## ARTHI JAYARAMAN

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#### **EDUCATION** I.

Birla Institute of Technology and Science (BITS), Pilani India B. E. (Honors) Chemical Engineering	08/1996 - 07/2000
North Carolina State University, Raleigh NC M.S. Chemical and Biomolecular Engineering Ph.D. Chemical and Biomolecular Engineering	08/2000 - 12/2002 12/2002 - 05/2006
University of Illinois, Urbana-Champaign Postdoctoral Research, Material Science and Engineering	06/2006 - 08/2008
II. PROFESSIONAL EXPERIENCE	
Director, NSF-funded NRT graduate traineeship on Computing and Data Science Training for Materials Innovation, Discovery, and Analytics	09/2021 - present
Full Professor with Tenure Department of Chemical and Biomolecular Engineering	09/2019 - present
& Department of Materials Science and Engineering Faculty Council, Data Science Institute University of Delaware, Newark	04/2020 - present
Centennial Term Professor for Excellence in Research and Teaching	09/2020 - 08/2024
Associate Editor, Macromolecules	08/2019 - present
Inaugural Deputy Editor of ACS Polymers Au	01/2021 - 12/2023
<b>Graduate Program Director</b> Department of Chemical and Biomolecular Engineering University of Delaware, Newark	08/2016 - 06/2019
Associate Professor with Tenure Department of Chemical and Biomolecular Engineering & Department of Materials Science and Engineering University of Delaware, Newark	08/2014 - 08/2019
Patten Assistant Professor(received tenure in 06/2014)Department of Chemical and Biological EngineeringUniversity of Colorado (CU), Boulder	11/2011 - 07/2014
Fellow, Materials Science and Engineering Program University of Colorado (CU), Boulder	11/2012 - 07/2014

#### Assistant Professor

Department of Chemical and Biological Engineering University of Colorado (CU), Boulder

### III. HONORS/AWARDS

#### **Professional Society**

- 2021 American Institute of Chemical Engineers (AIChE) Computational Molecular Science and Engineering Forum (COMSEF) IMPACT Award
- 2020 American Physical Society (APS) Fellow
- 2014 American Chemical Society (ACS) Polymeric Materials Science & Engineering (PMSE) Young Investigator
- 2013 AIChE COMSEF Young Investigator Award
- 2010 ACS Women Chemist Committee WCC Lectureship Award

## Lectureship/Federal Grant Agency Career Award

- 2024 Wayne State BASF Distinguished Lectureship
- 2016 Saville Lecturer, Princeton University
- 2010 Department of Energy (DOE) Early CAREER Research Award

## Journals' Emerging Investigator Recognition

- 2018 Featured as an Emerging Investigator in Journal of Chemical & Engineering Data
- 2016 Featured as an Emerging Investigator in *Materials Research Express*
- 2013 Featured as an Emerging Investigator in Soft Matter
- 2013 Featured as an Emerging Investigator in Journal of Polymer Science B: Polymer Physics

## University Recognition - Leadership, Research, & Teaching

- 2024-25 University of Delaware (UD), Selected to be in 1st cohort of Presidential Academic Leadership Program
- 2023 University of Delaware, College of Engineering Faculty Award for Excellence in Teaching
- 2014 Outstanding Faculty Graduate Teaching Award in Dept. of Chemical Engineering Univ. of Colorado, Boulder
- 2014 Outstanding Junior Faculty Award in the Dept. of Chemical Engineering University of Colorado, Boulder
- 2013 Provost's Faculty Achievement Award, University of Colorado, Boulder
- 2011-2012 College of Engineering Dean's Faculty Fellowship, University of Colorado, Boulder
- 2011 Outstanding Faculty Undergraduate Teaching Award, Dept. of Chemical Engineering University of Colorado, Boulder

## IV. RESEARCH EXPERTISE

I have led my team of undergraduate and graduate students and postdoctoral researchers to develop and use molecular models, theory, simulations, and machine learning to design soft materials at the molecular level for a variety of applications. Currently, my team is focused on the following research thrusts

- 1. Machine learning (ML) enabled automated analysis of materials' characterization data
- 2. ML and Artificial Intelligence (AI) for solving chemical industry problems
- 3. Polymer, Composites, Formulations
- 4. Bioderived, bioinspired, biocompatible soft materials

#### V. PEER-REVIEWED RESEARCH PUBLICATIONS

- Total number of publications as author (as of April 10, 2024): 125
- Publications from independent career: 116
- Publications as corresponding author: **109**
- Citations in google scholar

(\* denotes corresponding author, † denotes undergraduate, # denotes equal contributions)

- 125. V. Liao, T. Myers, A. Jayaraman\*, <u>A Computational Method for Rapid Analysis Polymer Structure and Inverse</u> <u>Design Strategy (RAPSIDY)</u> Soft Matter (2024) in press
- 124. S. Park#, T. Myers#, V. Liao, A. Jayaraman\*, <u>Self-Consistent Field Theory and Coarse-Grained Molecular</u> <u>Dynamics Simulations of Pentablock Copolymer Melt Phase Behavior</u> *Molecular Systems Design and Engineering* (2024) in press
- 123. A. Paruchuri, Y. Wang, X. Gu and A. Jayaraman\*, Machine Learning for Analyzing Atomic Force Microscopy (AFM) Images Generated from Polymer Blends, <u>https://arxiv.org/abs/2409.11438</u> (under review in Digital Discovery)
- 122. S. Kronenberger, N. Gupta, B. Gould, C. Peterson, A. Jayaraman\*, <u>Random field reconstruction of three-phase</u> polymer structures with anisotropy from 2D-small-angle scattering data , *Soft Matter* (2024) in press
- 121. J. Madinya, S. Kronenberger, B. Gould, C. Peterson, A. Jayaraman\*, Connecting features of ionomer scattering profiles to the real-space structural features of ionomer domains *Macromolecules* (2024) 57, 16, 8223-8239
- 120. S. Lu, A. Jayaraman\*, <u>Machine Learning for Analyses and Automation of Structural Characterization of Polymer</u> <u>Materials</u>, *Progress in Polymer Science*, (2024) 153, 101828
- 119. S. V. R. Akepati, N. Gupta, A. Jayaraman\*, <u>Computational Reverse Engineering Analysis of Scattering Experiments Method for Interpretation of 2D Small-Angle Scattering Profiles</u> (CREASE-2D) *JACS Au* (2024) 4, 4, 1570–1582
- 118. Z. Wu, A. Collins, A. Jayaraman\*, <u>Understanding self-assembly and molecular packing in methylcellulose aqueous</u> solutions using multiscale modeling and simulation, *Biomacromolecules*, (2024), 25, 3, 1682–1695
- 117. S. Lu, A. Jayaraman\*, <u>Pair-Variational Autoencoders (PairVAE) for Linking and Cross-Reconstruction of Characterization Data from Complementary Structural Characterization Techniques</u> JACS Au (2023) 3, 9, 2510-2521
- 116. J. Ju, A. Jayaraman, R. Hayward\*, <u>Temperature-Sensitive Micro- and Macro-phase Separation of Hydrogen-Bonded Polystyrene-Polydimethylsiloxane Blends</u> *Macromolecules* (2023) 56, 13, 4991–5000
- 115. N. Gupta, A. Jayaraman\*, Computational Approach for Structure Generation of Anisotropic Particles (CASGAP) with Targeted Distributions of Particle Design and Orientational Order, *Nanoscale* (2023) 15, 14958-14970
- 114. Z. Wu, J. Wu, Q. Michaudel\*, A. Jayaraman\*, <u>Investigating the hydrogen bond-induced self-assembly of</u> polysulfamides using molecular simulations and experiments, *Macromolecules* (2023) 56, 13, 5033–5049
- 113. P. Taylor#, S. Kronenberger#, A. Kloxin, A. Jayaraman\*, Effects of Solvent Conditions on the Self-Assembly of Heterotrimeric Collagen-Like Peptide (CLP) Triple Helices: A Coarse-Grained Simulation Study Soft Matter (2023),19, 4939-4953
- 112. Y. Ma, C. M. Heil, G. Nagy, W. Heller, Y. An, A. Jayaraman, B. Bharti\*, <u>Synergistic role of temperature and salinity in aggregation of nonionic surfactant coated silica nanoparticles</u>, *Langmuir* (2023) 39, 16, 5917–5928
- 111. C. M. Heil, Y. Ma, B. Bharti, A. Jayaraman\*, <u>Computational Reverse-Engineering Analysis for Scattering Experiments for Form Factor and Structure Factor Determination ('P(q) and S(q) CREASE')</u> JACS Au (2023), 3, 3, 889–904
- 110. C. M. Heil, A. Patil, B. Vanthournout, S. Singla, M. Bleuel, J-J. Song, Z. Hu, N. Gianneschi, M. Shawkey, S. Sinha, A. Dhinojwala\*, A. Jayaraman\*, <u>Mechanism of Structural Colors in Binary Mixtures of Colloidal</u> <u>Nanoparticle-based Supraballs</u> *Science Advances* (2023), Vol 9, Issue 21

