ARTHI JAYARAMAN

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University webpage: https://cbe.udel.edu/people/faculty/arthij/ Research lab webpage: https://sites.udel.edu/arthij/

I. EDUCATION

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 08/2000 - 12/2002
Ph.D. Chemical and Biomolecular Engineering 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 09/2021 - present
Computing and Data Science Training for Materials Innovation, Discovery, and Analytics

Full Professor with Tenure 09/2019 - present
Department of Chemical and Biomolecular Engineering
& Department of Materials Science and Engineering
Faculty Council, Data Science Institute 04/2020 - present
University of Delaware, Newark

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

Graduate Program Director 08/2016 - 06/2019
Department of Chemical and Biomolecular Engineering
University of Delaware, Newark

Associate Professor with Tenure 08/2014 - 08/2019
Department of Chemical and Biomolecular Engineering
& Department of Materials Science and Engineering
University of Delaware, Newark

Patten Assistant Professor (received tenure in 06/2014) 11/2011 - 07/2014
Department of Chemical and Biological Engineering
University of Colorado (CU), Boulder

Fellow, Materials Science and Engineering Program 11/2012 - 07/2014
University of Colorado (CU), Boulder

Assistant Professor 08/2008 - 07/2014
Department of Chemical and Biological Engineering
University of Colorado (CU), Boulder

III. HONORS/AWARDS

Professional Society / Federal Agency

- 2025 American Chemical Society (ACS) Polymeric Materials Science & Engineering (PMSE) Fellowship
- 2021 American Institute of Chemical Engineers (AIChE) Computational Molecular Science and Engineering Forum (COMSEF) IMPACT Award
- 2020 American Physical Society (APS) Fellow
- 2014 ACS PMSE Young Investigator
- 2013 AIChE COMSEF Young Investigator Award
- 2010 ACS Women Chemist Committee WCC Lectureship Award
- 2010 Department of Energy (DOE) Early CAREER Research Award

Lectureship

- 2025 Indian Institute of Sciences (IISc), Chemical Engineering, inaugural "R Kumar Distinguished Visitor"
- 2025 Dow Collegeville Asian Diversity Network Lectureship
- 2024 Wayne State BASF Distinguished Lectureship
- 2016 Saville Lectureship, Princeton University

Publishers/Journals Recognition

- 2025 Featured as *Women We Admire*'s Top 50 Women Leaders in Delaware
- 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 Selected to be in 1st cohort of UD's *Presidential Academic Leadership Program,* Univ. of Delaware
- 2023 College of Engineering Faculty Award for Excellence in Teaching, Univ. of Delaware
- 2014 Outstanding Faculty Graduate Teaching Award in Chemical Engineering Univ. of Colorado, Boulder
- 2014 Outstanding Junior Faculty Award in the Chemical Engineering Univ. of Colorado, Boulder
- 2013 Provost's Faculty Achievement Award, Univ. of Colorado, Boulder
- 2011-2012 College of Engineering Dean's Faculty Fellowship, University of Colorado, Boulder
- 2011 Outstanding Faculty Undergraduate Teaching Award, Chemical Engineering Univ. of Colorado, Boulder

IV. RESEARCH EXPERTISE

I have led my team of undergraduate, graduate, and postdoctoral researchers to develop and use molecular models, theory, simulations, and machine learning methods to design and characterize soft materials 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 of February 2025) = 127
- H-index = 39; i-10 index = 98 Google Scholar
- Associated open-source codes - https://github.com/arthijayaraman-lab

