Martini-based Coarse-grained Models of Enzymes, in preparation.
3. S. Mushnoori,[a] V. Balasubraminian, A. Merzky, M. Turilli, S. Jha and **M. Dutt**, RepEx: A Scalable, Flexible and User-extensible Replica Exchange Framework, in preparation.
4. S. Mushnoori,[a] M. Hooten,[a] V. Balasubraminian, A. Merzky, M. Turilli, S. Jha and **M. Dutt**, Biomolecular Assembly Enabled by RepEx, in preparation.

RESEARCH SOFTWARE FOR SCIENTIFIC COMMUNITY
These are research software products which my research program releases to our scientific community for their adoption and use. These software releases happen after we complete our commitments towards our publicly-funded research projects and publications.

1. Multiscale, Multiresolution Coarse-grained Models for Aromatic Peptides: (https://github.com/duttm/Hybrid_Bottom-Up_Coarse-Grained_Model_for_Aromatic_Peptides)
2. Multiscale, Multiresolution Coarse-grained Models for Peptoids (https://github.com/duttm/Multiscale-Multiresolution-CG-Models-for-Peptoids)
3. Toolkit for Automated Construction and Analysis of Dendronized Vesicles (https://github.com/duttm/Toolkit-for-automated-construction-and-analysis-of-dendronized-vesicles)
4. Materials Design Framework: Pipeline for Automating Compliance-based Elimination and Extension (PACE^2) (https://github.com/duttm/PACE2)
5. Isotropic particle and patchy particle mixtures (https://github.com/duttm/Octahedra_Nanoparticle_Project)
6. Multiresolution Coarse-Grained Model of Lipid-like Peptide Sequence (https://github.com/duttm/Hybrid_CG_Models_Peptides)
7. Membrane-Protein Biophysics (https://github.com/duttm/Protein_Membrane_System/)
8. Molecular Dynamics-Lattice Boltzmann Method: a hybrid particle dynamics and discreet fluid technique which captures the dynamic coupling between the fluid lattice and the particle dynamics. (http://dx.doi.org/10.17632/wr4mgv35j5.1)
9. RepEx: a replica exchange framework designed for extensibility to new kinds of exchange methods and performance at scale (https://github.com/SrinivasMushnoori/repex)
10. Amphiphilic Macromolecules in DSPC membranes (https://github.com/duttm/AM_DSPC_membrane)

RESEARCH GRANTS

(A) EXTERNAL PEER-REVIEWED AWARDS
2022   National Science Foundation, REU site: Advanced Materials at Rutgers Engineering, Role: PI, (Award: $382,260, Period: April 2022 – March 2025)
2021   National Science Foundation, Collaborative Research: DMREF: Machine Learning and Robotics for the Data-Driven Design of Protein-polymer Hybrid Materials, Role: Co-PI (PI: Adam Gormley), (Award: $1,315,946, Period: October 2021 – September 2025)
2018   National Science Foundation, Multiscale Modeling of Soft Materials and Interfaces, Role: PI (co-PI: J. Ardie Butch Dillen), (Award: $15,000, Period: Sept 2018 – Feb 2019)

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2018   National Science Foundation, S2I2: Impl: The Molecular Sciences Software Institute, Role: Subcontractor, (Subcontract Award: $107,894, Period: Jan 2018 – Jun 2019)

2017   National Science Foundation, S2I2: Impl: The Molecular Sciences Software Institute, Role: Subcontractor, (Subcontract Award: $36,486, Period: Jul 2017 – Dec 2017)

2017   National Science Foundation, REU Site: Advanced Materials at Rutgers Engineering, Role: Senior Investigator (PI: Masanori Hara), (Award: $324,900, Period: 2017 – 2022)

2017   National Science Foundation, CAREER: Cyber-enabled Multiscale Methodology for Hybrid Soft Materials-based Nanoparticle Design, Role: Sole PI (Award: $445,401.00; Period: 2017 – 2024)

2016   National Science Foundation, EAGER: Multiscale Methodology for Capturing Aggregation Phenomena in Surfactant-based Systems, Role: Sole PI (Award: $100,000.00; Period: 2016 - 2019)

2015   National Science Foundation, PFI:AIR-RA: Commercializing Pharmaceutical Process Modeling for Continuous Manufacturing, Role: Senior Investigator (PI: Benjamin Glasser; Co-PIs: M. Ierapetritou, C. Wassgren, R. Mendez, R. Dave) (Award: $800,000.00; Period: 2015 - 2018)

2015   Army Research Office, Modeling and Theory-Driven Design of Soft Materials, Role: co-PI (PI: J. Ardie Butch Dillen) (Award: $4,675.00; Period: 2015 - 2016)

2015   Air Force Office of Scientific Research, Modeling and Theory-Driven Design of Soft Materials, Role: co-PI (PI: J. Ardie Butch Dillen) (Award: $4,675.00; Period: 2015 - 2016)

2015   National Science Foundation, CBET-1542276, Modeling and Theory-Driven Design of Soft Materials, Role: PI (co-PIs: J. Ardie Butch Dillen) (Award: $15,000.00; Period: 2015 - 2016)

2013   National Science Foundation, Modeling and Theory-Driven Design of Soft Materials, Role: PI (co-PIs: Yaroslava Yingling, J. Ardie Butch Dillen) (Award: $4000.00; Period: 2013 - 2014)

(B) INTERNAL PEER-REVIEWED AWARDS

2023   Chancellor-Provost Challenge, CASS: Cyberinfrastructure & AI for Science and Society, Role: Senior/ Key Personnel (co-Leaders: Shantenu Jha and Alyson Brooks; Senior/ Key Personnel: I.P. Androukalis, M. Buckley, E. Curchitser, T. Davidson, N. Fahrenfeld, K. Garimella, L. Goodlad, W. Kung, S. Khare, R. Kopp, B. Lintner, A.V. Morozov, K. Ognyanov, L. Ojha, A. Rennermalm, D. Shih, R.B. Sills, J. Vaidya, L. Wang, D. York) (Award: $400,000, Period: 07/01/2023 – 06/30/2024)

2020   Initiative for Materials Research Team Proposal Development Grant, Co-Stimulatory Lipid Vesicles as CAR T Cell Therapy Boosters, Role: co-PI (PI: Adam Gormley; co-PIs: Vikas Nanda, Sagar Khare, Enver Izgu, Robert Hayes, Shishir Chundawat, Benjamin Schuster) (Award: $50,000, Period: January 2020 - present)

2019   Office of the Vice Chancellor for Research and Innovation Team Proposal Development Grant, Synthetic Cells and Cell Components, Role: co-PI (PI: Adam Gormley; co-PIs: Vikas Nanda, Sagar Khare, Enver Izgu, Robert Hayes, Shishir Chundawat, Benjamin Schuster) (Award: $60,000, Period: October 2019 –September 2020)

<u>COMPUTING GRANTS</u>
These awards support the computing needs of my research program (for external funding applications and peer-reviewed publications), and enable the use of national supercomputing facilities supported by the National Science Foundation through the ACCESS project. NSF ACI computes each Computing Service Unit (SU) on ACCESS to have a monetary value of $0.05, and states that these are "peer-reviewed" and "competitive" awards like regular NSF grants.

(A) EXTERNAL PEER-REVIEWED AWARDS
** 1 SU = $0.05 (https://portal.xsede.org/group/xup/knowledge-base/-/kb/document/bapq)

2022   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using Multiscale Simulation Techniques and Advanced Cyberinfrastructure, Role: PI (Award: 4,567,000 SUs, Equivalent Dollar Amount: $181,985.37 **; Period: July 2022 – June 2024)

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2021   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 5,125,172 SUs, Equivalent
         Dollar Amount: $53,603.94 **; Period: July 2021 – Jun 2022)
2019   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 5,125,172 SUs, Equivalent
         Dollar Amount: $148,534.29 **; Period: July 2019 – Jun 2020)
2019   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 44,098 SUs, Equivalent
         Dollar Amount: $2204.90 **; Period: Jan 2019 – Jun 2019, Supplement)
2019   Brookhaven National Laboratory, Center for Functional Materials award 37989,
         Title: Modeling of Programmable Self-Assembly Based on DNA Cages,
         Role: PI (Award: 150,000 SUs, Equivalent Dollar Amount: $7500.00 **;
         Period: Jan 2019 – Dec 2020)
2017   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 1,036,231 SUs, Equivalent
         Dollar Amount: $51,811.55 **; Period: 2017)
2017   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 223,000 SUs, Equivalent
         Dollar Amount: $11,150.00 **; Period: 2017)
2016   XRAC award DMR140125 from XSEDE, Title: Bio-inspired Materials Design using
         Multi-scale Simulation Techniques, Role: PI (Award: 740,040.90 SUs, Equivalent
         Dollar Amount: $54,502.05 **; Period: 2016)
2015   XRAC award DMR140125 from XSEDE, Title: Designing Soft Materials via
         Mesoscopic Computational Techniques: Cell-Mimetic Systems and Functionalized
         Surfaces, Role: PI (Award: 645,000 SUs, Equivalent Dollar Amount: $32,250.00**; Period: 2015)
2014   DAC award DMR140088 from XSEDE, Title: Designing Soft Materials via
         Mesoscopic Computational Techniques: Cell-Surface Interactions and Functionalized Surfaces,
         Role: PI (Award: 50,000 SUs, Equivalent Dollar Amount: $2,500.00**;
         Period: 2014)
2014   DAC award DMR140099 from XSEDE, Title: Designing Soft Materials via
         Mesoscopic Computational Techniques: Cell-Surface Interactions and Functionalized Surfaces,
         Role: PI (Award: 25,800 SUs, Equivalent Dollar Amount: $1,290.00 **;
         Period: 2014)
2014   DAC award DMR140060 from XSEDE, Title: Designing Soft Materials via
         Mesoscopic Computational Techniques: Cell-Surface Interactions and Functionalized Surfaces,
         Role: PI (Award: 100,000 SUs, Equivalent Dollar Amount: $5,000.00 **;
         Period: 2014)
2013   Supplement to Development Application Committee (DAC) award
         DMR110109 from XSEDE, Title: Optimizing Nanoparticle Architecture for
         Controlled Organization in a Lipid Membrane, Role: PI, (Award: 33,000 SUs,
         Equivalent Dollar Amount: $1,650.00 **; Period: 2013)
2011   DAC award DMR110109 from XSEDE, Title: Optimizing Nanoparticle
         Architecture   for Controlled Organization in a Lipid Membrane, Role: PI
         (Award: 200,000 SUs, Equivalent Dollar Amount: $10,000.00 **; Period: 2011)
2010   DAC award DMR090112 from XSEDE, Title: Computational Investigations on
         Self-assembly and Function of Biomimetic Cellular Vesicles, Role: PI (Award:
         60,000 SUs, Equivalent Dollar Amount: $3,000.00 **; Period: 2010)
2009   NCSA DAC award DMR080070N from XSEDE, Title: Simulations of Biological
         Membranes, Role: PI (Award: 30,000 SUs, Equivalent Dollar Amount: $1,500.00 **;
         Period: 2009)
2008   DAC award DMR080075 from XSEDE, Role: PI (Award: 30,000 SUs, Equivalent
         Dollar Amount: $1,500.00 **; Period: 2008)

(B) INTERNAL PEER-REVIEWED AWARDS

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** 1 SU = $0.05 (https://portal.xsede.org/group/xup/knowledge-base/-/kb/document/bapq)

2017   RDI^2 IBM Blue Gene/P Level 2 Award, Multiscale Models for Peptide-based Materials, Role: PI (Award: 800,000 SUs, Equivalent Dollar Amount: $40,000.00 **; Period: January – June 2017)

2014   RDI^2 IBM Blue Gene/P Level 2 Award, Computational Investigations of Artificial Photosynthesis using Titania-based Substrates, Role: PI (co-PI: Srinivas Mushnoori and Leebyn Chong, Award: 1,000,000 SUs, Equivalent Dollar Amount: $50,000.00 **; Period: 2014)

2014   RDI^2 IBM Blue Gene/P Level 2 Award, Computational Design of Bio-Inspired Membranes and Vesicles using Coarse-Grained Models, Role: PI (co-PI: Michael Sebastiano, Xiaolei Chu and Fikret Aydin, Award: 900,000 SUs, Equivalent Dollar Amount: $45,000.00 **; Period: 2014)