- 109. Z. Wu, A. Jayaraman\*, <u>Machine learning enhanced computational reverse-engineering analysis for scattering experiments (CREASE) for analyzing fibrillar structures in polymer solutions</u>, *Macromolecules* (2022), 55, 24, 11076–11091
- 108. C. M. Heil, A. Jayaraman\*, Polymer solution structure and dynamics within pores in hexagonally close-packed nanoparticles, *Soft Matter* (2022),18, 8175-8187
- 107. S. Lu, B. Montz, T. Emrick, A. Jayaraman\*, <u>Self-supervised machine learning model for analysis of nanowire</u> morphologies from transmission electron microscopy images *Digital Discovery* (2022), 1, 816 – 833
- 106. A. Kulshreshtha, A. Jayaraman\*, <u>Phase Behavior and Morphology of Blends containing Associating Polymers:</u> <u>Insights from Liquid State Theory and Molecular Simulations</u>, *Macromolecules* (2022), 55, 20, 9297–9311
- 105. A. Patil#, C. M. Heil#, B. Vanthournout, S. Singla, Z. Hu, J. Ilavsky, N. C. Gianneschi, M. D. Shawkey, S. K. Sinha, A. Jayaraman,\* and Ali Dhinojwala,\* <u>Modeling structural colors from disordered one-component supraballs using combined experimental and simulation techniques</u> *ACS Materials Letters* (2022), 4, 9, 1848–1854
- 104. U. Kapoor, A. Jayaraman\*, <u>Impact of Polydopamine Nanoparticle Surface Pattern and Roughness on</u> <u>Interactions with Poly (ethylene glycol) in Aqueous Solution: A Multiscale Modeling and Simulation Study</u>, *J. Phys. Chem. B.* (2022), 126, 33, 6301–6313
- 103. C. M. Heil, A. Patil, A. Dhinojwala, A. Jayaraman\*, <u>Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) with Machine Learning Enhancement to Determine Structure of Nanoparticle Mixtures and Solutions</u>, *ACS Central Science* (2022), 8, 7, 996–1007
- 102. P. A. Taylor, A. M. Kloxin\*, A. Jayaraman\*, <u>Impact of collagen-like peptide (CLP) heterotrimeric triple helix</u> design on helical thermal stability and hierarchical assembly: A coarse-grained molecular dynamics simulation study, *Soft Matter* (2022),18, 3177-3192
- 101. A. Kulshreshtha, R. Hayward, A. Jayaraman\*, <u>Impact of Composition and Placement of Hydrogen Bonding</u> <u>Groups along Polymer Chains on Blend Phase Behavior: Coarse-Grained Molecular Dynamics Simulation</u> <u>Study</u>, *Macromolecules* (2022), 55, 7, 2675–2690
- 100. A. Patil #, C. M. Heil #, B. Vanthournout, M. Bleuel, S. Singla, Z. Hu,6 N. C. Gianneschi, M. D. Shawkey, S. K. Sinha, A. Jayaraman\*, A. Dhinojwala\*, <u>Structural Color Production in Melanin-based Disordered Colloidal Nanoparticle Assemblies in Spherical Confinement</u>, *Advanced Optical Materials*, (2022), 10, 5, 2102162
- 99. S. Lu, A. Jayaraman\*, Effect of nanorod physical roughness on the aggregation and percolation of nanorods in polymer nanocomposites, ACS Macro Letters (2021) 10 (11), 1416–1422
- U. Kapoor#, A. Kulshreshtha#, A. Jayaraman\*, <u>Understanding the Effect of Heterogeneous Particle Functionalization on Graft-Matrix Wetting and Structure in Polymer Nanocomposites Containing Grafted Nanoparticles Using Multiscale Modeling and Simulation</u>, *ACS Applied Polymer Materials* (2021) 3 (11), 5642–5655
- 97. Z. Ye, Z. Wu, A. Jayaraman\*, <u>Computational Reverse-Engineering Analysis for Scattering Experiments CREASE</u>) on Vesicles Assembled from Amphiphilic Macromolecular Solutions, *JACS Au* (2021) 1 (11), 1925–1936
- 96. C. M. Heil, A. Jayaraman\*, <u>Computational reverse-engineering analysis for scattering experiments of assembled</u> <u>binary mixture of nanoparticles</u> ACS Materials Au (2021) 1 (2), 140–156
- 95. M. G. Wessels, A. Jayaraman\*, <u>Machine Learning Enhanced Computational Reverse Engineering Analysis for</u> <u>Scattering Experiments (CREASE) to Determine Structures in Amphiphilic Polymer Solution</u>s, *ACS Polymers Au* (2021) 1, 3, 153–164
- 94. X. Zhou, X. Gong, W. Cao, C. J. Forman, J. Okatawiec, L. d'Alba, H. Sun, M. P. Thompson, Z. Hu, U. Kapoor, N. C. McCallum, O. Farha, A. Jayaraman, M. D. Shawkey, and N. C. Gianneschi\*, <u>Anisotropic Synthetic</u> <u>Allomelanin Materials via Solid State Polymerization of Self-Assembled 1, 8-Dihydroxynaphthalene</u> <u>Dimers</u>, *Angewandte Chemie International Edition* (2021) 60, 32, 17464-17471
- 93. A. Jayaraman\*, A. Kulshreshtha, P. Taylor, A. Prhashanna, Coarse-Grained Modeling and Simulations of Thermoresponsive Biopolymers and Polymer Nanocomposites with Specific and Directional Interactions, Foundations of Molecular Modeling and Simulations: Select Papers from FOMMS 2018; Spring Nature (2021)
- 92. S. Lu#, Z. Wu#, A. Jayaraman\*, <u>Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod</u> <u>Fillers</u> J. Phys Chem B. (2021) 125, 9, 2435-2449

- 91. P. Cummings, C. McCabe, C. Iacovella, A. Ledeczi, E. Jankowski, A. Jayaraman, J. Palmer, E. Maginn, S. Glotzer, J. Anderson, I. Siepmann, J. Potoff, R. Matsumoto, J. Gilmer, R. DeFever, R. Singh, B. Crawford, <u>Open-Source</u> <u>Molecular Modeling Software in Chemical Engineering Focusing on the Molecular Simulation Design</u> <u>Framework</u>, *AIChE Journal* (2021) 67, 3, e17206
- 90. A. M. Hilderbrand, P. A. Taylor, F. Stanzione, M. LaRue, C. Guo, A. Jayaraman\*, A. M. Kloxin\*, <u>Combining simulations and experiments for the molecular engineering of multifunctional collagen mimetic peptide-based materials</u>, *Soft Matter* (2021) 17, 1985-1998
- 89. W. Cao, X. Zhou, N. C. McCallum, Z. Hu, Q. Z. Ni, U. Kapoor, C. M. Heil, K. S. Cay, T. Zand, A. J. Mantanona, A. Jayaraman, A. Dhinojwala, D. D. Deheyn, M. D. Shawkey, M. D. Burkart, J. D. Rinehart, and N. C. Gianneschi\*, <u>Unraveling the Structure and Function of Melanin Through Synthesis</u>, *J. Am. Chem. Soc.* (2021) 143, 7, 2622-2637
- 88. S. M. Maguire, N. M. Krook, A. Kulshreshtha, C.R. Bilchak, R. Brosnan, A.M. Pana, P. Rannou, M. Maréchal, K.Ohno, A. Jayaraman\*, R. J. Composto\*, <u>Interfacial Compatibilization in Ternary Polymer Nanocomposites:</u> <u>Comparing Theory and Experiments</u> *Macromolecules* (2020) 54, 2, 797-811
- M. Wessels, A. Jayaraman\*, <u>Computational Reverse Engineering Analysis of Scattering Experiments (CREASE)</u> on <u>Amphiphilic Block Polymer Solutions: Cylindrical and Fibrillar Assembly</u> *Macromolecules* (2020) 54,2, 783-796
- 86. U. Kapoor, A. Kulshreshtha, A. Jayaraman\*, Development of Coarse-Grained Models for Poly (4-vinylphenol) and Poly (2-vinylpyridine): Polymer Chemistries with Hydrogen Bonding, *Polymers*, (2020) 12, 11, 2764
- J. L. Young, Y. Song, M. Wessels, A. Jayaraman\*, K. Wooley\*, D. Pochan\*, Hierarchical Self-assembly of Poly(Dglucose carbonate) Amphiphilic Block Copolymers in Mixed Solvents, *Macromolecules*, (2020) 53, 19, 8581– 8591
- P. A. Taylor, H. Huang, K. Kiick\*, A. Jayaraman\*, Placement of tyrosine residues tunes the lcst-like transition of elp-clp conjugates: Experiments and simulations, *Molecular Systems Design and Engineering*, (2020) 5, 1239-1254
- Z. Wu, D. Beltran-Villegas, A. Jayaraman\*, Development of a new coarse-grained model to simulate assembly of cellulose chains due to hydrogen bonding, *Journal of Chemical Theory and Computation*, (2020) 16, 7, 4599– 4614
- 82. P. A. Taylor, A. Jayaraman\*, Molecular modeling and simulations of peptide-polymer conjugates, *Annu. Rev. Chem. Biomol. Eng.*, (2020) 11, 257-276
- 81. A. Jayaraman\*, Modeling and simulation of macromolecules with hydrogen bonds: Challenges, successes and opportunities, an invited viewpoint in *ACS Macro Letters*, (2020) 9, 656–665
- 80. T. E. Gartner III, C. M. Heil, A. Jayaraman\*, Surface composition and ordering of binary nanoparticle mixtures in spherical confinement, *Molecular Systems Design and Engineering*, (2020) 5, 864-875
- 79. U. Kapoor, A. Jayaraman\*, Self-assembly of allomelanin dimers and the impact of poly(ethylene glycol) on the assembly: a molecular dynamics simulation study, *Journal of Physical Chemistry B.*, (2020) 124, 2702-2714
- 78. A. Kulshreshtha, A. Jayaraman\*, Dispersion and aggregation of polymer grafted particles in polymer nanocomposites driven by the hardness and size of the grafted layer tuned by attractive graft-matrix interactions, *Macromolecules*, (2020) 53, 1302-1313
- 77. M. Wessels, A. Jayaraman\*, Self-assembly of amphiphilic polymers of varying architectures near attractive surfaces, *Soft Matter*, (2020) 16, 623-633 Back cover of this issue
- 76. H. Kuang, T. E. Gartner, M. Dorneles de Mello, J. Guo, X. Zuo, M. Tsapatsis, A. Jayaraman and E. Kokkoli\*, ssDNA-amphiphile architecture used to control dimensions of DNA nanotubes, *Nanoscale*, (2019) 11, 19850-19861
- D. Beltran-Villegas, M. Wessels, J.Y. Lee, Y.Song, K. Wooley\*, D. Pochan\*, A. Jayaraman\*, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions, *J. Am. Chem. Soc.*, (2019) 141, 14916-14930
- 74. T. E. Gartner, III, F. M. Haque, A. M. Gomi, S. M. Grayson\*, M. J. A. Hore\* and A. Jayaraman\*, Scaling Exponent and Effective Interactions in Linear and Cyclic Polymer Solutions: Theory, Simulations, and Experiments, *Macromolecules* (2019) 52, 4579-4589

- 73. M. Xiao, Z. Hu, T. E. Gartner III, X. Yang, W. Li, A. Jayaraman\*, N. C. Gianneschi\*, M. D. Shawkey\*, A. Dhinojwala\*, Experimental and theoretical evidence for molecular forces driving surface segregation in photonic colloidal assemblies, *Science Advances* (2019) 5, 9, eaax1254
- 72. D. J. Beltran-Villegas, D. Intriago<sup>†</sup>, K. Kim, N. Behaptu, J. D. Londono, A. Jayaraman\*, Coarse-grained molecular dynamics simulations of α-1,3-glucan, *Soft Matter*, (2019) 15, 4669-4681
- 71. M. Wessels, A. Jayaraman\*, Molecular dynamics simulation study of linear, bottlebrush, and star-like amphiphilic block polymer assembly in solution, *Soft Matter*, (2019) 15, 3987-3998
- 70. M. Dong, M.G. Wessels, J. Y.Lee, L. Su, H. Wang, R. A. Letteri, Y.Song, Y.N.Lin, Y. Chen, R Li, D. J. Pochan,\* A. Jayaraman,\* and K. L. Wooley\*, Experiments and Simulations of Complex Sugar based Coil brush Block Polymer Nanoassemblies in Aqueous Solution, *ACS Nano*, (2019) 13, 5147-5162
- 69. A. Kulshreshtha, K. Modica<sup>†</sup>, A. Jayaraman<sup>\*</sup>, Impact of hydrogen bonding interactions on graft-matrix wetting and structure in polymer nanocomposites, *Macromolecules*, (2019) 52, 2725–2735
- A. Prhashanna, P. A. Taylor, J. Qin<sup>#</sup>, K. L. Kiick<sup>\*</sup>, A. Jayaraman<sup>\*</sup>, Effect of peptide sequence on LCST-like transition of elastin-like peptides (ELP) and elastin-b-collagen-like peptide (ELP-CLP) conjugates: Simulations and experiments, *Biomacromolecules*, (2019) 20, 1178–1189
- A. Prhashanna, A. Jayaraman\*, Melting Thermodynamics of Oligonucleic Acids Conjugated with Relatively Solvophobic Linear Polymers: A Coarse-Grained Molecular Simulation Study, *J. Polymer Science B: Polymer Physics*, (2019) 57, 1196–1208
- 66. T. E. Gartner, III, A. Jayaraman\*, Modeling and Simulations of Polymers: A Roadmap, an invited perspective article for *Macromolecules*, (2019) 52, 755–786 <u>Listed in the Top 10 Most Read Article in Macromolecules</u> Front cover of this issue
- 65. I. Lyubimov, M. G. Wessels, A. Jayaraman\*, Molecular dynamics simulation and PRISM theory study of assembly in solutions of amphiphilic bottlebrush block copolymers", *Macromolecules,* (2018) 51 (19), 7586–7599
- 64. T. B. Martin\*, T. Gartner, III, R. Jones, C. Snyder\*, A. Jayaraman\*, pyPRISM: A Computational Tool for Liquid-State Theory Calculations of Macromolecular Materials *Macromolecules*, (2018) 51 (8), 2906–2922
- 63. D. J. Beltran-Villegas<sup>#</sup>, I. Lyubimov<sup>#</sup>, A. Jayaraman<sup>\*</sup>, Molecular dynamics simulations and PRISM theory study of solutions of nanoparticles and triblock copolymers with solvophobic end blocks, *Molecular Systems Design & Engineering*, (2018) 3, 453-472
- J. E. Condon, A. Jayaraman\*, Development of Coarse-Grained Model of Collagen-like Peptide (CLP) for Studies of CLP Triple Helix Melting *J. Physical Chemistry B.*, (2018) 122 (6), 1929–1939
- 61. D. J. Beltran-Villegas, A. Jayaraman\*, Assembly of amphiphilic block copolymers and nanoparticles in solution: Coarse-grained molecular simulation study, *Journal of Chemical & Engineering Data*, (2018) 63 (7), 2351– 2367
- 60. T. Gartner III., A. Jayaraman\*, Macromolecular 'size' and 'hardness' drives effective inter-polymer interaction in solvent-swollen polymer blends of varying architecture *Soft Matter*, (2018) 14, 411-423
- J. E. Condon, A. Jayaraman\*, Effect of Oligonucleic Acid (ONA) Design on Assembly of ONA-Star Polymer Conjugates: A Coarse-Grained Molecular Simulation Study *Soft Matter*, (2017) 7,13, 6770-6783
- 58. I. Lyubimow, D. Beltran-Villegas, A. Jayaraman\*, PRISM theory study of amphiphilic block copolymer solutions with varying copolymer sequence and composition *Macromolecules*, (2017) 50 (18), 7419–7431
- 57. K. Modica<sup>†</sup> #, T. B. Martin<sup>#</sup>, A. Jayaraman<sup>\*</sup>, Effect of Polymer Architecture on the Structure and Interactions of Polymer Grafted Particles: Theory and Simulations *Macromolecules*, (2017) 50 (12),4854
- 56. J. E. Condon<sup>#</sup>, T. B. Martin<sup>#</sup>, A. Jayaraman<sup>\*</sup>, Effect of Conjugation on Phase Transitions in Thermoresponsive Polymers: An Atomistic and Coarse-Grained Simulation Study *Soft Matter*, (2017) 13, 2907-2918, Front cover of this issue
- 55. T. B. Martin, A. Jayaraman\*, Using Theory and Simulations to Calculate Effective Interactions in Polymer Nanocomposites with Polymer Grafted Nanoparticles, *Macromolecules*, (2016) 49 (24), 9684–9692
- 54. T. Gartner III, T. H. Epps III\*, A. Jayaraman\*, Leveraging Gibbs Ensemble Molecular Dynamics and Hybrid Monte Carlo/Molecular Dynamics for Efficient Study of Phase Equilibria, *Journal of Chemical Theory and Computation*, (2016) 12 (11), 5501–5510
- A. Ghobadi, A. Jayaraman\*, Effects of Polymer Conjugation on Hybridization Thermodynamics of Oligonucleic Acids, *J. Phys. Chem. B*. (2016)120 (36), 9788

- 52. F. Stanzione, A. Jayaraman\*, Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene glycol (PEG) in Explicit Water, *J. Phys Chem. B* (2016) 120, 4160–4173
- 51. T.B. Martin, A. Jayaraman\*, Tuning the Wetting-Dewetting and Dispersion-Aggregation Transitions in Polymer Nanocomposites using Composition of Graft and Matrix Polymers, *Materials Research Express*, Special Issue on Emerging Investigators in Materials Science, (2016) 3, 034001
- A. Ghobadi, A. Jayaraman\*, Effect of Backbone Chemistry on Hybridization Thermodynamics of Oligonucleic Acids: A Coarse-Grained Molecular Dynamics Simulation Study, *Soft Matter*, (2016) 12, 2276-2287
- 49. A. Ghobadi, R. Letteri, T. Emrick\*, A. Jayaraman\* Dispersing zwitterions within comb polymers for non-viral transfection: Experiments and molecular simulations, *Biomacromolecules*, (2016) 17(2), 546-57
- H. S. Marsh, A. Jayaraman\* Effect of side chain length on the morphology of blends of 2,5-bis(3alkylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) oligomers and fullerene derivatives, *J. Polymer Science B: Polymer Physics*, (2016) 54,1, 89-97 )
- 47. F. Stanzione, A. Jayaraman\*, Computational design of oligopeptide containing poly(ethylene glycol) brushes for stimuli-responsive drug delivery, *J. Phys. Chem B.*, (2015) 119 (42), 13309-13320
- 46. T. B. Martin#, K. I. Mongcopa#, R. Ashkar, P. Butler, R. Krishnamoorti\*, A. Jayaraman\*, WettingDewetting and Dispersion-Aggregation Transitions are Distinct in Mixtures of Polymer Grafted Nanoparticles and a Chemically Dissimilar Polymer Matrix, *J. Am. Chem. Soc.*, (2015) 137 (33), 10624–10631
- 45. R. M. Elder, J. Pfaendtner, A. Jayaraman\*, Effect of hydrophobic and hydrophilic surfaces on the stability of double-stranded DNA, *Biomacromolecules*, (2015) 16 (6), 1862–1869
- 44. H. S. Marsh, A. Jayaraman\*, Effect of additive length and chemistry on the morphology of blends of conjugated thiophenes and fullerene derivative acceptor molecules, *Journal of Polymer Science, Part B: Polymer Physics.*, (2015) 53, 1046-1057
- 43. C. E. Estridge, A. Jayaraman\*, Diblock copolymer grafted particles as compatibilizers for immiscible homopolymer blends, *ACS Macro Letters*, (2015) 4, 155–159
- 42. L. Zhang, F. Liu, Y. Diao, H. S. Marsh, N. Collela, A. Jayaraman, T. P. Russell, S. C. Mannsfeld\*, A. Briseno\*, The good host: formation of discrete fullerene "autobahnen" in well-ordered BTTT Oligomers, *J. Am. Chem. Soc.*, (2014) 136 (52), 18120-18130
- C. E. Estridge, A. Jayaraman\*, Effect of homopolymer matrix on diblock copolymer grafted particle conformation and potential of mean force: a molecular simulation study, *J Polymer Science B: Polymer Physics*, (2015) 53, 76-88 Journal Front Cover Art
- 40. B. Lin, T. Martin, A. Jayaraman\*, Decreasing Polymer Flexibility Improves Wetting and Dispersion of Polymer Grafted Particles in a Chemically Identical Polymer Matrix, *ACS Macro Letters*, (2014) 3, 628–632
- T. Martin, A. Jayaraman\*, Effect of Matrix Bidispersity on the Morphology of Polymer Grafted Nanoparticle filled Polymer Nanocomposites, *J. Polymer Science B: Polymer Physics*, (Special Issue on "Hairy Nanoparticles") (2014) 52, 1661-1668
- 38. C. Estridge, A. Jayaraman\*, Assembly of diblock copolymer functionalized spherical nanoparticles as a function of copolymer composition, *J. Chem Phys*, 140 (14) 144905 (2014)
- R. Elder, A. Jayaraman\*, Simulation Study of the Effects of Surface Chemistry and Temperature on the Conformations of ssDNA Oligomers near Hydrophilic and Hydrophobic Surfaces, *J. Chem Phys*, 140 (15) 155103 (2014)
- 36. H. Marsh, E. Jankowski, A. Jayaraman\*, Controlling the morphology of model conjugated thiophene oligomers through alkyl side chain length, placement and interactions, *Macromolecules* (2014) 47 (8), 2736–2747
- 35. J.J. Roberts, R.Elder, A. Jayaraman, S.J. Bryant\*, Characterization of Matrix Retaining Hydrogels Containing Hyaluronan Binding Peptides, *Biomacromolecules*, (2014) 15 (4), 1132–1141
- 34. V. Ganesan\* and A. Jayaraman\*, Theory and simulation studies of effective interactions, phase behavior and morphology in polymer nanocomposites, Invited peer-reviewed review article to *Soft Matter*, (2014) 10, 13-38
- 33. A. Seifpour, S. Dahl, A. Jayaraman\*, Molecular simulation studies of assembly of DNA-grafted particles- Effect of bidispersity in DNA strand length, *Molecular Simulation*, (2013) 40, 1085-1098
- T. Martin, A. Jayaraman\*, Identifying the ideal characteristics of a polydisperse polymer graft length distribution for maximizing dispersion of polymer grafted nanoparticles in a polymer matrix, *Macromolecules*, (2013) 46 (22), 9144–9150