2014   RDI^2 IBM Blue Gene/P Level 2 Award, Computational Design of Soft Materials-based Delivery Vehicles, Role: PI (co-PI: Geetartha Uppaladadium and Fikret Aydin, Award: 950,000 SUs, Equivalent Dollar Amount: $47,500.00 **; Period: 2014)

2014   RDI^2 IBM Blue Gene/P Level 2 Award, Designing Hybrid Bio-nanostructured Soft Materials via Self-Assembly, Role: PI, (co-PI: Denise Preddie and Fikret Aydin, Award: 500,000 SUs, Equivalent Dollar Amount: $25,000.00 **; Period: 2014)

2013   RDI^2 IBM Blue Gene/P Level 2 Award, Simulation of Flowing Reactants Over a Catalytic Surface, Role: PI (co-PI: Leebyn Chong, Award: 500,000 SUs, Equivalent Dollar Amount: $25,000.00 **; Period: 2013)

2013   RDI^2 IBM Blue Gene/P Level 2 Award, Role: PI (co-PI: Fikret Aydin, Award: 400,000 SUs, Equivalent Dollar Amount: $20,000.00 **; Period: 2013)

2013   RDI^2 IBM Blue Gene/P Level 2 Award, Self-Assembly of Functionalized Biocolloids, Role: PI (co-PI: C.M. Vidyalakshmi, Award: 722,400 SUs, Equivalent Dollar Amount: $36,120.00 **; Period: 2013)

2013   RDI^2 IBM Blue Gene/P Level 2 Award, A Computational Study of Mixed Amphiphilic Lipid Bilayers, Role: PI, (co-PI: Evan Koufos, Award: 75,000 SUs, Equivalent Dollar Amount: $3,750.00 **; Period: 2013)

SYNERGISTIC ACTIVITIES AND PROFESSIONAL SERVICE

1. *Service to University:* **(1)** Facilitator of CAREER workshop for Biological Sciences (organized by Office of Research) (2022). **(2)** Busch Advisory Committee Member (2021 – 2023). **(3)** Member of New Brunswick Faculty Council (2023 – present).

2. *Membership of University Committees:* **(1)** Academic Cluster Committees of the School of Graduate Studies (2019 – present). **(2)** Member of Faculty Search Committee for Department of Food Science (2023 - 2024). **(3)** Member of Faculty and Personnel Affairs Committee, NB Faculty Council (2023 – present).

3. *Service to School of Engineering:* **(1)** Reviewing applications for New Jersey Governors School of Science and Technology (2015 - 2018). **(2)** Panelist in NSF CAREER Workshop (2017). **(3)** Member of SOE Planning Committee (Spring 2018). **(3)** Judge for Annual Biotechnology Symposium at Rutgers University (2022-2023).

4. *Membership of Department Committees:* **(1)** Committee on Research Innovation (2015 – 2016). **(2)** Graduate Recruitment Committee (2011 – present). **(3)** Doctoral Qualifying Exam Committee (2012 – 2018). **(4)** Chair of Graduate Recruitment Committee (2017 – 2020). **(5)** Member of ABET Committee (2017 – 2018). (6) Computation and Data Science Group Discussion Leader for CBE mini-retreat (June 2023).

5. *Service to Department:* **(1)** Faculty Adviser (Juniors), (2014 – present). **(2)** Participated in the OXE Faculty/Student Research Event (2013, 2014, 2015). **(3)** Lecturing Engineering Exploration Class (October 2012). **(4)** Delivering Freshman Orientation Lecture for Department of Chemical and Biochemical Engineering, Rutgers, USA (March 2013, October 2013). **(5)** Department-level tour for recruitment of prospective Engineering Scholars (February 20, 2012). **(6)** Maintaining minutes of Departmental Faculty Meeting (2013 – 2016). **(7)** Co-PI on GAANN submission from Department of Chemical and Biochemical Engineering, Rutgers, USA (2012, 2015). **(8)** Contribution to the

department annual report (2011-2012, 2012 -2013). **(9)** Member of Working Group in Materials (2017). **(10)** Academic Integrity Facilitator (2022 – present).

6. ***Mentorship of Faculty:*** (1) Assistant Teaching Professor Jason Robbins (2023).

7. ***Mentorship of Undergraduate Students:*** **(1)** Slade Scholars (2012 – present). **(2)** Aresty Research Assistants (2014 – present). **(3)** Summer NSF REU student (2014 – 2019, 2021 - present). **(4)** Rutgers Engineering Honors Academy *Table Talk with Professors at Rutgers* (November 2023).

8. ***Outreach for High School Students:*** **(1)** Developing course for summer program for high school students at Rutgers (part of the New Jersey Governors School of Science and Technology) on "Understanding Nanoparticle-Cell Interactions to Improve Health Care Diagnostics" (July 2015). **(2)** Cavendish Educational Outreach *Physics at Work* (2005, 2006, 2007).

9. ***Reviewer for Scientific Journals:*** Computer Physics Communications, Powder Technology, Particuology, Trends in Biotechnology, Molecular Simulations, RSC Soft Matter, RSC Physical Chemistry and Chemical Physics, ACS Macro Letters, Molecular Physics, Macromolecular Theory and Simulation, European Polymer Journal, Cellulose, Journal of Membrane Biology, ACS Applied Materials and Interfaces, RSC Advances, ACS Journal of Physical Chemistry, ACS Biomaterials Science and Engineering, Materials Research Express, Journal of Colloids and Interfaces: Biointerfaces, Bioconjugate Chemistry, Journal of Molecular Modeling, Journal of Materials Science, Journal of American Chemical Society, Inorganic Chemistry, Journal of Polymer Science, Part B: Polymer Physics, ACS Nano, RSC Nanoscale, Current Nanoscience, Chemical Physics Letters, Polymer Chemistry, ACS Langmuir, Polymer, Journal of Materials Science, Applied Mathematics and Mechanics, Advanced Materials, Small, ACS Biomacromolecules, AIP Journal Chemical Physics, ACS Journal of Chemical Theory and Computation, Advanced Theory and Simulations, RSC Chemical Communications, ACS Omega, Chemical Physics Letters, Springer Nature Cellulose, PLOS One, Computer Physics Communications, ACS Macromolecules, Nature Chemistry.

10. ***Reviewer for Federal Funding Agencies:*** ***(Domestic)*** National Science Foundation, Air Force Office of Scientific Research, United States Department of Energy, ACS Petroleum Research Fund, American Association for the Advancement of Science; ***(International)*** Canada Foundation for Innovation (CFI), Dutch Research Council (NWO), French National Research Agency (ANR).

11. ***Organization of Symposia in Professional National Meetings:*** **(1)** MRS Symposium BM03: *"Multi-scale Modeling of Soft Materials and Interfaces"*, MRS Fall 2018 Meeting, Boston, MA, December 2018. **(2)** MRS Symposium WW: *"Modeling and Theory-Driven Design of Soft Materials"*, MRS Fall 2015 Meeting, Boston, MA, December 2015. **(3)** ACS symposium *"Theory and Modeling of Nanoparticle Interactions with Biomolecules and Polymers"* at 2015 ACS Fall National Meeting, Boston, MA, August 2015. **(4)** MRS Symposium A: *"Modeling and Theory-Driven Design of Soft Materials"*, MRS Fall 2013 Meeting, Boston, MA, December 2013.

12. ***Chairing/ Presiding Sessions in National Meetings:*** **(1)** Symposium BM03: *"Multiscale Modeling of Soft Materials and Interfaces"*, MRS Fall 2018, Boston, MA, December 2018. **(2)** Symposium WW: *"Modeling and Theory-Driven Design of Soft Materials"*, MRS Fall 2015 Meeting, Boston, MA, December 2015. **(3)** Session on *"Fundamentals of Interfacial Phenomena I"*, AIChe Annual Meeting 2015, Salt Lake City, Utah, November 2015. **(4)** *"Theory and Modeling of Nanoparticle Interactions with Biomolecules and Polymers"* at 2015 ACS Fall National Meeting, Boston, MA, August 2015. **(5)** *"Biomembranes"* at 2015 ACS Fall National Meeting, Boston, MA, August 2015. **(6)** Symposium on *"Fundamentals of Interfacial Phenomena I"*, AIChe Annual Meeting 2014, Atlanta, Georgia, November 2014. **(7)** Session on *"Biomolecules at Biomaterial Interfaces"*, AIChe Annual Meeting 2014, Atlanta, Georgia, November 2014. **(8)** Symposium on *"Hybrid Materials"*, ACS National meeting, San Francisco, August 2014. **(9)** Symposium A: *"Modeling and Theory-Driven Design of Soft Materials"*, MRS Fall 2013 Meeting, Boston, MA, December 2013.

13. ***Service to Community:*** **(1)** MRS Graduate Student Award Chair (Spring 2020). **(2)** MRS Graduate Student Award Judge (Fall 2019). **(3)** Reviewing Computers in Chemistry Division Student Awards applications (Spring/Fall 2016, Fall 2019, Fall 2023). **(4)** Reviewer for MRS Graduate Student Awards (Fall 2013/2015/2018). **(5)** Reviewer for MRS graduate student poster competition (Fall 2013/2015/2018).

14. ***Reviewer for Abstracts and Conference Proceedings:*** MRS Fall 2013/2015/2018, Nanotech (2011-14, 2016).

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15. ***Membership of Editorial Boards:*** Materials Research Society Advances (focus on *Computational Materials Science*) (2016 – present); Frontiers in Soft Matter (focus on *Self-assembly and self-organization*) (2023 – present).

COLLABORATORS AND CO-EDITORS
Rutgers: Prof. Adam Gormley, Department of Biomedical Engineering; Prof. Enver Izgu, Department of Chemistry and Chemical Biology; Prof. Shantenu Jha, Department of Electrical and Computer Engineering; Prof. Sagar Khare, Department of Chemistry and Chemical Biology; Prof. Sanjeeva Murthy, Department of Chemistry and Chemical Biology; Prof. Vikas Nanda, Robert Wood Johnson Medical School, Department of Biochemistry. ***External:*** Prof. Marilyn Minus, Department of Mechanical and Industrial Engineering, Northeastern University; Alexei Tkachenko, Center for Functional Nanomaterials, Brookhaven National Laboratory; Prof. Matthew Webb, Department of Chemical Engineering, Princeton University; Prof. Yaroslava Yingling, Department of Materials Science and Engineering, North Carolina State University; Prof. Kathryn E. Uhrich, Department of Chemistry, University of California- Riverside.

CURRENT GROUP MEMBERS
Graduate Students (Doctoral Degree)
- Mason Hooten (B.S., Lehigh University, 2020 – present)
- Rishabh Singh (2023 – present)

Graduate Students (Master of Science Degree with Thesis):
- Het Patel (2023 – present)
- Yiwei Shao (B.B., Rutgers University, 2023 – present)

Undergraduate Students:
- Jeeyoung Han (2022 – present)
- Nivedha Ganesan (2023 – present)

FORMER GROUP MEMBERS
Graduate Students (Doctoral Degree):
- Fikret Aydin (B.S., University of Koc, 2011 - 2015) (Ph.D. Rutgers, 2015), Staff Scientist, Lawrence Livermore National Laboratory. USA.
- Leebyn Chong (B.S., Columbia University, 2011 - 2015) (Ph.D. Rutgers, 2015), Research Scientist, Leidos, USA.
- Xiang Yu (B.S., Pennsylvania State University, 2014 - 2019) (Ph.D. Rutgers, 2019), Postdoctoral Research Associate, Westlake University, China.
- Srinivas Mushnoori (B.S., Birla Institute of Technology and Science, 2013 - 2020), Intel, USA.
- Akash Banerjee (B.S., BMS College of Engineering, 2016 - 2023), Amgen, USA.