- R. Elder, A. Jayaraman\* Structure and thermodynamics of ssDNA Oligomers near hydrophobic and hydrophilic Surfaces: A molecular simulation study, *Soft Matter* (2013) 9, 11521-11533
- R. Elder and A. Jayaraman\* Molecular simulations of polycation-DNA binding exploring the effect of peptide chemistry and sequence in nuclear localization sequence based polycations, *J. Phys Chem. B.*, (2013) 117 (40), 11988–11999
- E. Jankowski<sup>#</sup>, H. S. Marsh<sup>#</sup>, A. Jayaraman<sup>\*</sup>, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology, *Macromolecules*, (2013) 46 (14) 5775-5785
- 28. T. Martin, A. Jayaraman\*, Polydisperse Polymer Grafts for Stabilizing Dispersion of Homopolymer Grafted Nanoparticles in Chemically Identical Homoolymer Matrix, Peer-reviewed article for special issue on 'Emerging Investigators in Soft Matter' in *Soft Matter*, (2013) 9 (29), 6876 – 6889
- 27. A. Seifpour, S. Dahl, B. Lin<sup>†</sup>, A. Jayaraman<sup>\*</sup>, Molecular simulation studies of assembly of DNA-functionalized particles- Effect of DNA strand sequence and composition, *Molecular Simulation*, (2013) 39(9)741-753
- 26. A. Jayaraman\*, Polymer Grafted Nanoparticles: Effect of Chemical and Physical Heterogeneity in Polymer Functionalization on Particle Assembly and Dispersion, Invited Peer-reviewed Feature Article for special issue highlighting innovative young polymer researchers in *Journal of Polymer Science B: Polymer Physics* (2013) 51(7), 524–534
- 25. T. Martin, P. Dodd<sup>†</sup>. A. Jayaraman<sup>\*</sup>, Polydispersity in polymer grafts for tuning potential of mean force between polymer grafted nanoparticles in a polymer matrix *Physical Review Letters* (2013) 110, 018301
- 24. T. Martin, C. McKinney<sup>†</sup>, A. Jayaraman<sup>\*</sup>, Effect of monomer sequences and particle monomer interactions on assembly of copolymer grafted nanoparticles' *Soft Matter* (2013) 9, 155-169
- H. Marsh, A. Jayaraman\*, Morphological Studies of Blends of Conjugated Polymers and Acceptor Molecules using Langevin Dynamics Simulations, *J. Polymer Science B: Polymer Physics*, (2013) 51 (1), 64-77
- 22. R. Elder, A. Jayaraman\*, Coarse-grained simulation studies of effects of polycation architecture on structure of the polycation and polycation-polyanion complexes, *Macromolecules* (2012) 19, 8083-8096
- R. Elder, A. Jayaraman\*, Sequence specific recognition of cancer drug-DNA adducts by HMGB1a repair protein, *Biophysical Journal*, (2012) 102, 10, 2331–2338
- 20. A. Jayaraman\* and N. Nair, Integrating PRISM theory and Monte Carlo simulation to study polymer functionalized particles and polymer nancomposites', for a special issue "New developments in Molecular Simulations" *Molecular Simulation*, (2012) 38, 8-9, 751-761
- P. Dodd<sup>†</sup> and A. Jayaraman<sup>\*</sup>, Monte Carlo simulation studies of effects of polydispersity in polymer grafted nanoparticle on chain conformations and grafted layer, *J Polym Sci B: Polymer Physics*, (2012) 50, 10, 694– 705
- R. Elder, A. Jayaraman\*, Role of Conformational Dynamics of DNA with Cisplatin and Oxaliplatin Adducts in Various Sequence Contexts on Binding of HMGB1a Protein: A Molecular Dynamics Simulation Study, *Molecular Simulations*, (2012) 38, 10, 793-808
- 17. R. Elder, T. Emrick, and A. Jayaraman\* Understanding the effect of polylysine architecture on DNA binding using molecular dynamics simulations, *Biomacromolecules*, (2011), 12(11), 3870-9
- T. B. Martin<sup>†#</sup>, A. Seifpou<sup>r#</sup>, A. Jayaraman<sup>\*</sup>, Assembly of copolymer functionalized nanoparticles: A Monte Carlo simulation study, *Soft Matter*, (2011) 7, 5952-5964
- N. Nair, N. Wentzel and A. Jayaraman\*, Effects of bidispersity in grafted chain length on grafted chain conformations and Potential of Mean Force between polymer grafted nanoparticles in a Homopolymer Matrix, *J. Chem Phys*, (2011) 134, 194906
- N. Nair and A. Jayaraman\*, Self-Consistent PRISM Theory-Monte Carlo Simulation Studies of Copolymer Grafted Nanoparticles in a Homopolymer Matrix, *Macromolecules*, (2010) 43 (19), 8251–8263
- A. Seifpour, P. Spicer<sup>†</sup>, N. Nair, A. Jayaraman<sup>\*</sup>, Effect of monomer sequences on conformations of copolymers grafted on spherical nanoparticles: A Monte Carlo simulation study, *J. Chem. Phys.*, (2010) 131, 164901 (2010) (Selected to appear in *Virtual Journal of Biological Physics*)

# Papers 1 – 12 were from my doctoral research with Prof. Carol Hall and Prof. Jan Genzer and postdoctoral research with Prof. Ken Schweizer.

## VI. PROCEEDINGS/BOOK CHAPTERS

- Lu, S.; Jayaraman, A; Machine Learning for Analysis of Structural Characterization chapter in the Book: Digital Transformation of Product Formulations edited by Alix Schmidt and Kristin Wallace, Taylor Francis Publishing 2024
- Jayaraman, A.; Chapter 1: Polymer Reference Interaction Site Model (PRISM) Theory and Molecular Simulation Studies of Polymer Nanocomposites, Book: Theory and Modeling of Polymer Nanocomposites Edited by Lisa Hall and Valeriy Ginzburg, Pages 1-22, Published 2021 Springer Publishing,
- Jayaraman, A.; Kulshreshtha, A.; Taylor, P. L.; Ammu, P.; Chapter: Coarse-Grained Modeling and Simulations of Thermoresponsive Biopolymers and Polymer Nanocomposites with Specific and Directional Interactions, in Molecular Modeling and Simulation, Edited by Jeffrey Errington and Edward J. Maginn Proceedings of Foundations Of Molecular Modeling And Simulation (FOMMS) Published 2021 Springer Publishing

## VII. EDITORIALS

- 1. A. Jayaraman.; A. J Patel, Molecular design and engineering of biomimetic, bioinspired, and biologically derived materials. Editorial for Special Issue in Mol. Syst. Des. Eng. 2020, 5, 599-601.
- 2. As the deputy editor for ACS Polymers Au, I led these editorials with my Assoc. editor Prof. Harm-Anton Klok
  - o Inaugural Editorial for ACS Polymers Au, ACS Polymers Au 1, 1, 4-6 (2021)
  - o ACS Polymers Au's First Issue, ACS Polymers Au 1,1, 1-3 (2021)
  - o Publishing in and reviewing for ACS Polymers Au, ACS Polymers Au 1,3, 131-133 (2021)
  - o ACS Polymers Au recognizes Rising Stars in Polymers in 2021, ACS Polymers Au 2, 1, (2022)
  - o ACS Polymers Au's Most Viewed Papers in 2021, ACS Polymers Au 2,1, (2022)
  - o ACS Polymers Au recognizes Rising Stars in Polymers in 2022, ACS Polymers Au 2, 6, (2022)
  - Editorial for ACS Polymers Au Grand Challenges in Polymers virtual special issue, ACS Polymers Au 3, 1, (2023)
  - o ACS Polymers Au recognizes Rising Stars in Polymers in 2023, ACS Polymers Au 4, (2024)
- 3. As associate editor for *Macromolecules*, I co-authored an editorial on '**Convergence of Artificial Intelligence**, **Machine Learning, Cheminformatics, and Polymer Science** in *Macromolecules*' in August 2024.

## VIII. INVITED SEMINARS AND CONFERENCE PRESENTATIONS (by A. Jayaraman)

- 1. Plenary lecture, European Polymer Congress, Groningen, Netherlands, June 2025
- 2. Seminar, Dept. of Chemical Engineering, University of Kentucky, April 2025
- 3. Invited Talk, ACS Spring Meeting COLL: Colloidal and Soft Metamaterials, March 2025
- 4. Invited Talk, ACS Spring Meeting COMP: Using Artificial Intelligence & Advanced Computing-enabled Tools to Study Biomolecular Assembly, March 2025
- 5. Invited Talk, ACS Spring Meeting PMSE: Advancing Polymer Science: Integrating High Throughput Techniques and Digital Technologies for Sustainability and More, March 2025
- 6. Seminar, Dept. of Chemical Engineering, University of Rochester, February 2025
- 7. Technical Talk and DEI Seminar, Dow Chemical, Collegeville, PA, January 2025
- 8. Seminar, Dept. of Polymer Science and Engineering, University of Southern Mississippi November 2024
- 9. Invited talk, Small-Angle Scattering conference, Taipei Taiwan, November 2024
- 10. Invited talk, Small-Angle Scattering satellite meeting in Kitakyushu, Fukuoka, Japan, October 2024
- 11. Seminar, Macromolecules Innovation Institute, Virginia Tech October 2024
- 12. BASF Distinguished Lecture, Wayne State University, September 2024
- 13. Invited Talk, 'Advances in Machine Learning and Physics-based Modeling for Colloidal Materials', ACS Fall Meeting, Denver, August 2024
- 14. Invited Talk, 'Navigating the Nanoscale: Innovations in Molecular Dynamics Simulations and Machine Learning for Polymeric Materials', ACS Fall Meeting Denver August 2024.

- 15. Speaker, Gordon Research Conference, Organic Electronic Materials, Lucca Italy July 2024
- 16. Keynote speaker, PolyChar 2024, Madrid Spain, May 2024
- 17. Seminar, Dept. of Macromolecular Science and Engineering, Case Western Reserve University, April 2024
- Seminar, 100th year celebration, Dept. of Chemical and Biological Engineering, NC State University, April 2024
- Invited Talk, ACS Spring Meeting: PMSE Centennial: Celebration of Success and New Frontiers in Polymeric Materials Science and Engineering, New Orleans, March 2024
- 20. Invited Talk "Interactive Materials Talks Simulation and Data Driven Material Design" Symposium in Aachen, Germany, March 2024
- 21. Invited Talk, APS March Meeting 2023, 'Computational Design, Understanding, and Discovery of Novel Materials' session, Minneapolis, March 2024
- 22. Seminar, AI+Science Schmidt Fellows Speaker Series at University of Chicago, February 2024
- 23. Panelist, Gordon Research Seminar, Colloidal and Macromolecular Materials, February 2024
- 24. Seminar, Dept. of Chemical Engineering, University of Texas at Austin, January 2024
- 25. Invited talk, AICHE Annual Meeting 2023, Session in honor of Juan De Pablo, November 2023
- 26. Invited talk, AICHE Annual Meeting 2023, Polymer Thermodynamics and Self Assembly. November 2023
- 27. Seminar, Dept. of Materials Science and Engineering, Cornell University, October 19th, 2023
- 28. Seminar, Dept. of Chemical Engineering, NYU, October 13th, 2023
- 29. Seminar, UConn Polymer Program, Institute of Materials Science, September 29th, 2023
- 30. Invited talk, Bayreuth Polymer Symposium, Germany September 17-19th 2023
- 31. Invited talk at the ACS-PMSE/CCS-PD Joint Symposium on Frontiers of Polymer Science and Engineering, ACS Fall Meeting, San Francisco, CA August 2023
- 32. Invited talk at the symposium *Hybrid Functional Materials of Polymers for Inorganic Nanoparticles* (sponsored by PMSE) ACS Fall Meeting, San Francisco, CA, August 2023
- 33. Invited talk, 2023 American Crystallography Association, *Small Angle Scattering To Characterize Structurally Complex Materials*, Baltimore, June 2023
- 34. Invited talk, 2023 ACS Colloids and Surface Science meeting, *Artificial Intelligence in Colloids and Surface Science*, Raleigh NC, June 2023
- 35. Invited talk, 2023 International Polymer Colloid Group conference, June 19-23, 2023, Queen's University, Kingston/Canada
- Invited Talk, Polymers in Water, High Polymer Research Group meeting, Pott Shirgley, UK April 23 27, 2023
- 37. Keynote lecture, NanoBioNYC NRT Launch event, City University of New York (CUNY) April 18 2023
- 38. Seminar, Department of Materials Science and Engineering, University of Virginia, April 10-11, 2023
- 39. Invited talk, Symposium on *Advances in Coarse-Graining and Multiscale Modeling*, ACS (COMP) Spring Meeting, March 26 30 2023 Indianapolis, IN,
- 40. Invited talk, *Chemical Physics at the Middle Scales of Soft Matter* Focus Session, American Physical Society March Meeting, March 6-10, 2023, Las Vegas, NV (given by graduate student Zijie Wu)
- 41. Invited talk, Designing soft matter in and out of equilibrium, Lorentz Center, Oort in Leiden, The Netherlands, Jan 30 Feb 3, 2023
- 42. Seminar, Department of Materials Science and Engineering, Carnegie Mellon University, January 20, 2023
- 43. Plenary Lecture. Equifase 2022 XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, Brazil, October 24-27, 2022
- 44. Invited talk, Digitization Track 2: Artificial Intelligence for Materials Discovery, Innovation Day 2022, Science History Institute, Philadelphia, PA September 13, 2022
- 45. Seminar (virtual), Department of Civil Engineering, Carnegie Mellon University September 23, 2022
- 46. Plenary Lecture, Division of Condensed Matter and Materials Physics, 2022 Canadian Association of Physicists (CAP) Congress, June 2022
- 47. Invited talk, ACS Mid-Atlantic Regional Meeting, Session on *Simulation and Machine Learning of Soft Materials*, June 2022

- 48. Invited talk, ACS Mid-Atlantic Regional Meeting, Session on *Industrial Applications of Molecular simulations* June 2022
- 49. Invited talk, MRS Spring Meeting, Session on Bioinspired Structural Composites—Advances in Experiments, Simulations and AI-Based Design, Simulations, and AI Based Design, May 2022
- 50. Seminar, POLY-PMSE student chapter, University of Minnesota, May 2022
- 51. Seminar, School of Polymer Science and Engineering, University of Akron, April 2022
- 52. Seminar, Dept. of Materials Science and Engineering, UIUC, April 2022
- 53. Invited talk, APS March Meeting DPOLY session on Polymer Nanocomposites, March 2022
- 54. Seminar, Dept. of Chemistry, Stony Brook University, February 2022
- 55. Seminar, Mechanical Engineering and Chemical Engineering, IIT Madras, January 2022
- 56. Plenary Lecture, AIChE Annual Meeting, COMSEF Plenary Session, Boston, MA, November 2021
- 57. Seminar, Dept. of Chemical Engineering, Georgia Tech, November 2021
- 58. Invited talk, TechConnect, Washington DC, October 2021
- 59. Seminar, Dept. of Chemical Engineering, University of Notre Dame, October 2021
- 60. Invited talk, Computing in Engineering forum, University of Wisconsin-Madison, September 2021
- 61. Invited talk, ACS SCIENCE TALKS series featuring editors talking about their science, India, September 2021
- 62. Invited talk, Telluride Science Workshop on Polymer Physics, Telluride CO, June-July 2021
- 63. Invited talk, 'Dynamics in Soft Matter with Emphasis on Complex Fluids' workshop organized by Argonne National Lab for Advanced Photon Source (APS) users, May 2021
- 64. Seminar, Dept. of Chemical Engineering, UMass-Amherst, April 2021
- 65. Seminar, Dept. of Chemistry, University of Delaware, March 2021
- 66. Short course invited lecture, 2021 APS March meeting DPOLY short course on 'Macromolecular Engineering of Formulations', March 2021
- 67. Seminar, Dept. of Chemical Engineering, Mississippi State University, March 2021
- 68. Invited Lecture, AICTE short term course advances in biomaterials and tissue engineering, IIT Madras, India, January 2021
- 69. Invited Talk, International Conference on New Trends in Applied Chemistry, Sacred Heart College, India, December 2020
- 70. Invited talk, MRS Fall/Spring virtual Meeting CT04: Tailored Interphases for High Strength and Functional Composites" 2020
- 71. Invited talk, MRS Fall/Spring virtual Meeting MT04: Materials Theory, Characterization and Data Science, 2020
- 72. Invited talk, One of three speakers highlighted in "100 Years of Polymer Science" virtual symposium organized by Wiley, October 2020
- 73. Virtual Seminar, Department of Chemical Engineering, UIUC, October 2020
- 74. Invited talk, Frontiers in Chemical Engineering Virtual Symposium, Caltech, October 2020
- 75. Invited talk, ACS Fall meeting, COMP division *Multiscale Modeling of Protein and Nucleic Acid Therapeutics* August 2020
- 76. Invited talk, ACS Fall meeting, POLY/PMSE division, Advances in the synthesis, characterization, modeling and application of bottlebrush polymers, August 2020
- 77. Invited talk, Next Generation Synchrotron X-ray Needs in Soft Matter Science, Argonne National Lab, May 2020 Cancelled due to COVID
- 78. Seminar, Department of Chemical Engineering, Caltech May 2020 Cancelled due to COVID
- 79. Invited talk, BASF, April 2020 Virtual seminar
- 80. Invited talk, MRS Spring Meeting 2020, Phoenix, April 2020 Cancelled due to COVID
- 81. Seminar, Department of Chemical Engineering, UMass Amherst, April 2020 Cancelled due to COVID
- 82. Invited talk, ACS Spring Meeting, Philadelphia, March 2020 Cancelled due to COVID
- 83. Invited talk, US-France Polymer Nanocomposites Workshop, Columbia University, March 2020 *Cancelled due to COVID*
- 84. Seminar, Department of Chemical Engineering, Columbia, February 2020

- 85. Invited talk, MRS Fall Meeting 2019, Boston December 2019
- 86. Seminar, Department of Chemical Engineering, Univ. of Buffalo, November 2020
- 87. Invited talk, New Frontiers in Molecular Thermodynamics, AICHE Annual Meeting 2019
- 88. Invited talk, Area 8A (Polymers) Plenary Session, AICHE Annual Meeting 2019
- 89. Invited talk, ARL's Strategic Materials, Temple University, August 2019
- 90. Invited talk, Gordon Research Conference, Polymers, June 2019
- 91. Invited lecture, PPEPPD 2019, Canada, May 2019
- 92. Seminar, School of Polymer Science and Engineering, University of Southern Mississippi, May 2019
- 93. Invited talk, "Multicomponent Block Polymer Systems" session at ACS Spring Meeting, April 2019
- 94. Invited talk, "Using Polymer Sequence to Control Material Properties" session at APS March Meeting, March 2019
- 95. Invited talk, AICHE Annual Meeting Thermodynamics at the nanoscale, Pittsburgh, Oct-Nov 2018
- 96. Invited talk, Frontiers in Molecular Engineering, Chicago Sept 2018
- 97. Invited talk, ACS Fall Meeting, Boston, August 2018
- 98. Plenary lecture, FOMMS 2018 Innovations for Complex Systems, July 2018
- 99. Invited talk, 4th Functional Polymeric Materials Conference, Bahamas, June 2018
- 100.Invited talk, 30th anniversary of the Midwest Thermodynamics and Statistical Mechanics (MTSM) conference June 2018
- 101.Invited talk, Polymer Nanocomposites Workshop, iPRIME meeting, University of Minnesota, May 2018
- 102.Invited talk, STM Global Publishing Conference, Philadelphia, April 2018
- 103.Seminar, Department of Chemical Engineering, BYU April 2018
- 104.Invited talk, ACS Spring Meeting, Polymers with Complex Architecture: From Synthesis to Self-Assembly, March 2018
- 105.Seminar, Department of Chemistry, University of Minnesota, February 2018
- 106.Keynote address, NCSU Department of Chemical and Biomolecular Engineering, Schoenborn Graduate Student Symposium, January 2018
- 107.Seminar, Dept. of Chemical Engineering (students-nominated speaker) Cornell University, Sept 2017
- 108. Invited talk, Telluride Science Workshop on Molecular Engineering in Soft Matter June 2017
- 109. Invited talk, Mid-Atlantic Soft Matter Meeting University of Pennsylvania, May 2017
- 110.Invited talk, Argonne Research Lab, Center for Nanostructured Materials, May 2017
- 111.Invited talk, Pan-American Polymer Science Conference (ACS) in Brazil, Invited Speaker March 2017
- 112. Seminar, Macromolecular Science and Engineering, Case Western Reserve University, March 2017