Graduate Students (Masters of Science Degree with Thesis):
- C.M. Vidylakshmi (B. Tech. Sastra University) (M.S. Rutgers, 2014), Doctoral student, University of Southampton, UK.
- Bharatram Muralidharan (B.S. Manipal Institute of Technology) (M.S. Rutgers, 2013), Engineer, C & J Energy, Inc.
- Geetartha Uppaladadium (B. Tech, Chaitanya Bharathi Institute of Technology, 2013 - 2016) (M.S. Rutgers, 2016) Aurex Pharmaceuticals, Inc.
- Xiaolei Chu (B.S., Shangai Institute of Technology, 2013 - 2016) (M.S. Rutgers, 2016) Doctoral student, University of California, Davis.
- Qi Qiao (M.S. Rutgers, 2016; co-advised with Dr. Yee Chiew) Doctoral student, University of Oklahoma.
- Srinivas Mushnoori (B.S., Birla Institute of Technology and Science, 2013 - present) Doctoral student, Rutgers.
- Bin Zhang (B.S., Nanking University of Science and Technology)(M.S. Rutgers, 2017) Doctoral student, Lehigh University, Pennsylvania.

- Vyshnavi Karra (B.S. Rutgers, 2016)(M.S. Rutgers, 2017) Doctoral student, Northeastern University, Massachusetts.
- Jia Li (M.S., Florida Institute of Technology, 2014 - 2017), Qualcom.
- Kassandra Schmidt (B.S., Rose-Hulman Institute of Technology, 2016 – 2019), Larsen and Toubro.
- Chien Yu Lu (B.S., Chung Yung Christian University, 2018 – 2019)
- Joseph Shovlin (B.S., Rutgers University, 2020 - 2021)

Graduate Students (MS)
- Tulsi Char (B.S. D.J. Sanghvi College of Engineering, 2016 – 2018)
- Nour Srouji (B.S. Rutgers University, 2019 – 2021)

Undergraduate Students:
- Sonali Ahuja (2012)
- Diane Kao (2012 – 2013)
- Evan Koufos, Slade Scholar (2012 – 2013)
- Paul Ludford, Slade Scholar (2012 – 2013)
- Sang Yun Lee, Slade Scholar (2012 – 2013)
- Andrew Rullo (2013 – 2014)
- Yuan Zhuang (2013 – 2014, co-advised with Dr. Yee Chiew)
- Denise Preddie (2013 – 2015)
- Zeyu Yang (2014 – 2015, co-advised with Dr. Yee Chiew)
- Michael Sebastiano, Slade Scholar (2013 – 2015)
- Vyshnavi Karra, Slade Scholar (2013 - 2016)
- Joseph Greenstein (2014 – 2016)
- Sarah Libring, Slade Scholar (2014 – 2017)
- Kai Jin (2015 – 2017)
- Tianyou Mou (2016 – 2018)(co-advised with Professor Vikas Nanda, Robert Wood Johnson Medical School, Department of Biochemistry)
- Brian Ronan (2017 – 2018)
- Ahsan Shawl (2018 – 2019)
- Ethan Zang (2018 – 2021)
- Rebecca Welch (2020 – 2021)
- Jeeyoung Han, Slade Scholar (2022 – present)
- Nivedha Ganesan (2022 – present)
- Orlando Mulero, NSF-REU undergraduate research assistant (Summer 2014)
- Gabriel Rodriguez, NSF-REU undergraduate research assistant (Summer 2015)
- Yejoon Seo, NSF-REU undergraduate research assistant (Summer 2016)
- Emran Rashid, NSF-REU undergraduate research assistant (Summer 2017)
- Zachary Finkel, NSF-REU undergraduate research assistant (Summer 2018)
- Acacia Tam, NSF-REU undergraduate research assistant (Summer 2019)
- Isabel Powers, NSF-REU undergraduate research assistant (Summer 2021)
- Ebony Oenga, NSF-REU undergraduate research assistant (Summer 2022)
- Imani Birchett, NSF-REU undergraduate research assistant (Summer 2023)

ADVISORY ACTIVITY ON GRADUATE THESIS COMMITTEES
Member of PhD thesis committee
Sara Koynov (adviser: Fernando Muzzio), Marlena Brown (adviser: Paul Takhistov), Ming-Tsung Lee (adviser: Alexander V. Neimark), Maitraye Sen (adviser: Rohit Ramachandran), Anwesha Chaudhury (adviser: Rohit Ramachandran), Jinjun Zhuge (adviser: Marianthi Ierapetritou), Mahim Misra (Princeton University, advisers: Stanislav Shvartsman, Yannis Kevrekidis), Dana Barrasso (adviser: Rohit Ramachandran), Kenneth McGuinness (adviser: Vikas Nanda), Yile Gu (Princeton University, adviser: S.

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Sundaresan), Sarang Oka (adviser: Fernando Muzzio, Rohit Ramachandran), Richard Cimino (adviser: Alexander V. Neimark), Monika Kazancioglu (adviser: M. Hara), Tao Zhang (adviser: Tewodros Asefa), Daehoon Han (adviser: Howon Lee, Mechanical and Aerospace Engineering), Zainab Abd Al-Jaleel (adviser: Nina Shapley), Silvio Dantas (adviser: Alexander V. Neimark), Sean Burgess (adviser: Alexander V. Neimark), Yaoyukun Jiang (adviser: Lu Wang, Chemistry and Chemical Biology), Jin Tang (adviser: Hao Wang, Civil and Environmental Engineering), Robert Palmere (adviser: Andy Nieuwkoop, Chemistry and Chemical Biology)

Member of Masters thesis committee
Fabian Casteblanco (adviser: Yee Chiew), Anuj Prakash (adviser: Rohit Ramachandran), Joyce John (adviser: Rohit Ramachandran), Kun Mei (adviser: Nina Shapley), Jianli Cheng (adviser: Alexander V. Neimark), Atish Kulkarni (adviser: F. Celik), Shiv Shah (adviser: Stavroula Sofou), Siddhi Hate (adviser: Rohit Ramachandran), Manogna Murthy (adviser: Rohit Ramachandran), Chinmay Pathak (adviser: Nina Shapley), Ashley Pennington (adviser: F. Celik), Elliott Taylor (adviser: Masanori Hara), Shashank Kosuri (adviser: Nina Shapley), Tianying Ma (adviser: Alexander V. Neimark), Christopher Dobrzanski (adviser: Nina Shapley), Yexuan Lu (adviser: Masanori Hara), Ravish Kumar (adviser: Alexander V. Neimark), Anjani Ganti (adviser: Tewodros Asefa), Lizhuo Song (adviser: Masanori Hara), Apostolos Zournas (adviser: Charles Dismukes), Mayur Barai (adviser: Maria Silvina Tommasone).

MEMBERSHIP AT PROFESSIONAL SOCIETIES
American Physical Society (1996 – 2011)
American Chemical Society (2013 – present)
Materials Research Society (2009 – 2018)

STUDENT AWARDS/HONORS/FELLOWSHIPS
- **2023:** Travel Award, Biomedical Engineering/ Graduate School of Rutgers to Mason Hooten (PhD student). (**Award:** $1000.00)
- **2022:** Douglass PROJECT SUPER Summer Stipend to Jeeyoung Han (undergraduate research assistant)   (**Award:** $3000.00)
- **2022:** Travel Award, Chemical and Biochemical Engineering/ Graduate School of Rutgers to Akash Banerjee (PhD student). (**Award:** $500.00)
- **2020:** Douglass STEM Summer Stipend to Rebecca Welch (undergraduate research assistant) (**Award:** $3000.00)
- **2020:** Travel Award, Chemical and Biochemical Engineering/ Graduate School of Rutgers to Akash Banerjee (PhD student). (**Award:** $300.00)
- **2018:** Travel Award, Chemical and Biochemical Engineering/ Graduate School of Rutgers to Akash Banerjee (PhD student). (**Award:** $300.00)
- **2018:** Travel Award, Chemical and Biochemical Engineering/ Graduate School of Rutgers to Srinivas Mushnoori (PhD student). (**Award:** $250.00)
- **2018:** Phase-II MoSSI Software Fellows, Srinivas Mushnoori (PhD student) (**Award:** $107,894.00)
- **2017:** Travel Award, Graduate School of Rutgers to Srinivas Mushnoori (PhD student). (**Award:** $250.00)
- **2017:** Graduate Fellowship 2017-2018 Academic Year from the New Jersey Space Grant Consortium, Kassandra Schmidt (MS student) (**Award:** $10,000.00)
- **2017:** Phase-I MoSSI Software Fellows, Srinivas Mushnoori (PhD student) (**Award:** $36,486.00)
- **2017:** Poster Award, AIChe Mid-Atlantic conference to Sarah Libring (Undergraduate student). (**Award:** $100.00)
- **2017:** Travel Award, AIChe Rutgers Chapter to Sarah Libring (Undergraduate student) (**Award:** $75.00)
- **2016:** Travel Award, Associate Alumnae for Douglass College to Vyshnavi Karra (Masters student) (**Award:** $500.00)
- **2016:** Travel Award, AIChe Rutgers Chapter to Vyshnavi Karra (Masters student) (**Award:** $350.00)
- **2016:** Graduate student travel award to Xiang Yu (Doctoral student) (**Award:** $200.00)

- **2016:** Rutgers Chemical and Biochemical Engineering travel award to Sarah Libring (Undergraduate student) (**Award:** $300.00)
- **2016:** Douglass Project travel award to Sarah Libring (Undergraduate student) (**Award:** $250.00)
- **2015:** MRS Fall 2015 travel award to Xiang Yu (Doctoral student) (**Award:** $587.00)
- **2015:** MRS Fall 2015 poster award to Xiang Yu (Doctoral student), Xiaolei Chu (Masters student) (**Award:** $200.00)
- **2015:** Graduate student travel award to Xiang Yu (Doctoral student) (**Award:** $250.00)
- **2015:** Rutgers Chemical and Biochemical Engineering travel award to Sarah Libring (Undergraduate student) (**Award:** $300.00)
- **2015:** Graduate student travel award to Fikret Aydin (Doctoral student) (**Award:** $250.00)
- **2015:** Graduate student travel award to Leebyn Chong (Doctoral student) (**Award:** $250.00)
- **2015:** Louis Stokes Alliance for Minority Participation Travel Stipend to Sarah Libring (undergraduate research assistant) (**Award:** $1000.00)
- **2015:** Douglass Residential College Conference Funding Award to Vyshnavi Karra (undergraduate research assistant) (**Award:** $250.00)
- **2014:** Douglass Residential College Special Funding Award to Vyshnavi Karra (undergraduate research assistant) (**Award:** $500.00)
- **2014:** Materials Research Society Fall 2014 travel award to Leebyn Chong (Doctoral student) (**Award:** $1400.00)
- **2014:** Graduate student travel award to Leebyn Chong (Doctoral student) (**Award:** $250.00)
- **2014:** Graduate student travel award to Fikret Aydin (Doctoral student) (**Award:** $250.00)
- **2014:** Researchers Present award to Sarah Libring (undergraduate research assistant) (**Award:** $1000.00)
- **2014:** Douglass STEM Summer Stipend to Sarah Libring (undergraduate research assistant) (**Award:** $3000.00)
- **2014:** Louis Stokes Alliance for Minority Participation Research Stipend to Sarah Libring (undergraduate research assistant) (**Award:** $1000.00)
- **2013:** Graduate student travel award to Leebyn Chong (Doctoral student) (**Award:** $250.00)
- **2013:** Graduate student travel award to Fikret Aydin (Doctoral student) (**Award:** $250.00)
- **2013:** Brazil-US exchange program fellowship awarded to Paul Ludford (undergraduate research assistant) (**Award:** travel and subsistence ~ $3000)

COURSE DEVELOPMENT & INSTRUCTION
Chemical Engineering Thermodynamics II: Fall 2011 – 2016; Spring 2022.
Analytical Methods in Chemical & Biochemical Engineering: Spring 2012 - 2013, Fall 2014-2015, 2017- 2020, 2022 - present.
Multiscale Materials Modeling: Spring 2018 - 2020.
Chemical Engineering of Advanced Materials: Spring 2024 – present.