113.Invited talk, Experimental Station Dupont, January 2017

- 114.Invited talk, AICHE Annual Meeting, Invited-only session to honor Carol Hall, November 2016
- 115. Seminar, University of Pennsylvania, PICS Seminar Series, October 2016
- 116.Seminar, University of Florida, Physical Chemistry Seminar Series, October 2016
- 117.Seminar, University of Akron, Physics Club, October 2016
- 118.Invited talk, ACS Fall Meeting, Philadelphia, August 2016
- 119.Invited speaker, Gordon Research Conference, Polymer Physics July 2016
- 120.Keynote Lecture, PPG-Pitt Innovations in Materials Symposium, May 2016
- 121.Seminar, Dept. of Chemical Engineering, University of Akron, March 2016
- 122.Invited talk, PittConn Meeting, March 2016
- 123.Saville Lecture, Department of Chemical Engineering, Princeton University, March 2016
- 124.ACS Southeast Regional meeting, Multiscale modeling and simulations, November 2015
- 125.Seminar, Nanotechnology Seminar Series, Stevens Institute of Tech, October 2015
- 126.Seminar, Biomedical and Chemical Engg. Syracuse University, September 2015
- 127.Seminar, Chemical Engineering, URhode Island, September 2015
- 128. Invited talk, ACS Fall Meeting, Functional Polymers: Connecting Modeling and Experiment, August 2015
- 129.Invited talk, SPIE Meeting, Physical Chemistry of Interfaces and Nanomaterials, August 2015
- 130.Invited talk, Functional Polymeric Material Conference, Ascot UK 2015
- 131. Invited talk, Telluride workshop on Multiscale modeling in organic electronic materials, July 2015

- 132.Invited talk, Telluride workshop on Polymer Physics, June 2015
- 133.Seminar, Dept. of Chemical Engineering, UC Santa Barbara, April 2015
- 134. Invited talk, ACS Spring Meeting 2015 Design principles for functional macromolecular materials March 2015
- 135. Invited talk, ACS Spring Meeting 2015 Polymer Modeling: Structure, Function, Properties March 2015
- 136.Invited talk, APS March Meeting San Antonio March 2015
- 137.Invited talk, XPV- Excitonic Photovoltaics Telluride science workshop August 2014
- 138.Invited talk NSF-US-Poland Workshop on Thermodynamics of Complex Fluids and Interfaces June 2014
- 139.Invited talk, ACS Spring Meeting 2014, Structure for Function: Rational design of new functional polymeric materials March 2014
- 140.Invited talk, ACS Spring Meeting 2014, PMSE Young Investigators Symposium, March 2014
- 141. Seminar, Dept. of Materials Engineering, Purdue University, February 2014
- 142.Seminar, Center for Molecular Engineering and Thermodyanmics, University of Delaware, Jan 2014
- 143. Invited talk, AICHE Annual Meeting 2013, Modeling and Simulation of Polymers session, November 2013
- 144. Invited award talk, AIChE Annual Meeting 2013, COMSEF Plenary Session, November 2013
- 145.Invited talk, APS meeting, Four Corners section, October 2013
- 146.Seminar, Tulane University, Department of Chemical Engineering, September 2013
- 147.Invited talk, ACS Fall Meeting, Indianapolis, September 2013
- 148. Invited talk, APS March Meeting in 'Directed Assembly of Hybrid Materials' session March 2013
- 149.Invited talk, Army Research Laboratory, Aberdeen Proving Ground, Maryland, March 2013
- 150.Invited speaker, Gordon Research Conference Macromolecular Materials, January 2013
- 151.Seminar, Department of Material Science and Engineering, University of Delaware, December 2012
- 152. Invited talk, AICHE Annual Meeting 2012, invited talk in Thermodynamics of Polymers' session
- 153.Invited talk, AICHE Annual Meeting 2012, invited talk in *Emerging Areas in Polymer Science and Engineering* session
- 154. Invited talk, AICHE Annual Meeting 2012, invited talk in Multiscale Modeling and Simulation for Renewable Energy session
- 155.Seminar, Department of Chemical Engineering, University of Washington, October 2012
- 156. Seminar, Chemistry Department, Colorado State University, September 2012
- 157.Seminar, Chancellor's Invitation to present to CU Alumni and friends, September 2012
- 158.Seminar, Molecular Biophysics Seminar Series, Institute of Computational Engineering and Sciences, University of Texas at Austin, April 2012
- 159. Invited talk, ACS Spring National Meeting COMP division Integration of Computer Simulation with Experiments March 2012
- 160.Seminar, Department of Chemical Engineering, Colorado School of Mines, January 2012
- 161. Seminar, Liquid Crystal Materials Research Center, CU Boulder January 2012
- 162. Seminar, Department of Polymer Engineering, University of Akron, Ohio, November 2011
- 163.Seminar, "Young Investigators in Materials Research" UMass Amherst Materials Research Science & Engineering Center (MRSEC) May 2011
- 164.Seminar, Dept. of Chemical Engineering, Rice University, March 2011
- 165.Seminar, Dept. of Chemical Engineering, Texas A&M University, February 2011
- 166.Seminar, Dept. of Materials Science and Engineering, University of Illinois at Urbana, February 2011
- 167.Seminar, Dept of Chemical Engineering, Vanderbilt University, November 2010
- 168.Seminar, Dept. of Applied Math, University of Colorado Boulder, November 2010
- 169.Invited talk, Interfacial Phenomena in Nanostructured Materials and Devices, Telluride Workshop February 2010
- 170.Seminar, Dept. of Chemical Engineering, Colorado State University, October 2009
- 171.Seminar, Condensed Matter Lunch, Dept. of Physics, University of Colorado, Boulder, September 2008

## X. TEACHING - both undergraduate as well as graduate-level core and elective courses

## (2014 - present) at UNIVERSITY OF DELAWARE

- Fall 2014 Introduction to Polymer Science and Engineering CHEG600/MSEG630 (40 students) co-taught with Prof. April Kloxin
- Fall 2015 Introduction to Polymer Science and Engineering CHEG600/MSEG630 (47 students) co-taught with Prof. April Kloxin
- Spring 2016 Introduction to Chemical Engineering CHEG 112 (139 students) co-taught with Prof. Christopher Roberts.
- Fall 2016 Introduction to Polymer Science and Engineering CHEG600/MSEG630 (48 students)
- Spring 2017 Introduction to Chemical Engineering CHEG 112 (135 students) co-taught with Prof. Joshua Enszer
- Fall 2017 Chemical Engineering Lab II Distillation CHEG 445 (69 students)
- Spring 2018 Introduction to Chemical Engineering CHEG 112 (122 students) co-taught with Prof. Joshua Enszer
- Fall 2018 Chemical Engineering Lab II Distillation CHEG 445 (60 students)
- Spring 2019 Molecular Modeling and Simulation of Soft Materials CHEG 867/667 (15 students)
- Fall 2018 Chemical Engineering Lab II Distillation CHEG 445 (35 students)
- Spring 2019 Molecular Modeling and Simulation of Soft Materials CHEG 667/867 (14 students)
- Fall 2019 Chemical Engineering Lab II Distillation Lab CHEG 445 (30 students)
- Spring 2020 Random Variability in Chemical Engineering CHEG 304 (101 students) co-taught with Prof. Joshua Enszer.
- Fall 2020 and Spring 2021 on AY 2020-21 Sabbatical
- Fall 2021 Chemical Engineering Lab II Distillation Lab CHEG 445 (65 students)
- Spring 2022 Computing and Data Science for Soft Materials Innovation and Design CHEG 867-015 (total 15 students) co-taught with CISC 867-015 Prof. Sunita Chandrasekaran
- Fall 2022 Molecular Modeling and Simulation of Soft Materials CHEG 867-010/667-010 (total 22 students- from UD and Delaware State University)
- Spring 2023 Computing and Data Science for Soft Materials Innovation and Design CHEG/CISC/ECEG/MSEG 867-015 (total 14 students including 2 students from Delaware State University)
- Fall 2023 Molecular Modeling and Simulation of Soft Materials CHEG 847-010/647-010 (total 16 students- from UD and Delaware State University)
- Spring 2024 Computing and Data Science for Soft Materials Innovation and Design CHEG/CISC/ECEG/MSEG 848 (total 17 students including 2 students from Delaware State University)
- Fall 2024 Molecular Modeling and Simulation of Soft Materials CHEG 847-010/647-010 (total 18 students- from UD and Delaware State University)

## (2008-2014) at UNIVERSITY OF COLORADO, BOULDER

- Fall 2008 Materials and Energy Balances CHEN2120 (48 students) 3 credits
- Spring 2009 Process Control CHEN4570 (64 students) 4 credits
- Spring 2010 Process Control CHEN4570 (1 section of lecture, 2 sections of lab) (69 students) 4 credits
- Spring 2011 Process Control CHEN4570-01 (1 section lecture, 1.5 sections of lab) (49 students) 4 credits
- Spring 2011 Process Control CHEN4570-02 (1 section lecture, 1.5 sections of lab) (47 students) 4 credits
- Spring 2012 Process Control CHEN4570-01 (1 section lecture, 1.5 sections of lab) (52 students) 4 credits
- Spring 2012 Process Control CHEN4570-02 (1 section lecture, 1.5 sections of lab) (50 students) 4 credits
- Fall 2012 CHEN5838 Molecular Modeling and Simulation of Materials and Biological Systems (15 students) 3
- Spring 2013 Process Control CHEN4570 (1 section lecture, 2 sections of lab, 2 sections of recitation) (81 students)
   4 credits
- Fall 2013 Analytical Methods Chemical Engineering CHEN5740 (1 section lecture) (25 students)