COURSE REVIEWS

SIRS ONLINE SURVEY								Evaluation Responses	Teaching Effectiveness (Max=5)		Course Quality (Max=5)	
S/Yr	Course Title	Course ID	Credits	MOI	Aud	Resp	Enrl		Instructor	Dept Mean	Instructor	Dept Mean
Fa 22	ANAL METH CHEM BIOENG	16:155:507:01	3				25	14	4.57	4.34	4.29	4.23
Fa 20	ANAL METH CHEM BIOENG	16:155:507:01	3				30	16	4.3	4.3	4.2	4.2
Sp 20	MULTI MAT MOD	16:155:520:01	3				12	9	5	4.5	4.8	4.5
Fa 19	ANAL METH CHEM BIOENG	16:155:507:01	3				34	24	4.22	4.32	4.00	4.24
Sp 19	MULTI MAT MOD	16:155:520:01	3				8	8	4.63	4.30	4.75	4.26

Fa 18	ANAL METH CHEM BIOENG	16:155:507:02	3					22	13	4.31	4.22	4.31	4.22
Sp 18	MULTI MAT MOD	16:155:588:02	3					8	6	4.83	4.31	4.83	4.34
Fa 17	ANAL METH CHEM BIOENG	16:155:507:01	3					22	11	4.60	4.08	4.60	4.12
Fa 16	CHEM ENG THERMO II	14:155:309:01	3					122	122	3.64	3.50	3.48	3.39
Fa 15	CHEM ENG THERMO II	14:155:309:01	3					123	109	4.46	4.05	4.34	3.97
Fa 15	ANAL METH CHEM BIOENG	16:155:507:01	3					69	68	3.53	4.24	3.63	4.19
Fa 14	CHEM ENG THERMO II	14:155:309:01	3					105	95	4.37	3.85	4.31	3.85
Fa 14	ANAL METH CHEM BIOENG	16:155:507:01	3					60	55	4.07	4.24	4.07	4.21
Fa 13	CHEM ENG THERMO II	14:155:309:01	3					100	48	4.13	3.82	4.18	3.82
Sp 13	ANAL METH CHEM BIOENG (Lecture)	16:155:507:01	3					56	41	2.76	3.79	2.83	3.73
Fa 12	CHEM ENG THERMO II	14:155:309:01	3					84	48	2.65	3.39	2.88	3.37
Sp 12	ANAL METH CHEM BIOENG	16:155:507:01	3					48	28	1.82	3.72	2.00	3.84
Fa 11	CHEM ENG THERMO II	14:155:309:01	3					78	46	3.62	3.65	3.58	3.58

GUEST LECTURES

- *Guest lecture on Ethics in Professor Marianthi Ierapetritou's undergraduate core course on Professional Development in Rutgers, The State University of New Jersey:* Spring 2014/2015, Fall 2016/2017.
- *Guest lecture on Coarse-Graining in Professor Alexander Neimark's graduate elective course on Nanoscale Transport in Rutgers, The State University of New Jersey:* Fall 2015.
- *Guest lecture in Professor Keith Gubbins' graduate elective course on Multiscale Modeling of Matter (CHE-775) in North Carolina State University:* April 2016.
- *Online guest lecture in Professor Jonathan P. Singer's undergraduate core course on Multiphysics Simulations (MAE-439) in Rutgers, The State University of New Jersey:* September 2018.

INVITED COLLOQUIA, SEMINARS AND TALKS

1. Coarse-Grained Methods for Soft and Biological Materials, Gordon Research Conference, Computational Materials Science and Engineering: Comparing Theories, Algorithms and Computation Protocols in Materials Science and Engineering, Newry, ME, August 2022.
2. A Hybrid Coarse-Grained Model for Lipid-like Peptides: Structure, Solvation and Assembly, American Chemical Society (ACS) Mid-Atlantic Regional Meeting (MARM) 2022, Trenton, NJ, June 2022.
3. A Hybrid Computational Approach to Design Co-Assembled Peptide Materials: PACE[2] Framework, ACS MARM 2022, Trenton, NJ, June 2022.
4. Soft and Biological Materials Design via Cyber-Enabled Computational Methods, 2020 Virtual MRS Spring/ Fall Meeting.
5. Interfacial Behavior and Self-Organization of Nano-Inclusions in Vesicles, 2020 Virtual MRS Spring/ Fall Meeting.
6. Computational Design of Shape-Tunable Nanostructures, Physics and Astronomy, University of Texas at San Antonio, San Antonio, TX, March 2020.
7. Computational Design of Shape-Tunable Nanostructures, Chemical and Biomedical Engineering, University of Texas at San Antonio, San Antonio, TX, February 2020.
8. Computational Design of Shape-Tunable Nanostructures, Materials Science and Engineering, Rutgers, Piscataway, NJ, February 2019.

9. Computational Design of Shape-Tunable Nanostructures, Biomedical and Chemical Engineering, Syracuse University, NY, September 2018.
10. Computational Design of Shape-Tunable Nanostructures, Center for Functional Nanomaterials, Brookhaven National Laboratory, NY, July 2018.
11. Computational Design of Bioinspired Vesicles with Tunable Shape and Interfacial Characteristics, Department of Civil and Materials Engineering, University of Illinois at Chicago, IL, May 2017.
12. Computational Design of Bioinspired Vesicles with Tunable Shape and Interfacial Characteristics, Department of Physics, Lehigh University, PA, March 2017.
13. Computational Design of Bioinspired Vesicles with Tunable Shape and Interfacial Characteristics, Department of Chemistry and Chemical Biology, Rutgers, NJ, December 2016.
14. Coarse-grained Models for Self-assembly of ABA Triblock Copolymers using Dissipative Particle Dynamics, Neimark Group Meeting, Rutgers, Piscataway, NJ, May 2016.
15. Design of Shape-Tunable Nanoparticles. University of Massachusetts, Dartmouth, MA, May 2016.
16. Computational Design of Vesicles with Tunable Shape and Interfacial Properties. North Carolina State University, Raleigh, NC, April 2016.
17. Computational Design of Shape-Tunable Nanoparticles. Georgia Institute of Technology, Atlanta, GA, April 2016.
18. Design of Shape-Tunable Vesicles. Mechanical and Industrial Engineering, Northeastern University, Boston, MA, September 2015.
19. Coarse-Grained Models of Peptides. Multiscale Characterization of Advanced Materials Workshop, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, Dayton, Ohio, June 2015.
20. Design of Shape-Tunable Vesicles. Rutgers University Bioengineering Society, Piscataway, NJ, May 1, 2015.
21. Design of Shape-Tunable Vesicles. School of Pharmacy, Rutgers University, Piscataway, NJ, April 29, 2015.
22. Computational Soft Materials: Computational Design of Bio-inspired and Biological Nanoparticles via Self-Assembly. Multiscale Characterization of Advanced Materials Workshop, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, Dayton, Ohio, July 2014.
23. Harnessing Self-Assembly to Design Nanostructured Biomaterials: Functionalized Icosahedral Building Block Assemblies and Bio-inspired Bilayers with Tunable Properties, Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, Dayton, Ohio, October 4, 2013.
24. Nano-pipette Directed Motion of Bio-inspired Transmembrane Channel, Southeastern Regional Meeting of the American Chemical Society 2012, Raleigh, North Carolina, November 15, 2012.
25. Exploiting Spontaneous and Self-Assembly to Design Biomimetic Functionalized Nanotube-Lipid Hybrid Structures, Triangle MRSEC Seminar Series, Duke University, Durham, North Carolina, October 11, 2012.
26. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Gordon Research Seminar, Biointerfaces, Les Diablerets, Switzerland, May 19, 2012.
27. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Oak Ridge National Laboratory, Tennessee, April 2, 2012.
28. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Center for Advanced Biotechnology and Medicine, Rutgers University, New Jersey, March 23, 2012.
29. Exploiting Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Graduate Research Seminar, Materials Science and Engineering, Rutgers University, New Jersey, March 16, 2012.
30. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Fluid Mechanics Seminar, New Jersey Institute of Technology, New Jersey, March 5, 2012.
31. Computational Design of Hybrid Materials: From Pharmaceutical Powders to Bio-nanomaterials, Rutgers University Biomedical Students' Society, New Jersey, October 2011.
32. Computational Design of Hybrid Materials: From Pharmaceutical Powders to Bio-nanomaterials, Rutgers University, New Jersey, October 2010.

33. Modeling the Interactions between Amphiphilic Nanotubes and Lipid Bilayers, Nanotech 2010, Anaheim, California, June 2010.
34. Microstructural studies of dense granular media and their importance to the pharmaceutical industry, International Congress of Industrial and Applied Mathematics 2007, Zurich, Switzerland, July 2007.
35. Influence of particle size dispersity on frictional frustration in compressed dense granular packings, University of Leiden, The Netherlands, July 2007.
36. Dense granular media and their importance to the pharmaceutical industry, McMaster University, Canada, February 2007.
37. Physics of compressed dense granular media and their applications, University of Western Ontario, Canada, February 2007.
38. Numerical studies of ultrafine particles in the absence and presence of external fields, Summer School on Colloids in external fields: Physics and its Applications, Cargese, France, October 2006.
39. Modelling cohesive particles for inhalation applications, PIPMS Seminar series, Cambridge, UK, May 2006.
40. Using particle-based simulations for studying microscopic dynamics of powder compaction, Pfizer Global R and D, Sandwich, UK, September 2005.
41. Microscopic dynamics of powder compaction, Kavli Institute of Theoretical Physics program on Granular Physics, University of California, Santa Barbara, USA, May 2005.
42. Using Discrete element modelling for understanding microscopic dynamics of powder compaction, Pfizer Global R and D, Groton, USA, March 2005.
43. Numerical investigations of the effects of particle size and material dispersity on powder compaction, PIPMS Seminar series, Cambridge, UK, May 2005.
44. Discrete element modeling of powder compaction, PIPMS Seminar series, Cambridge, UK, May 2004.
45. Numerical experiments on particle packings, Workshop on Cooperative Grains: From Granular Matter to Nano Materials, University of Leiden, The Netherlands, October 2003.
46. Particle based modeling using discrete element simulations to investigate powder compaction, Pfizer Global R and D, Sandwich, UK, September 2003.
47. Discrete element simulations of dry non-cohesive powders, PIPMS Seminar series, Cambridge, UK, May 2003.

CONTRIBUTED PRESENTATIONS
1. Imani Birchett and M. Dutt, PACE[2]: Automated Design of Materials with Targeted Properties, RiSE/REU research symposium, New Brunswick, August 2023. (poster)
2. Imani Birchett and M. Dutt, PACE[2]: Automated Design of Materials with Targeted Properties, RiSE/REU research mini-symposium, New Brunswick, August 2023. (talk)
3. Jeeyoung Han, A. Banerjee and **M. Dutt**, Simulation of Lipid Bilayer Structures for Designing Novel Biomedicine, Chemical Engineering Undergraduate Research Symposium, New Brunswick, April 2023. (poster)
4. Nivedha Ganesan, M. Hooten and **M. Dutt**, Curating a Python Manual for Non-Programmers in Engineering Research Laboratories, Chemical Engineering Undergraduate Research Symposium, New Brunswick, April 2023. (poster)
5. M. Hooten and **M. Dutt**, Coarse-grained Molecular Modeling Framework for Enzymes, ACS Spring 2023, Indianapolis, IN, March 2023. (poster)
6. M. Hooten, A. Banerjee and **M. Dutt**, Hybrid Coarse-grained Approach to Model Structure, Conformation, Solvation and Aggregation of Aromatic Tripeptides, ACS Spring 2023, Indianapolis, IN, March 2023. (talk)
7. Jeeyoung Han, Ebony Oenga, Mason Hooten and M. Dutt, How Noncovalent Interactions Influence Conformation of Lipase, Douglas College Project SUPER Research Symposium, August 2022. (poster)
8. Ebony Oenga, Jeeyoung Han, Mason Hooten and M. Dutt, How Noncovalent Interactions Influence Conformation of Lipase, RiSE/REU research symposium, August 2022. (poster)
9. M. Dutt, A Hybrid Computational Approach to Design Co-Assembled Peptide Materials: PACE[2] Framework, Gordon Research Conference, Computational Materials Science and Engineering:

Comparing Theories, Algorithms and Computation Protocols in Materials Science and Engineering, Newry, ME, August 2022.