Spring 2014 Process Control CHEN4570 (1 section lecture, 2 sections of lab, 2 sections of recitation) (94 students)

 4 credits

## XI. RESEARCHERS SUPERVISED (08/2008 – present) (UD- University of Delaware; CU=University of Colorado)

<b>GRADUATE</b>	<u>STUDENTS</u>		
Name	Dept./Univ.	Title (Current Position)	Period
Will Dodd	CBE (UD)	M.S. student with coursework	01/2024-05/2024
Pavan Revva	Robotics	M.S. Robotics student	01/2024-05/2024
Vinson Liao	CBE (UD)	PhD student	01/2024 - current
Aanish Paruchuri	Data Science	M.S. Data Science student	09/2023 - current
Tristan Myers	CBE(UD)	PhD student	09/2023 - current
Lalith Nagidi	Data Science	M.S. Data Science student	08/2023-08/2024
Sri Vishnu Reddy Akepati	Data Science	M.S. Data Science student	05/2023 - current
Audrey Collins	Chem (UD)	PhD student, CBI fellow	03/2023 - current
Erik Anderson	CBE(UD)	PhD student, NRT fellow	01/2023-08/2024
Shweta Burgula	CBE(UD)	M.S. degree with coursework only	01/2023-08/2024
Jay Shah	CBE(UD)	PhD student, NRT fellow	01/2023 - current
Stephen Kronenberger	CBE (UD)	PhD student, NRT fellow	01/2022 - current
Shizhao Lu	CBE (UD)	PhD 2024	01/2020-03/2024
Jihyuk Kim	CBE (UD)	MS student (main advisor: Norm Wagner)	01/2020-05/2023
Zjie Wu	CBE (UD)	PhD 2023	01/2019-12/2023
Christian Heil	CBE (UD)	PhD 2023	01/2019-02/2023
Phillip Taylor	CBE (UD)	PhD 2022 (co-advisor: April Kloxin)	05/2018-06/2022
Arjita Kulshreshta	CBE(UD)	PhD 2022	01/2018-05/2022
Michiel Wessels	CBE (UD)	PhD 2021	01/2017-06/2021
Thomas Gartner	CBE (UD)	PhD 2019	01/2015-07/2019
Joshua Condon	CBE (UD)	MS with thesis 2017	07/2015-12/2017
Tyler Martin	ChBE (CU)	PhD 2016	01/2012-05/2016
Ryan Friedrich	CBE (UD)	One year of graduate course work	01/2015-06/2015
Hilary Marsh	ChBE (CU)	PhD 2015	01/2011-05/2015
Carla Estridge	Chem (CU)	PhD 2015	01/2013-04/2015
Daniel Johnson	ChBE (CU)	MS 2014	01/2013-05/2014
Robert Elder	ChBE (CU)	PhD 2014	01/2010-12/2013
Alex Van Fosson	ChBE (CU)	MS with thesis 2013	01/2012-06/2013
Arezou Seifpour	ChBE (CU)	PhD 2013	06/2009-01/2013
Charles Starbird	ChBE (CU)	MS 2012	01/2011-06/2012
Mohamed Seyam	ChBE (CU)	MS 2011	01/2009-06/2011

#### **UNDERGRADUATE STUDENTS**

<u>Name</u>	<u>Department</u>	<u>Title</u>	Period
Nina Borodin	CHEM (UD)	Undergrad research	09/2023 -present
Kaveri Shrivatsava	CBE (UD)	Undergrad research	08/2023-05/2024
Shivam Chauhan	CBE (UD)	Undergrad research	01/2022-02/2022
Geoffrey Bonanzino	CBE (UD)	Undergrad research	05/2020-05/2022
Ryan Tarr	CBE (UD)	Undergrad research	01/2021-05/2021
Chandler Amato	CBE (UD)	Undergrad research	06/2018-06/2020
Daniel Intriago	CBE (UD)	Undergrad research	01/2017-05/2019

Christopher Johnson	CBE (UD)	Undergrad research	06/2018-05/2020
Paul Blanchard	Penn State	REU Undergrad Research	06/2016-08/2016
Kevin Modica	CBE (UD)	Undergrad research	06/2016-05/2019
Christopher Knieste	CBE (UD)	Undergrad research	01/2015-12/2015
Sloane McNeill	AppMath (CU)	Undergrad summer research	05/2014-07/2014
Anna Mcleland	ChBE (CU)	Undergrad Senior Thesis	08/2013-05/2014
Brandon Lin	ChBE (CU)	Undergrad Senior Thesis, MS thesis	08/2011-05/2014
Melika Ashtiani	ChBE (CU	Undergrad research	06/2013-05/2014
Paul Dodd	ChBE (CU)	Undergrad Senior Thesis	08/2010-05/2012
Xiao Ba	ChBE (CU)	Undergrad Senior Thesis	06/2011-07/2012
Gilberto Haro	ChBE (CU)	Undergrad Independent study	01/2012-05/2012
Chris Mckinney	ClarksonU	Undergraduate REU student	06/2011-08/2011
Tyler Martin	ClarksonU	Undergraduate REU student	06/2010-08/2010
Philip Spicer	ChBE (CU)	Undergraduate Research Asst.	04/2009-12/2009
Owen Lewis	Math (CU)	Undergraduate Research Asst	05/2009-08/2009
Audrey Schaiberger	ChBE (CU)	Undergraduate Independent study	08/2008-12/2008

#### POSTDOCTORAL RESEARCHERS

Name	Title (Current Position)	Period
Rohan Adhikari	Postdoc	05/2024 - current
Sojoung Park	Postdoc	09/2023 - current
Jason Madinya	Postdoc	09/2022 - current
Nitant Gupta	Postdoc	02/2022 - current
Umashankar Erigi	Postdoc (unknown)	12/2021-08/2022
Ziyu Ye	Postdoc (unknown)	08/2020-08/2021
Utkarsh Kapoor	Postdoc (currently Asst. Prof. Univ. of Wyoming)	02/2019-06/2021
Prasanna Ammu	Postdoc (currently at Corning)	07/2017-05/2019
Daniel Beltran-Villagas	Postdoc (currently at Jannsen, Johnson & Johnson)	11/2016-07/2019
Ivan Lyubimov	Postdoc (unknown)	09/2016-05/2019
Ahmadreza Ghobadi	Postdoc (currently at P&G)	08/2014-08/2016
Francesca Stanzione	Postdoc (currently at Cambridge)	02/2014-03/2016
Renfeng Hu	Postdoc (unknown)	09/2013-05/2014
Eric Jankowski	Postdoc (currently Prof. Boise State University)	08/2012-03/2014
Dongsheng Zhang	Postdoc (last known UT Dallas postdoc)	06/2010-09/2011
Nathaniel Wentzel	Postdoc (currently Milligen as Instructor)	07/2010-05/2011
Steven Dahl	Postdoc @50% appointment (last known BP)	01/2010-03/2011
Nitish Nair	Postdoc (currently at Shell)	06/2009-12/2010

#### COMPLETED DOCTORAL and MASTER'S DEGREES and THEIR LAST KNOWN PLACEMENT

Ms. Arezou Seifpour PhD 2013 –Auxon Corporation Mr. Robert Elder Phd 2014 – Food and Drug Administration Mr. Alex Van Fosson MS 2013 -OSISoft Mr. Charles Starbird MS 2012 –Eastman Mr. Mohamed Seyam MS 2011 –BioGen Idec Mr. Brandon Lin MS 2014 –Shell Ms. Carla Estridge PhD 2015 –Boeing Ms. Hilary Marsh PhD 2015 – Ch2M Hill Ms. Tyler Martin PhD 2016- NIST Scattering Scientist Mr. Joshua Condon MS 2017 – Capitol One Mr. Thomas Gartner PhD 2019 – Asst. Prof. Georgia Tech Mr. Michel Wessels PhD 2021 – Siemens, USA Ms. Arjita Kulshreshta PhD 2022 – Dow Chemicals, Michigan, USA Mr. Phillip Taylor PhD 2022 – Sandia National Lab (Postdoc), Asst. Prof. University of Virginia (Fall 2024) Mr. Christian Heil PhD 2023 – Dow Chemicals, Pennsylvania, USA Mr. Zijie Wu PhD 2023 – Oak Ridge National Laboratory, USA Mr. Shizhao Lu PhD 2024 – Lawrence Berkeley National Laboratory, USA

#### XII. RESEARCH AWARDS TO GRADUATE STUDENTS MENTORED

Robert Elder	Univ. of Colorado Max Peters award for Outstanding Doctoral Thesis 2013
	ACS Peter Kollman award for Supercomputing 2011
	AICHE COMSEF outstanding graduate student award 2013
Hilary Marsh	Excitonic Photovoltacis (XPV) Best Research Poster award 2014
	MRS Fall meeting 2014 Best Oral Research Presentation (Symposium Q)
Tyler Martin	Finalist of "Excellence in Polymer Graduate Research" AICHE Annual Meeting 2015
	Finalist in "Padden symposium for Excellence in Graduate Research" APS Meeting 2016
Joshua Condon	Best Poster Award, PMSE Division, ACS Fall Meeting 2016
Thomas E. Gartner	1st place award MESD poster competition, AICHE Annual Meeting 2017
	Winner of "Excellence in Polymer Graduate Research" AICHE Annual Meeting 2018
	Finalist in "Padden symposium for Excellence in Graduate Research" APS March Meeting 2019
Arjita Kulshreshtha	Best poster award at the DARWIN Computing Symposium 2021,
,	University of Delaware Doctoral Fellowship 2021
	Richard Wool Outstanding Woman Graduate Student in Green Engineering 2020 2021 3M RISE program participant
	Finalist in "Excellence in Polymer Graduate Research" Area 08A: AICHE Annual Meeting 2021
	Finalist in "Padden symposium for Excellence in Graduate Research" APS March Meeting 2022
Phillip Taylor	Best talk award for MRS 2021 Spring meeting SM09: Peptide and Protein Design
- •	for Responsive Materials symposium
	1 <sup>st</sup> place in 'Outstanding Biomaterials Graduate Research' Area 08B: AICHE Annual Meeting 2021
Zijie Wu	Finalist in "Padden symposium for Excellence in Graduate Research" APS March
	Meeting 2023
	Finalist in "Excellence in Polymer Graduate Research" Area 08A AICHE Annual
	Meeting 2023