10. Ebony Oenga, Jeeyoung Han, Mason Hooten and M. Dutt, How Noncovalent Interactions Influence Conformation of Lipase, RiSE/REU research mini-symposium, July 2022. (talk)

11. A. Banerjee, Chien Y. Lu and **M. Dutt**, A Hybrid Coarse-grained Model for Lipid-like Peptides: Structure, Solvation and Assembly, ACS Spring 2022, San Diego, CA, March 2022. (talk)

12. A. Banerjee, A. Tam and **M. Dutt**, Formation and Stability of Dendronized Vesicles: Role of Dendron Generation and Concentration, ACS Spring 2022, San Diego, CA, March 2022. (talk)

13. A. Banerjee and **M. Dutt**, Automating the Design of Formation of Dendronized Vesicles- The PACE^2 Framework, MRS Fall 2021, Boston, MA, November 2021. (poster)

14. A. Banerjee, A. Tam and **M. Dutt**, Formation and Stability of Dendronized Vesicles, MRS Fall 2021, Boston, MA, November 2021. (talk)

15. Isabel Powers and **M. Dutt**, Modeling the PhoPQ Signaling Pathway in Salmonella, RiSE/REU research symposium, August 2021. (poster)

16. Isabel Powers and **M. Dutt**, Modeling the PhoPQ Signaling Pathway in Salmonella, RiSE/REU research symposium, July 2021. (talk)

17. S. Mushnoori, K. Schmidt, and **M. Dutt**, Peptide Materials Design via a Hybrid Computational Approach, MRS Fall 2019, Boston, MA, November 2019. (talk)

18. A. Banerjee, A. Tam and **M. Dutt**, Computational Design of Dendron-grafted Soft Materials-based Nanoparticles, MRS Fall 2019, Boston, MA, November 2019. (poster)

19. S. Mushnoori, K. Schmidt and **M. Dutt**, Computational Design of Peptide-based Materials, AIMS 2019 Workshop, National Institute of Standards and Technology, Gaithersburg, MD, August 2019. (poster)

20. Acacia Tam, A. Banerjee and **M. Dutt**, Characterization of PAMAM Dendron Based Lipids Grafted Structure on a DPPC Lipid Vesicle, RiSE/REU research symposium, August 2019. (poster)

21. Acacia Tam, A. Banerjee and **M. Dutt**, Characterization of PAMAM Dendron Based Lipids Grafted Structure on a DPPC Lipid Vesicle, RiSE/REU research symposium, July 2019. (talk)

22. E. Zang, K. Schmidt, S. Mushnoori and **M. Dutt**, Computational Characterization of Peptide Self-Assembled Structures, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2019. (poster, *award winner*)

23. A. Shawl, B. Ronan, S. Libring, V. Karra, S. Mushnoori and **M. Dutt**, Multi-scale Simulation of Collagen using Coarse-Grained Molecular Dynamics, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2019. (poster)

24. S. Mushnoori, K. Schmidt, V. Nanda and **M. Dutt**, Ultrashort peptide materials design via a hybrid computational approach, 257th ACS National meeting 2019, Orlando, FL, March 2019. (talk)

25. X. Yu and **M. Dutt**, A Multiscale Approach to Study Molecular and Interfacial Characteristics of Vesicles, 257th ACS National meeting 2019, Orlando, FL, March 2019. (talk)

26. A. Banerjee and **M. Dutt**, Computational Design of Dendron-grafted Soft Materials-based Nanoparticles, MRS Fall 2018, Boston, MA, November 2018. (poster)

27. A. Banerjee and **M. Dutt**, Self-organization of Peptides in Bioinspired Vesicles: Role of Relative Concentration and Helical Separation, MRS Fall 2018, Boston, MA, November 2018. (talk)

28. S. Mushnoori, K. Schmidt, V. Nanda and **M. Dutt**, Designing hybrid biological materials: Controlling morphology via molecular composition, MRS Fall 2018, Boston, MA, November 2018. (talk)

29. S. Mushnoori, V. Balasubramanian, S. Jha and **M. Dutt**, Replica Exchange Enhanced Self Assembly of Ultrashort Peptides, MRS Fall 2018, Boston, MA, November 2018. (talk)

30. X. Yu and **M. Dutt**, A Multiscale Approach to Study Molecular and Interfacial Characteristics of Colloids, MRS Fall 2018, Boston, MA, November 2018. (poster, *nominated for Best Poster Award*)

31. S. Mushnoori, V. Balasubramanian, S. Jha and **M. Dutt**, RepEx: A scalable, flexible, extensible replica exchange framework, 256th ACS National meeting 2018, Boston, MA, August 2018. (talk)

32. S. Mushnoori, K. Schmidt, V. Nanda and **M. Dutt**, Designing hybrid biological materials: Controlling morphology via molecular composition, 256th ACS National meeting 2018, Boston, MA, August 2018. (talk)

33. E. Dolan, S. Mushnoori, **M. Dutt**, and S. Khare An integrated computational-experimental approach for designing photoswitchable protein assemblies, 256th ACS National meeting 2018, Boston, MA, August 2018. (talk)
34. Zachary Finkel, A. Banerjee and **M. Dutt**, Study of Hydrophobic Mismatch Protein Systems: Role of Peptide Orientation and Lipid Density Profile, RiSE/REU research symposium, August 2018. (poster)
35. Zachary Finkel, A. Banerjee and **M. Dutt**, Study of Hydrophobic Mismatch Protein Systems: Role of Peptide Orientation and Lipid Density Profile, RiSE/REU research symposium, July 2018. (talk)
36. X. Yu and **M. Dutt**, A Multiscale Approach to Study Molecular and Interfacial Characteristics of Vesicles, FOMMS 2018, Delevan, WI, July 2018. (poster)
37. A. Shawl, B. Ronan, S. Libring, V. Karra, S. Mushnoori and **M. Dutt**, Multi-scale Simulation of Collagen using Coarse-Grained Molecular Dynamics, Chemical Engineering Undergraduate Research Symposium, New Brunswick, April 2018. (poster)
38. X. Chu, X. Yu, J. Greenstein, F. Aydin, G. Uppaladadium and **M. Dutt**, Flow-induced Shape Reconfiguration, Phase Separation and Rupture of Bio-inspired Vesicles, Materials Research Society Fall 2017 meeting, Boston. (poster)
39. S. Mushnoori, K. Schmidt and **M. Dutt**, Hybrid peptide-based materials encompassing ultrashort peptides: Molecule to Materials, 254th ACS National meeting, Washington D.C., August 2017. (talk)
40. S. Mushnoori, K. Schmidt and **M. Dutt**, Hybrid peptide-based materials encompassing ultrashort peptides: Molecule to Materials, Sci-mix poster session, 254th ACS National meeting, Washington D.C., August 2017. (poster)
41. S. Mushnoori, K. Schmidt and **M. Dutt**, Designing Sterically Stable Peptide Aggregates with Target Morphologies, Sci-mix, 254th ACS National meeting, Washington D.C., August 2017. (poster)
42. S. Mushnoori, K. Schmidt and **M. Dutt**, Designing Sterically Stable Peptide Aggregates with Target Morphologies, 254th ACS National meeting, Washington D.C., August 2017. (talk)
43. X. Chu, X. Yu, J. Greenstein, F. Aydin, G. Uppaladadium and **M. Dutt**, Flow-induced Shape Reconfiguration, Phase Separation and Rupture of Bio-inspired Vesicles, 254th ACS National meeting, Washington D.C., August 2017. (talk)
44. Emran Rashid, K. Schmidt, S. Mushnoori and **M. Dutt**, Self-Assembling Peptides: Characterization of Nanostructures, RiSE/REU research symposium, August 2017. (poster)
45. Emran Rashid, K. Schmidt, S. Mushnoori and **M. Dutt**, Self-Assembling Peptides: Characterization of Nanostructures, RiSE/REU research symposium, July 2017. (talk)
46. S. Libring, V. Karra, B. Ronan, S. Mushnoori and **M. Dutt**, Ultra-Corase-Grained Design of Peptide-Based Materials, Slade Scholar Public Presentation, April 2017. (talk)
47. T. Ma, D. Grisham, S. Mushnoori, **M. Dutt** and V. Nanda, Synthesis and Characterization of Multicoomponent Peptide Materials, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2017. (poster)
48. B. Ronan, S. Libring, V. Karra, S. Mushnoori and **M. Dutt**, Multi-Scale Simulation of Collagen Using Coarse-Grained Molecular Dynamics, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2017. (poster)
49. S. Libring, V. Karra, B. Ronan, S. Mushnoori and **M. Dutt**, Ultra-Coarse-Grained Design of Peptide-Based Materials, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2017. (poster)
50. K. Jin, J. Li, S. Mushnoori and **M. Dutt**, Interactions Between Lipid Membrane and PAMAM Dendron-grafted Surface: Insight via Computational Techniques, Chemical Engineering Undergraduate Research Symposium, New Brunswick, March 2017. (poster)
51. S. Libring, V. Karra, L. Chong and **M. Dutt**, Self-Assembly of Virus Capsids Decorated with Block Copolymers: A Simulation Study, AICHe Mid-Atlantic Student Regional Conference, March 2017, Sewell. (poster, *award winner*)
52. S. Mushnoori[a] and **M. Dutt**, Computational Design of Hybrid Peptide Materials, 2017 Mid-Atlantic Region Biomaterials Day, New York, NY, February 2017. (poster)
53. X. Chu,[b] X. Yu,[a] J. Greenstein,[c] F. Aydin,[a] G. Uppaladadium[b] and **M. Dutt**, Flow-induced Shape Reconfiguration, Phase Separation and Rupture of Bio-inspired Vesicles, Gordon Research Conference on Complex Adaptive & Dissipative Materials, January 2017, Ventura. (poster)

MEENAKSHI DUTT

54. S. Mushnoori and **M. Dutt**, Computational Study of Di and Tripeptide Assembly, Materials Research Society Fall 2016 meeting, Boston. (poster, *nominated for Best Poster Award*)
55. S. Mushnoori and **M. Dutt**, Computational Design of Peptide-based Nanomaterials, Materials Research Society Fall 2016 meeting, Boston. (poster)
56. X. Yu and **M. Dutt**, Computational Design of Dendronized Vesicle, Materials Research Society Fall 2016 meeting, Boston. (poster)
57. X. Yu, X. Chu, J. Greenstein, F. Aydin, G. Uppaladadium and **M. Dutt**, Morphological Studies of Bioinspired Vesicle Under Laminar Flow, Materials Research Society Fall 2016 meeting, Boston. (poster, **poster award winner)**
58. Y.J. Seo, X. Chu and **M. Dutt**, The Formation of Vesicles through the Modification of Tyrosine-Derived ABA Tri-Block Copolymer Membranes, American Institute of Chemical Engineers Annual Meeting 2016, San Francisco. (poster)
59. Y.J. Seo, X. Chu and **M. Dutt**, The Formation of Vesicles through the Modification of Tyrosine-Derived ABA Tri-Block Copolymer Membranes, American Institute of Chemical Engineers Annual Meeting 2016, San Francisco. (talk)
60. S. Libring, V. Karra, L. Chong and **M. Dutt**, Self-Assembly of Virus Capsids Decorated with Block Copolymers: A Simulation Study, American Institute of Chemical Engineers Annual Meeting 2016, San Francisco. (poster)
61. V. Karra, S. Libring, L. Chong and **M. Dutt**, Self-Aggregation of Functionalized Capsids Using Coarse Grained Molecular Dynamics, American Institute of Chemical Engineers Annual Meeting 2016, San Francisco. (poster, *award winner*)
62. X. Chu, F. Aydin and **M. Dutt**, Interactions Between Peptide-Mimetic Nanoparticles and Synthetic Cells, American Institute of Chemical Engineers Annual Meeting 2016, San Francisco. (talk)
63. S. Mushnoori and **M. Dutt**, Computational Design of Ultrashort Peptide Aggregates via Coarse-Grained Molecular Dynamics, 252th ACS National meeting, Fall 2016, Philadelphia. (poster)
64. S. Mushnoori, L. Chong and **M. Dutt**, Computational Study of pH-driven Aggregation of EAK16 Peptides, 252th ACS National meeting, Fall 2016, Philadelphia. (talk)
65. X. Yu, F. Aydin, L. Chong and **M. Dutt**, Multiscale modeling of hairy vesicles, 252th ACS National meeting, Fall 2016, Philadelphia. (talk)
66. X. Chu, X. Yu, J. Greenstein, F. Aydin, G. Uppaladadium and **M. Dutt**, Flow-induced shape changes in bioinspired vesicles, 252th ACS National meeting, Fall 2016, Philadelphia. (sci-mix poster)
67. X. Yu and **M. Dutt**, Computational design of amphiphile-based nanoparticles, 252th ACS National meeting, Fall 2016, Philadelphia. (talk)
68. X. Yu, F. Aydin, L. Chong and **M. Dutt**, Multiscale modeling of hairy vesicles, Gordon Research Conference on Computational Chemistry, July 2016, Girona, Spain. (poster)
69. Sarah Libring, V. Karra, L. Chong and **M. Dutt**, Self-Aggregation of Virus Capsids Decorated with Amphiphilic Diblock Copolymers: A Coarse-Grained Simulation, Aresty Undergraduate Research Symposium, April 2016. (poster)
70. Sarah Libring, V. Karra, L. Chong and **M. Dutt**, Self-Aggregation of Virus Capsids Decorated with Amphiphilic Diblock Copolymers: A Coarse-Grained Simulation, AIChe Mid-Atlantic Student Regional Conference, April 2016. (talk)
71. Vyshnavi Karra, S. Libring, L. Chong and **M. Dutt**, Self-Aggregation of Functionalized Capsids using Coarse-Grained Molecular Dynamics, AIChe Mid-Atlantic Student Regional Conference, April 2016. (poster)
72. Sarah Libring, V. Karra, L. Chong and **M. Dutt**, Self-Aggregation of Virus Capsids Decorated with Amphiphilic Diblock Copolymers: A Coarse-Grained Simulation, CBE Undergraduate Research Day, April 2016. (poster)
73. Vyshnavi Karra, S. Libring, L. Chong and **M. Dutt**, Self-Aggregation of Functionalized Capsids using Coarse-Grained Molecular Dynamics, Slade Presentation, CBE Undergraduate Research Day, April 2016. (talk)
74. Joseph Greenstein, X. Chu and **M. Dutt**, Shape Characteristics of Multi-Component Bio-inspired Vesicles During Transport through a Microfluidic Channel, CBE Undergraduate Research Day, April 2016. (poster)

75. X. Chu, F. Aydin, G. Uppaladadium and **M. Dutt**, Interactions between Peptide-mimetic Nanoparticles and Synthetic Cells, ACS National Meeting, San Diego, CA, March 2016. (talk/ sci-mix poster)
76. F. Aydin, G. Uppaladadium and **M. Dutt**, Interfacial Adsorption of Patchy Nanoparticles onto Hairy Vesicles, ACS National Meeting, San Diego, CA, March 2016. (poster)
77. L. Chong, F. Aydin and **M. Dutt**, Implicit Solvent Coarse-Grained Model for Polyamidoamine Dendrimers: Role of Generation and pH, ACS National Meeting, San Diego, CA, March 2016. (poster)
78. X. Chu, X. Yu, Joseph Greenstein, F. Aydin, G. Upplaldadium and **M. Dutt**, Shape Characteristics of Multi-Component Bio-inspired Vesicles During Transport through a Microfluidic Channel, MRS Fall 2015 meeting, Boston, MA, December 2015. (poster, *award winner*)
79. F. Aydin, X. Chu. G. Uppaladadium, D. Devore, R. Goyal, Z. Zhang, J. Kohn and **M. Dutt**, Coarse-grained Models for Self-assembly of ABA Triblock Copolymers using Dissipative Particle Dynamics, MRS Fall 2015 meeting, Boston, MA, December 2015. (talk)
80. X. Yu, F. Aydin, L. Chong and **M. Dutt**, Computational Design of Soft Materials via Coupling of Particle Dynamics and Continuum Approaches, MRS Fall 2015 meeting, Boston, MA, December 2015. (talk, *award winner*)
81. X. Chu, X. Yu, J. Greenstein, F. Aydin, G. Uppaladadium and **M. Dutt**, Capillary Flow of Cell-Mimetic and Hairy Vesicles via Dissipative Particle Dynamics, MRS Fall 2015 meeting, Boston, MA, December 2015. (talk)
82. F. Aydin, G. Uppaladadium, and **M. Dutt**, Interfacial Adsorption of Janus Nanoparticles Onto Hairy Vesicles, AIChe Annual 2015 meeting, Salt Lake City, UT, November 2015.
83. L. Chong, S. Libring, V. Karra and **M. Dutt**, Self-Assembly Simulations of Polymer Functionalized Nanoparticles, ACS National Meeting, Boston, MA, August 2015. (talk, *award winner*)
84. L. Chong, S. Mushnoori and **M. Dutt**, Molecular Dynamics Simulations of the Titania & Water Interface, ACS National Meeting, Boston, MA, August 2015. (talk)
85. L. Chong and **M. Dutt**, Design of PAMAM-COO Dendron-grafted Surfaces to Promote Pb(II) Adsorption, ACS National Meeting, Boston, MA, August 2015. (talk)
86. Xiaolei Chu, F. Aydin, and **M. Dutt**, Computationally Driven Design of Multi-Component Bio-Inspired Vesicles Interacting with Functionalized Nanoparticles, ACS National Meeting, Boston, MA, August 2015. (talk)
87. F. Aydin, and **M. Dutt**, Modeling Interactions between Charged Nanoparticles and Multi-component Nanostructured Soft Biomaterials, ACS National Meeting, Boston, MA, August 2015. (talk)
88. F. Aydin, G. Uppaladadium, and **M. Dutt**, Designing Invisible Drug Delivery Vehicles through End-functionalization of Bio-Inspired Hybrid Soft Biomaterials, ACS National Meeting, Boston, MA, August 2015. (talk)
89. **M. Dutt**, Design of Multicomponent Shape-Tunable Carriers, ACS National Meeting, Boston, MA, August 2015. (poster)
90. F. Aydin, G. Uppaladadium and **M. Dutt**, Design of Shape-Tunable Vesicles, FOMMS 2015, Oregon, July 2015. (poster)
91. S. Mushnoori, L. Chong and M. **Dutt**, Molecular Dynamics study of water over Pt/TiO2 surfaces, Advances in Functional Materials, Stonybrook, June 2015. (talk)
92. L. Chong, F. Aydin and **M. Dutt**, Coarse-grained PAMAM dendrimer dynamics in implicit solvent, 4th Northeast Complex Fluids and Soft Matter Workshop (NCS4), Stony Brook University June 2015. (talk)
93. X. Chu, F. Aydin and **M. Dutt**, Modeling of bio-inspired vesicle and its interactions with nanoparticles, 4th Northeast Complex Fluids and Soft Matter Workshop (NCS4), Stony Brook University June 2015. (talk)
94. M. Sebastiano, X. Chu, F. Aydin and **M. Dutt**, Computational Design and Modeling of Bio-Inspired DPPC/DMPC/Cholesterol Phospholipid Membranes with Nanoparticles, Department of Chemical and Biochemical Engineering Slade Public Presentation, May 2015. (poster)
95. M. Sebastiano, X. Chu, F. Aydin and **M. Dutt**, Computational Design and Modeling of Bio-Inspired DPPC/DMPC/Cholesterol Phospholipid Membranes with Nanoparticles, Department of Chemical and Biochemical Engineering Undergraduate Research Symposium, April 2015. (poster)

96. J. Greenstein, X. Chu, F. Aydin and **M. Dutt**, Characterization of Vesicle Shapes from Particle Dynamics Simulations, Department of Chemical and Biochemical Engineering Undergraduate Research Symposium, April 2015. (poster)
97. S. Libring, V. Karra, L. Chong and **M. Dutt**, Self-Assembly Simulations of Polymer Functionalized Virus Capsids, Department of Chemical and Biochemical Engineering Undergraduate Research Symposium, April 2015. (poster)
98. Z. Yang, **M. Dutt** and Y. Chiew, Structure and Pattern Formation in Two Dimensional Colloidal Dimers, Department of Chemical and Biochemical Engineering Undergraduate Research Symposium, April 2015. (poster)
99. V. Karra, S. Libring, L. Chong and **M. Dutt**, Self-Aggregation of Virus Capsids Decorated with Homopolymers: a Coarse-Grained Molecular Dynamics Study, Aresty Research Symposium, Rutgers, Piscataway, NJ, April 2015. (poster)
100. Z. Yang, **M. Dutt** and Y. Chiew, Structure and Pattern Formation in Two Dimensional Colloidal Dimers, American Institute of Chemical Engineers 2015 Mid-Atlantic Student Regional Conference, Baltimore, MD, April 2015. (talk)
101. S. Libring, V. Karra, L. Chong and **M. Dutt**, Self-Assembly Simulations of Polymer Functionalized Virus Capsids, American Institute of Chemical Engineers 2015 Mid-Atlantic Student Regional Conference, Baltimore, MD, April 2015. (talk)
102. V. Karra, S. Libring, L. Chong and **M. Dutt**, Self-Aggregation of Virus Capsids Decorated with Homopolymers: a Coarse-Grained Molecular Dynamics Study, American Institute of Chemical Engineers 2015 Northeast Student Regional Conference, Boston, MA, March 2015. (poster)
103. F. Aydin, G. Uppaladadium and **M. Dutt**, Designing Bio-Inspired Hybrid Soft Biomaterials via the Self-Assembly of End-Functionalized Amphiphilic Molecules, Society of Women Engineers and Sigma Phi Delta Research Fair, Rutgers, Piscataway, NJ, March 2015. (poster)
104. X. Chu, M. Sebastiano, F. Aydin and **M. Dutt**, Computationally Driven Design of Multi-Component Bio-Inspired Membranes and Vesicles Interacting with Functionalized Nanoparticles, Society of Women Engineers and Sigma Phi Delta Research Fair, Rutgers, Piscataway, NJ, March 2015. (poster)
105. L. Chong, V. Kharra, S. Libring and **M. Dutt**, Self-Assembly of Functionalized Virus Capsids, OXE Research Symposium, Rutgers, Piscataway, NJ, February 2015. (poster)
106. L. Chong, S. Mushnoori and **M. Dutt**, Molecular Dynamics Simulations of Water Adsorption on Pt/TiO$_2$, Rutgers Discovery Informatics Institute Open House, Piscataway, NJ, February 2015. (poster)
107. L. Chong, V. Kharra, S. Libring and **M. Dutt**, Self-Assembly Simulations of Polymer Functionalized Viral Capids, Rutgers Discovery Informatics Institute Open House, Piscataway, NJ, February 2015. (poster)
108. X. Chu, M. Sebastiano, F. Aydin and **M. Dutt**, Computationally Driven Design of Multi-Component Bio-Inspired Membranes and Vesicles Interacting with Functionalized Nanoparticles, Rutgers Discovery Informatics Institute Open House, Piscataway, NJ, February 2015. (poster)
109. F. Aydin and **M. Dutt**, Computational Design of Charged Nanoparticles with Functional Groups Interacting with Multi-component Nanostructured Soft Biomaterials, Rutgers Discovery Institute Informatics Open House, Piscataway, NJ, February 2015. (poster)
110. X. Chu, F. Aydin, M. Sebastiano and **M. Dutt**, Modeling Bio-Inspired Cell, 3rd Northeast Complex Fluids and Soft Matter Workshop (NCS3), New Jersey Institute of Technology, Newark, January 2015. (talk)
111. F. Aydin, G. Uppaladadium and **M. Dutt**, Modeling of Bacterial-Mimetic Systems, 3rd Northeast Complex Fluids and Soft Matter Workshop (NCS3), New Jersey Institute of Technology, Newark, January 2015. (talk)
112. L. Chong and **M. Dutt**, Simulating Metal Ion Adsorption on Grafted Dendritic Surfaces, 3rd Northeast Complex Fluids and Soft Matter Workshop (NCS3), New Jersey Institute of Technology, Newark, January 2015. (talk)
113. F. Aydin, G. Uppaladadium and **M. Dutt**, Designing Bio-Inspired Hybrid Soft Biomaterials via the Self-Assembly of End-Funtionalized Amphiphilic Molecules, Materials Research Society Fall 2014 Meeting, Boston, MA. (poster)