#### XIII. PROFESSIONAL SERVICE ACTIVITIES (2008—present)

#### Editorial Board/Editorial Advisory Boards

- Deputy Editor, *ACS Polymers Au* (01/2021 12/2023)
- Associate Editor, *Macromolecules* (08/2019 present)
- Editorial advisory board of *JACS Au* (01/2025 )
- Editorial advisory board of ACS Polymers Au (01/2025 )
- Editorial advisory board of Journal of Polymer Science B: Polymer Physics (August 2018 present)

- Editorial advisory board of Molecular Systems Design and Engineering (March 2017- present)
- Editorial Board, Polymer Theory and Simulation section, Polymers (2020 2022)
- Editorial Board, Theory & Simulation, Current Opinion in Colloids and Interface Science (2020 2021)
- Editorial Advisory Board of Macromolecules and ACS Macro Letters (2015- 2018)

## Meetings, conferences, workshops

- Elected chair for Gordon Research Conference (GRC) Polymer Physics in July 2026
- Vice chair for Gordon Research Conference (GRC) Polymer Physics in July 2024
- During my sabbatical year: I planned and organized 'Women ExceLling in COmputational Molecular Engineering (WELCOME)' virtual monthly seminar series (Sept 2020 May 2021)
- Discussion Leader for Gordon Research Conference (GRC) Polymer Physics in July 2020
- Co-Organizer of Telluride Science Workshop on Molecular Engineering of Soft Matter June 2019
- Meeting chair of the 2018 Department of Energy (DOE) Basic Energy Sciences Materials Chemistry PI meeting in Washington DC area, July 2018
- Discussion Leader for Gordon Research Conference (GRC) Polymer Physics in July 2018
- Session co-chair for one of the sessions at the Fundamental of Molecular Modeling and Simulations (FOMMS) in July 2018
- Co-Organizer of Telluride Science Workshop on Molecular Engineering of Soft Matter June 2017
- Co-Organizer of American Physical Society (APS) March Meeting 2018 symposia on Advancing Polymer Physics by Integrating Simulation and Theory
- Co-Organizer of American Chemical Society (ACS) Fall Meeting 2017 symposia on Simulations of Polymer Systems Molecular to Macroscale.
- Discussion Leader for GRC Complex, Active and Adaptive Matter, January 2017
- Chair for "Nanoscale structure in polymer systems" at AIChE Annual Meeting 2016
- Co-Organizer of ACS Fall 2016 symposia on Recent Advances in Modeling and Simulation of Synthetic and Biopolymers
- Chaired the Excellence in Graduate Polymer Research Award (AICHE Area 08A polymers) committee 2015
- Elected to Chair for Gordon Research Conference Macromolecular Materials 2019 (meeting cancelled by GRC council)
- Co-chair for "Emerging Areas in Polymer Science" plenary at AIChE Annual Meeting 2013
- Chair for "Condensed Matter -I" session at APS Four Corners Meeting 2013
- Chair for "Modeling and Simulation of Polymers II" session at AIChE Annual Meeting 2012
- Co-Chair for "Thermodynamics and Phase Behavior V" session at AIChE Annual Meeting 2012
- Co-Chair for "Thermodynamics of Polymers" session at AIChE Annual Meeting 2011
- Chair of Macromolecular, Supramolecular and Nanotechnology Polymer Chemistry Symposium: Young
   Polymer Chemists, Session at IUPAC 2011
- Chair of Materials session at DOE SciDAC 2011
- Discussion leader at Gordon Research Conference- Macromolecular Materials January 2011
- Invited panelist at NSF Workshop on Computational Energy Research, Palm Desert CA April 2010
- Chair for "Thermodynamics of Polymers" session at AIChE Annual Meeting 2009
- Co-Chair for "Soft Materials and Complex fluids" at FOMMS 2009
- Chair for "The Physics of Polymer Nanocomposites: Grafting and Dispersion' session at APS March Meeting 2009

- Chair for 'Modeling of Colloidal Assembly and Photonic Structures in Liquid Crystals' session in LC2CAM (Light-Controlled Liquid Crystal Complex Adaptive Materials) -Boulder International Workshop 2008
- Chair for 'Theory and Simulation I' session at APS March Meeting 2008
- Co-chair for 'Thermodynamics of Polymers' session at AIChE Annual Meeting 2007

#### Professional Society and Other Advisory Boards

- Served on DPOLY Nomination Committee (2020 2021)
- Serving on Advisory Board for UPenn-Grenoble REACT center grant (2015- 2020)
- Elected "Member at Large" Division of Polymer Physics (DPOLY), Executive Committee, APS (20172020)
- Served on Planning Committee of Symposium of Thermophysical Properties 2014-2018
- Served on Education Committee of APS DPOLY division 2014-2017
- Elected Liason Director for COMSEF division of AICHE (2010-2012)
- Elected Member-Elect for Area 01a AICHE Annual meeting (2010)

#### Reviewer for

- Journals: Journal of American Chemical Society (JACS), Biomacromolecules, ACS Nano, ACS Macro Letters, Soft Matter, Macromolecules, Langmuir (earned the placed as one of top 20% of reviewers in 2010), Journal of Chemical Physics, Fluid Phase Equilibria, Journal of Physical Chemistry, Journal of Computational Chemistry, Journal of Chemical Theory and Computation, Journal of Polymer Science B: Polymer Physics, Biophysical Journal, Physica E, BMC Bioinformatics, Macromolecular Theory and Simulations, Science Advances, Physical Review Letters, ACS Applied Materials and Interfaces, Polymer.
- <u>Grant agencies</u>: National Science Foundation (NSF)-DMR, CBET, Department of Energy- Early Career Award, American Chemical Society - Petroleum Research Fund grants, GACR – Grantová agentura České republiky - Czech Science Foundation grants, University of Houston – GEAR program, University of Colorado Innovative Seed Grants

#### Member of

• American Institute of Chemical Engineers, American Physical Society, American Chemical Society, Materials Research Society

## XIV. UNIVERSITY of DELAWARE SERVICE – DEPARTMENT & COLLEGE (2014-)

#### NRT Graduate Traineeship

- Director of NRT program (Fall 2021 present) <u>Computing and Data Science Training for Materials</u>
   <u>Innovation, Discovery, and Analytics</u>
- Chair of NRT Program Coordination staff search committee (Fall 2021)
- NRT Trainees Admissions Committee chair (Fall 2021 present)
- NRT Trainees' Technical Training Planning chair (Fall 2021 present)
- NRT Trainees' Professional Development Planning chair (Fall 2021 present)
- NRT Weekly Community Hours Planning & Organization (Spring 2022, 2023, 2034)
- NRT appointed secondary thesis advisor to several NRT graduate students in COE departments:
  - o George Kramarenko (UD Biomedical Engineering, Emily Day primary advisor,
  - o Kayla Hapler (UD Materials Science and Engineering, Charles Dhong primary advisor),
  - o Peter Osazuwa (UD Materials Science and Engineering, Laure Kayser, primary advisor)

- o Kelsey Koutsoukos (UD Materials Science and Engineering, Laure Kayser primary advisor),
- o Justin Lombard (UD Elec and Computer Engineering, Austin Brockmeier primary advisor),
- o Leonardo Pierre (DSU Applied Physics, Q. Lu primary advisor)

### Department of Chemical and Biological Engineering (University of Delaware)

- Member of Graduate Education Committee (2023 current)
- Chair of Faculty Search Committee (Fall 2019- Spring 2020)
- Director of Graduate Program (Fall 2016-Summer 2019)
- Member of Graduate Admissions Committee (2014-2016)
- Member of Faculty Search Committee (2015-2016)
- Overseeing Fraser Russell's Enrichment Fund Undergraduate Research (2015-2016)
- Member of Instructor search committee (Fall 2014)

## Department of Materials Science and Engineering (University of Delaware)

- Member of CIS-MSEG joint faculty position search committee (Fall 2022-Spring 2023)
- Member of Chair search committee (Spring 2022)
- Member of materials theory faculty search committee (2014-15)

#### College of Engineering (University of Delaware)

- Member of Dean Search Committee (AY 2024 current)
- Member of Dean Search Committee (AY 2023 2024)
- Member of Diversity in Graduate Programs Committee, College of Engineering (2016-2017)

## Data Science Institute (University of Delaware)

- Faculty council member (2020 present)
- Member of DSI Training Working Group (2022 present)
- Executive Committee Member for DiCoS (Data Science and Computational Science) initiative
- Organizer of DARWIN day (02/2020) to inaugurate DARWIN Supercomputer on UD campus

## University (University of Delaware)

- Member of the College of Engineering Dean Search Committee (AY 2023 2024)
- Elected Member of Graduate College Council (AY 2022-present)
- Elected Member of Graduate College Council (AY 2019-2020)
- Member of search committee for Grants Facilitator, Research Office, University of Delaware

## XV. UNIVERSITY of COLORADO SERVICE -DEPARTMENT & COLLEGE (2008-2014)

## University of Colorado (CU) - Boulder

- Member of College of Engineering Diversity Action Committee (2009-2012)
- Member of CU- Materials Science and Engineering Program Task Force (2010-2012)
- Member of CU- Materials Science and Engineering Program Faculty Search Committee (2010-11)
- Organizer for CU Materials Science and Engineering Program Seminar Series (01/2013-)

#### Department of Chemical and Biological Engineering (CU Boulder)

- Member of Graduate Committee (2012-14) leading graduate recruiting, involved in graduate admissions, deciding Patten distinguished seminar speaker
- Member of Faculty search committee (2011-12)
- Member of Department Leadership Committee (2011-12) (2012-13)
- Member of Chair Search Committee (2010-11)
- Lead Department Visibility Committee (2009-2010, 2010-2011) organized department reception at AIChE meeting, fall town hall meeting, department faculty lunch seminars, department website and presentations
- Lead Teaching Planning Committee (2009-2010)- headed a committee to plan for managing large laboratory classes
- Member of Graduate Students Recruiting Committee (2008-2009) Member of Doctoral thesis committee:
- Undergraduate Freshman Advisor (2008-2009) Undergraduate Sophomore Advisor (2009-2010), Undergraduate Junior Advisor (2010-2011)