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114. F. Aydin, G. Uppaladadium and **M. Dutt**, Designing Bio-Inspired Hybrid Soft Biomaterials via the Self-Assembly of End-Funtionalized Amphiphilic Molecules, Materials Research Society Fall 2014 Meeting, Boston, MA. (poster)

115. L. Chong and **M. Dutt**, Metal Ion Adsorption Via Grafted Dendritic Surfaces, Materials Research Society Fall 2014 Meeting, Boston, MA. (poster)

116. L. Chong, S. Mushnoori and **M. Dutt**, Atomistic Simulations of Photocatalytic Water Splitting on Pt/TiO2, Materials Research Society Fall 2014 Meeting, Boston, MA. (talk, *award winner*)

117. L. Chong, V. Kharra, S. Libring and **M. Dutt**, Self-Assembly of Functionalized Virus Capsids, Materials Research Society Fall 2014 Meeting, Boston, MA. (poster)

118. F. Aydin, X. Chu, M. Sebastiano and **M. Dutt**, Computational Modelling of Functionalized Nanoparticles Interacting with Bio-Inspired Membranes and Vesicles, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

119. F. Aydin, G. Uppaladadium and **M. Dutt**, Design of Sterically Stable Bio-Inspired Hybrid Soft Biomaterials Via Computational Modelling, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

120. F. Aydin and **M. Dutt**, Designing Multi-Component Nanostructured Soft Biomaterials Interacting with Charged Nanoparticles, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

121. L. Chong and **M. Dutt**, Metal Ion Adsorption Via Grafted Dendritic Surfaces, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

122. L. Chong, S. Mushnoori and **M. Dutt**, Atomistic Simulations of Photocatalytic Water Splitting on Pt/TiO2, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

123. L. Chong, V. Kharra, S. Libring and **M. Dutt**, Self-Assembly of Functionalized Virus Capsids, American Institute of Chemical Engineers Annual Meeting 2014, Atlanta. (talk)

124. F. Aydin, G. Uppaladadium and **M. Dutt**, Computational design of bio-inspired hybrid soft biomaterials, American Chemical Society Meeting 2014. San Francisco. (talk)

125. Orlando Mulero, F. Aydin, G. Uppaladadium and **M. Dutt**, Mechanical Properties of Lipid Bilayer Membranes: Bending and Compressibility Modulus, RiSE/REU Mini-Symposium. Piscataway July 2014. (talk)

126. Orlando Mulero, F. Aydin, G. Uppaladadium and **M. Dutt**, Mechanical Properties of Lipid Bilayer Membranes: Bending and Compressibility Modulus, RiSE/REU Research Symposium. Piscataway, July 2014. (poster)

127. **M. Dutt**. Functionalized Nanoparticle Interactions with Bio-Inspired Membranes and Vesicles, Gordon Research Seminar, Bioinspired Materials, Sunday River Resort, Maine, June 2014. (poster)

128. **M. Dutt**. Functionalized Nanoparticle Interactions with Bio-Inspired Membranes and Vesicles, Gordon Research Conference, Biointerfaces, Il Ciocco, Italy, June 2014. (poster)

129. Denise Preddie, Fikret Aydin and **M. Dutt**, Computational Investigations of the Morphology and Dynamics of Hybrid Nanostructured Biomaterials, Chemical and Biochemical Engineering Undergraduate Research Day, May 2014. (poster)

130. M. Sebastiano, F. Aydin, X. Chu and **M. Dutt**. Functionalized Nanoparticle Interactions with Bio-Inspired Membranes and Vesicles, RiSE Poster Presentations, May 2014. (poster)

131. Denise Preddie, Fikret Aydin and **M. Dutt**, Computational Investigations of the Morphology and Dynamics of Hybrid Nanostructured Biomaterials, RiSE Poster Presentations, May 2014. (poster)

132. M. Sebastiano, F. Aydin, X. Chu and **M. Dutt**. Functionalized Nanoparticle Interactions with Bio-Inspired Membranes and Vesicles, Chemical and Biochemical Engineering Undergraduate Research Day, March 2014. (poster)

133. **M. Dutt**, Design and Characterization of Multi-Component Nanostructured Biomaterials, Materials Research Society Fall 2013 Meeting, Boston, MA. (talk)

134. Fikret Aydin and **M. Dutt**, Modeling Driven Design of Multi-component Nanostructured Soft Biomaterials, Materials Research Society Fall 2013 Meeting, Boston, MA. (talk)

135. Denise Preddie, Paul Ludford, Fikret Aydin and **M. Dutt**, Computational Investigations of the Morphology and Dynamics of Hybrid Nanostructured Biomaterials, Materials Research Society Fall 2013 Meeting, Boston, MA. (talk)

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136. Evan Koufos and **M. Dutt**, Computational Investigations on the Role of Molecular Architecture on Morphology, and Properties of Bio-inspired Soft Materials, Materials Research Society Fall 2013 Meeting, Boston, MA. (talk)
137. Vidyalakshmi Muthukumar and **M. Dutt**, Computational Studies of the Aggregation of Functionalized Icosahedral Nanoparticles, Materials Research Society Fall 2013 Meeting, Boston, MA. (poster)
138. Vidyalakshmi Muthukumar, Sang Yun Lee, Phong Huynh, Paul Takhistov and **M. Dutt**, Computational Studies of Drying and Dissolution of Polymer Films, Materials Research Society Fall 2013 Meeting, Boston, MA. (poster)
139. Leebyn Chong and **M. Dutt**, Computer Simulations of Fluid Flow Over Catalytic Surfaces for Water Splitting, Materials Research Society Fall 2013 Meeting, Boston, MA. (poster)
140. Leebyn Chong and **M. Dutt**, Computer Simulations of Metal Ion Adsorption onto Surfaces Grafted with Dendrimers, Materials Research Society Fall 2013 Meeting, Boston, MA. (talk)
141. Leebyn Chong and **M. Dutt**, Computer Simulations of Fluid Flow Over Catalytic Surfaces for Water Splitting, American Institute of Chemical Engineers Annual Meeting 2013, San Francisco. (poster)
142. Fikret Aydin and **M. Dutt**, An Implicit Solvent Coarse-Grained Model for Design and Characterization of Bio-Nanostructured Soft Materials, American Institute of Chemical Engineers Annual Meeting 2013, San Francisco. (talk)
143. Evan Koufos and **M. Dutt**, Effect of Molecular Architecture On the Morphology and Properties of Bio-Nanostructured Soft Materials, American Institute of Chemical Engineers Annual Meeting 2013, San Francisco. (poster)
144. **M. Dutt**, Fikret Aydin, Paul Ludford and Denise Preddie, Designing Hybrid Bio-Nanostructured Soft Materials Via Self-Assembly, American Institute of Chemical Engineers Annual Meeting 2013, San Francisco. (talk)
145. **M. Dutt**, C. Vidyalakshmi, Sang Yun Lee, Phong Huynh and Paul Takhistov, Phase Transition in HPMC Gel, American Institute of Chemical Engineers Annual Meeting 2013, San Francisco. (poster)
146. Denise Preddie, Paul Ludford, Fikret Aydin and **M. Dutt**, Computational Investigations of the Morphology and Dynamics of Hybrid Nanostructured Biomaterials, OXE Faculty/ Student Research Event, October 2013. (poster)
147. Fikret Aydin and **M. Dutt**, An Implicit Solvent Coarse-Grained Model for Design and Characterization of Bio-Nanostructured Soft Materials, OXE Faculty/ Student Research Event, October 2013. (poster)
148. Paul Ludford and **M. Dutt**, Computational Studies of Domain Formation in Two-Component Lipid, Slade Public Lecture, May 2013. (poster)
149. Evan Koufos and **M. Dutt**, Effect of Lipid Chain on Nanoparticle Insertion into a Membrane Bilayer, Slade Scholar Public Lecture, March 2013. (poster)
150. Sang Yun Lee, Y. Chiew and **M. Dutt**, Design of Tunable Aggregate Morphologies using Peptide Blocks, Slade Scholar Public Lecture, May 2013. (poster)
151. Paul Ludford and **M. Dutt**, Computational Studies of Domain Formation in Two-Component Lipid, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, May 2013. (poster)
152. Evan Koufos and **M. Dutt**, Effect of Lipid Chain on Nanoparticle Insertion into a Membrane Bilayer, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, March 2013. (poster)
153. Sang Yun Lee, Y. Chiew and **M. Dutt**, Design of Tunable Aggregate Morphologies using Peptide Blocks, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, May 2013. (poster)
154. Diane Kao and **M. Dutt**, Computer Simulations of Powder Flow Using Discrete Element Method, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, March 2013. (poster)
155. Andrew Rullo and **M. Dutt**, Study of the Behavior of Lipid Bilayers Based on Membrane Tension, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, March 2013. (poster)
156. Yuan Zhuang, Y. Chiew and **M. Dutt**, Molecular Dynamics Modeling of Colloidal Dimers Thin Films, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, March 2013. (poster)

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157. Evan Koufos and **M. Dutt**. Design of Nanostructured Hybrid Inorganic-biological Materials via Self-assembly, Materials Research Society Spring 2013, San Francisco, CA. (talk)

158. Paul Ludford, Fikret Aydin and **M. Dutt**. Design and Characterization of Nanostructured Biomaterials via the Self-assembly of Lipids, Materials Research Society Fall 2012, Boston, MA. (talk)

159. **M. Dutt**. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Gordon Research Seminar, Bioinspired Materials, Davidson, North Carolina, June, 2012. (poster)

160. **M. Dutt**. Exploiting Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Tech World Connect (Nanotech 2012), Santa Clara, June, 2012. (talk)

161. **M. Dutt**. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Gordon Research Conference, Biointerfaces, Les Diablerets, Switzerland, May 21, 2012. (poster)

162. **M. Dutt**. Harnessing Spontaneous and Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, Gordon Research Seminar, Biointerfaces, Les Diablerets, Switzerland, May 20, 2012. (poster)

163. Paul Ludford and **M. Dutt**, Study of the Behavior of a Vesicle with Two Types of Lipids, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, April 2012.

164. Sang Yun Lee and **M. Dutt**, Study of Free and Tethered Polymer Chains in Solvent, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, April 2012.

165. Diane Kao and **M. Dutt**, Self-Assembly of Polymer Chains in Solvent with Dissipative Particle Dynamics, Rutgers Chemical and Biochemical Engineering Department Undergraduate Poster Day, April 2012.

166. **M. Dutt**, O, Kuksenok and A.C. Balazs. Designing Tunable Bio-nanostructured Materials via Self-Assembly of Amphiphilic Lipids and Functionalized Nanotubes, Materials Research Society Spring 2012, San Francisco. (talk)

167. **M. Dutt**, O, Kuksenok and A.C. Balazs. Nano-pipette Directed Motion of Biomimetic Transmembrane Channel, Materials Research Society Spring 2012, San Francisco. (poster)

168. **M. Dutt**, O, Kuksenok and A.C. Balazs. Designing Tunable Bio-nanostructured Materials via Self-Assembly of Amphiphilic Lipids and Functionalized Nanotubes, Materials Research Society Spring 2012, San Francisco. (talk)

169. **M. Dutt**, M. J. Nayhouse, O. Kuksenok, S.R. Little and A.C. Balazs*. Modeling the Self-Assembly of Lipids and Nanotubes in Solution: Forming Vesicles and Bicelles with Transmembrane Nanotube Channels. Materials Research Society Fall Meeting 2011, Boston, December 2011. (* presenter, talk)

170. **M. Dutt**. Compressed Dense Powder Blends: Size Dispersity and Void Structure, AIChe Annual Meeting 2011, Minneapolis, October 2011. (poster)

171. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs. Designing Biomimetic Membranes using Functionalized Nanotubes and Lipid Membranes, AIChe Annual Meeting 2011, Minneapolis, October 2011. (talk)

172. **M. Dutt**, M. J. Nayhouse, O. Kuksenok, S.R. Little and A.C. Balazs. Harnessing Self-Assembly to Design Functionalized Nanotube-Lipid Hybrid Structures, AIChe Annual Meeting 2011, Minneapolis, October 2011. (talk)

173. **M. Dutt**, O. Kuksenok and A.C. Balazs. Guided Transport of a Transmembrane Nanochannel, American Physical Society (APS) March Meeting 2011, Dallas, March 2011. (talk)

174. **M. Dutt**, O. Kuksenok, M.J. Nayhouse, S.R. Little and A.C. Balazs. Interactions of End-Functionalized Nanotubes with Lipid Vesicles: Spontaneous Insertion and Nanotube Self-organization, APS March Meeting 2011, Dallas, March 2011. (poster)

175. M.J. Nayhouse, **M. Dutt**, O. Kuksenok*, S.R. Little and A.C. Balazs. Design of Synthetic Vesicles Encompassing End-functionalized Nanotubes, Materials Research Society Fall Meeting 2010, Boston, November 2010. (poster, * presenter)

176. **M. Dutt**, O. Kuksenok*, S.R. Little and A.C. Balazs. Effects of Membrane Tension and Nanotube's Functionalization on Formation of Trans-membrane Channels, Materials Research Society Fall Meeting 2010, Boston, December 2010. (poster, * presenter)

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177. **M. Dutt**, O. Kuksenok, M.J. Nayhouse, S.R. Little and A.C. Balazs. Design of Synthetic Vehicles through Self-Assembly of End-Functionalized Nanotubes and Lipids, American Institute of Chemical Engineers Annual Meeting 2010, Salt Lake City, November 2010. (talk)

178. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs. Forming Trans-Membrane Channels Using End-Functionalized Nanotubes, American Institute of Chemical Engineers Annual Meeting 2010, Salt Lake City, November 2010. (poster)

179. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs*. Modeling interactions between amphiphilic nanotubes and lipid bilayers, 2010 Materials Research Society (MRS) Spring Meeting, San Francisco, CA, April 2010. (talk, * speaker)

180. **M. Dutt**, O. Kuksenok, S.R. Little and A.C. Balazs. Self-assembly of Amphiphilic Nanotubes and Lipids into Synthetic Vehicles: Computer Simulation Study, American Physical Society (APS) March 2010, Portland, March 2010. (poster)

181. **M. Dutt**, M. Nayhouse, O. Kuksenok, A. Alexeev, S.R. Little and A.C. Balazs. Mesoscopic Simulations of the Insertion of the Amphiphilic Nanotubes into Lipid Bilayers, APS March 2010, Portland, March 2010. (talk)

182. **M. Dutt**, O. Kuksenok, A. Alexeev, S.R. Little and A.C. Balazs. Modeling interactions between amphiphilic nanotubes and lipid bilayers, American Institute of Chemical Engineers Annual Conference 2009, Nashville, Novembers 2009. (talk)

183. **M. Dutt** and E. Luijten. Nanoparticle-induced domain formation in zwitterionic lipid membranes, APS March 2009, Pittsburgh, March 2009. (talk)

184. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. The Effect of Surface Properties on the Behavior of Ultrafine Particles, Particle Technology Forum UK 2007, Cambridge, United Kingdom September 2007. (poster)

185. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. Importance of length scales in the static and dynamic configurations of pharmaceutical particulate systems, Euromat 2007, Nurnberg, Germany, September 2007. (talk)

186. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. Using granular dynamics to explore the importance of length scales in the static and dynamic configurations of pharmaceutical particulate systems, Annual meeting of CCP5: Multi-scale Modelling, Cambridge, United Kingdom, August 2007. (talk)

187. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. Numerical Studies of Ultrafine Particles: A Simple Model and their Behavior in the Absence and Presence of External Fields, Satellite meeting of Statphys 2007: Statics and dynamics of granular media and colloidal suspensions, Naples, Italy, July 2007. (poster)

188. M. Benedict, **M. Dutt**, B. Hancock, C. Bentham and J. Elliott, The Effect of Particle Size Dispersity in Dense Packings on the Void Structure and the Interparticle Contact State, Satellite meeting of Statphys 2007: Statics and dynamics of granular media and colloidal suspensions, Naples, Italy, July 2007. (poster)

189. M. Benedict, **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott, Influence of Particle Size Dispersity in Dense Packings on the Void Structure and the Interparticle Contact State, APS March 2007, Denver, USA. (poster)

190. **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott, The Behavior of Ultrafine Particles in the Absence and Presence of External Fields, APS March 2007, Denver, USA. (talk)

191. **M. Dutt**. Ultrafine Particles: a Numerical Model and Their Behavior in the Absence and Presence of External Fields, Summer School on Colloids in external fields: Physics and its Applications, Cargese, France, October 2006. (poster)

192. **M. Dutt**, Y.S. Cheong, B. Hancock, C. Bentham and J. Elliott. Microscopic and Macroscopic Studies of Pharmaceutical Excipient Mixtures, 7th UK Particle Technology Forum, Imperial College, London, UK, September 2006. (poster)

193. **M. Dutt**, M. Benedict, B. Hancock, C. Bentham and C. Bentham. Influence of Particle Size Dispersity in Dense Packings on the Interparticle Contact State, 7th UK Particle Technology Forum, Imperial College, London, UK, September 2006. (poster)

194. **M. Dutt** and R.P. Behringer. Particle-Substrate Models for Cooling and Driven Granular Systems, Gordon Research Conference (GRC) Granular and Granular Fluid 2006, Oxford, UK, July 2006. (poster)

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195. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. Granular templating: effects of boundary structure on particle packings under simultaneous shear and compression, GRC Granular and Granular Fluid 2006, Oxford, UK, July 2006. (poster)
196. **M. Dutt** and R.P. Behringer. A Particle-Substrate Model and Its Applications to Cooling and Driven Granular Systems, American Physical Society (APS) March 2006, Baltimore, USA, March 2006. (poster)
197. C. Bentham, **M. Dutt**, B. Hancock and J. Elliott. Effects of Particle Size Dispersity on the Response to Compressive Strains, APS March 2006, Baltimore, USA, March 2006. (talk)
198. **M. Dutt**, B. Hancock, C. Bentham and J. Elliott. Effect of Relative Material Stiffness of Binary Mixture Components to Compression, APS March 2006, Baltimore, USA, March 2006. (poster)
199. B. Hancock, **M. Dutt**, C. Bentham and J. Elliott. Granular templating: effects of boundary structure on particle packings under simultaneous shear and compression, APS March 2006, Baltimore, USA, March 2006. (poster)
200. **M. Dutt** and R.P. Behringer. Extension of a Particle-Substrate Model to a 2-dimensional Driven Granular System, APS Divison of Fluid Dynamics (DFD), Chicago, USA, November 2005. (talk)
201. M. Benedict, **M. Dutt** and J. Elliott. Porosity Determination in Mesoscale Simulations using Artificial Intelligence Technique, Intelligent Processing and Manufacturing of Materials 2005, Monterey, USA, July 2005. (talk)
202. **M. Dutt** and R.P. Behringer. The Granular Collider: Introduction to a Particle-Substrate Model and the Numerical Experiment, Powders and Grains 2005, Stuttgart, Germany, July 2005. (poster)
203. A.C. Bentham, **M. Dutt**, B.C. Hancock and J.A. Elliott. Effects of Size Polydispersity on Pharmaceutical Particle Packings, Powders and Grains 2005, Stuttgart, Germany, July 2005. (poster)
204. **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott. Studies of Particle Packings in Mixtures of Pharmaceutical Excipients, Powders and Grains 2005, Stuttgart, Germany, July 2005. (poster)
205. B.C. Hancock, **M. Dutt**, A.C. Bentham and J.A. Elliott. Ordered Packing Induced by Simultaneous Shear and Compaction, Powders and Grains 2005, Stuttgart, Germany, July 2005. (poster)
206. **M. Dutt** and R.P. Behringer. The Granular Collider: Particle-Substrate Model and the Numerical Experiment, APS March 2005 meeting, Los Angeles, USA, March 2005. (talk)
207. **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott. Effects of Size Polydispersity on Pharmaceutical Particle Packings, APS March 2005 meeting, Los Angeles, USA, March 2005. (talk)
208. **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott. Studies of Particle Packings in Mixtures of Pharmaceutical Excipients, APS March 2005 meeting, Los Angeles, USA, March 2005. (talk)
209. **M. Dutt**, B.C. Hancock, A.C. Bentham and J.A. Elliott. Ordered Packing Induced by Simultaneous Shear and Compaction, APS March 2005 meeting, Los Angeles, USA, March 2005. (talk)
210. X.W. Fu, G.E. Milroy, **M. Dutt**, A.C. Bentham, B.C. Hancock and J.A. Elliott. Quantitative analysis of packed and compacted granular system by x-ray microtomography, Medical Imaging, SPIE- The International Society for Optical Engineering, San Diego, USA, February 2005. (poster)
211. G. Milroy, **M. Dutt**, C. Wu, C. Bentham, B. Hancock and R. Cameron. Characterising randomly packed and compacted pharmaceutical particulate systems using x-ray microtomography, 7th World Biomaterials Congress 2004, Sydney, Australia, May 2004. (poster)
212. G.E. Milroy, **M. Dutt**, C.Y. Wu, A.C. Bentham, B.C. Hancock, J.A. Elliott and R.E. Cameron. The use of desktop x-ray microtomography to characterize randomly packed and compacted pharmaceutical particulate systems, Materials Congress 2004, London, UK, March 2004. (poster)
213. **M. Dutt**, J. Elliott, C. Bentham and B. Hancock. Characterization studies of spherical particle packings resulting from compaction, APS March Meeting, Montreal, Canada, March 2004. (talk)
214. **M. Dutt**, J. Elliott, C. Bentham and B. Hancock. Studies of spherical particle packings arising from uni-axial compaction, APS March Meeting, Montreal, Canada March 2004. (talk)
215. **M. Dutt**, J. Elliott, S. Best, C. Bentham, B. Hancock and A. Windle. Numerical experiments on packings of spherical particles, workshop on Flow regimes, transitions and segregation in granular & particle-laden flow, Newton Institute of Mathematical Sciences, Cambridge, UK, September 2003. (poster)

216. Chuan-Yu Wu, **M. Dutt**, J. Elliott, S. Best, W. Bonfield, C. Bentham and B. Hancock. Studies on the tabletting process: from grains to tablets, 5th UK Particle Technology Forum, Sheffield, UK, July 2003. (poster)

217. **M. Dutt**, G. Milroy, J. Elliott, R. Cameron, C. Bentham and B. Hancock. Investigating spherical particle packing from free flowing powders using a novel combination of modeling and x-ray microtomography, 5th UK Particle Technology Forum, Sheffield, UK, July 2003. (poster)

218. **M. Dutt** and R.P. Behringer. Numerical Model of a Granular Collider Experiment, APS DFD Meeting, Dallas, USA, November 2002. (talk)

219. **M. Dutt** and R.P. Behringer. Numerical Model of a Granular Collider Experiment, Dynamic Days '02 (DD02), Baltimore, USA, January 2002. (poster)

220. **M. Dutt** and R.P. Behringer. Model for a Horizontally Vibrated Granular System, APS DFD Meeting, San Diego, USA, November 2001. (talk)

221. **M. Dutt** and R.P. Behringer. Models of Dissipation for Grains Rolling on Static and Dynamic Substrates, DD01, Chapel Hill, NC, January 2001. (poster)

222. **M. Dutt** and R.P. Behringer. Models of Dissipation for Grains Rolling on Static and Dynamic Substrates, APS DFD Meeting, Washington, D.C., USA, November 2000. (talk)

223. **M. Dutt** and R.P. Behringer. Models of Dissipation for Grains Rolling on Static and Dynamic Substrates, APS Division of Fluid Dynamics (DFD) Meeting, New Orleans, LA, USA, November 1999. (talk)

224. **M. Dutt** and R.P. Behringer. Models of Dissipation for Grains Rolling on Static and Dynamic Substrates, American Physical Society (APS) South Eastern Section (SES) Meeting, Chapel Hill, USA, November 1999. (talk)

225. **M. Dutt** and R.P. Behringer. Models of Dissipation for Grains Rolling on Static and Dynamic Substrates, APS Centennial Meeting, Atlanta, USA, March 1999. (talk)