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

127. J. Shah, A. Jayaraman* Coarse-grained molecular dynamics simulations of mixtures of polysulfamides, ***RSC Applied Polymers*** (2025) accepted
126. A. Paruchuri, C. Thrasher, A. J. Hart, R. Macfarlane, A. Jayaraman*, Machine Learning for Identifying Grain Boundaries in Scanning Electron Microscopy (SEM) Images of Nanoparticle Superlattices, **ArXiv** (2025)
125. V. Liao, T. Myers, A. Jayaraman*, A Computational Method for Rapid Analysis Polymer Structure and Inverse Design Strategy (RAPSIDY) ***Soft Matter*** (2024) 20, 8246
124. S. Park# , T. Myers#, V. Liao, A. Jayaraman*, Self-Consistent Field Theory and Coarse-Grained Molecular Dynamics Simulations of Pentablock Copolymer Melt Phase Behavior ***Molecular Systems Design and Engineering*** (2024) 9, 1235-1253
123. A. Paruchuri, Y. Wang, X. Gu and A. Jayaraman*, Machine Learning for Analyzing Atomic Force Microscopy (AFM) Images Generated from Polymer Blends, ***Digital Discovery*** (2024) 3, 2533-2550
122. S. Kronenberger, N. Gupta, B. Gould, C. Peterson, A. Jayaraman*, Random field reconstruction of three-phase polymer structures with anisotropy from 2D-small-angle scattering data, ***Soft Matter*** (2024) 20, 8493-8504
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*, Machine Learning for Analyses and Automation of Structural Characterization of Polymer Materials, ***Progress in Polymer Science,*** (2024) 153, 101828
119. S. V. R. Akepati, N. Gupta, A. Jayaraman*, Computational Reverse Engineering Analysis of Scattering Experiments Method for Interpretation of 2D Small-Angle Scattering Profiles (CREASE-2D) ***JACS Au*** (2024) 4, 4, 1570–1582
118. Z. Wu, A. Collins, A. Jayaraman*, Understanding self-assembly and molecular packing in methylcellulose aqueous solutions using multiscale modeling and simulation, ***Biomacromolecules***, (2024), 25, 3, 1682–1695
117. S. Lu, A. Jayaraman*, Pair-Variational Autoencoders (PairVAE) for Linking and Cross-Reconstruction of Characterization Data from Complementary Structural Characterization Techniques ***JACS Au*** (2023) 3, 9, 2510-2521
116. J. Ju, A. Jayaraman, R. Hayward*, Temperature-Sensitive Micro- and Macro-phase Separation of Hydrogen-Bonded Polystyrene-Polydimethylsiloxane Blends ***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*, Investigating the hydrogen bond-induced self-assembly of 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*, Synergistic role of temperature and salinity in aggregation of nonionic surfactant coated silica nanoparticles, ***Langmuir*** (2023) 39, 16, 5917–5928
111. C. M. Heil, Y. Ma, B. Bharti, A. Jayaraman*, Computational Reverse-Engineering Analysis for Scattering Experiments for Form Factor and Structure Factor Determination ('P(q) and S(q) CREASE') ***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*, Mechanism of Structural Colors in Binary Mixtures of Colloidal Nanoparticle-based Supraballs ***Science Advances*** (2023), Vol 9, Issue 21

109. Z. Wu, A. Jayaraman*, Machine learning enhanced computational reverse-engineering analysis for scattering experiments (CREASE) for analyzing fibrillar structures in polymer solutions, ***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*, Self-supervised machine learning model for analysis of nanowire morphologies from transmission electron microscopy images ***Digital Discovery*** (2022), 1, 816 – 833
106. A. Kulshreshtha, A. Jayaraman*, Phase Behavior and Morphology of Blends containing Associating Polymers: Insights from Liquid State Theory and Molecular Simulations, ***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,* Modeling structural colors from disordered one-component supraballs using combined experimental and simulation techniques ***ACS Materials Letters*** (2022), 4, 9, 1848–1854
104. U. Kapoor, A. Jayaraman*, Impact of Polydopamine Nanoparticle Surface Pattern and Roughness on Interactions with Poly (ethylene glycol) in Aqueous Solution: A Multiscale Modeling and Simulation Study, ***J. Phys. Chem. B.*** (2022), 126, 33, 6301–6313
103. C. M. Heil, A. Patil, A. Dhinojwala, A. Jayaraman*, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) with Machine Learning Enhancement to Determine Structure of Nanoparticle Mixtures and Solutions, ***ACS Central Science*** (2022), 8, 7, 996–1007
102. P. A. Taylor, A. M. Kloxin*, A. Jayaraman*, Impact of collagen-like peptide (CLP) heterotrimeric triple helix 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*, Impact of Composition and Placement of Hydrogen Bonding Groups along Polymer Chains on Blend Phase Behavior: Coarse-Grained Molecular Dynamics Simulation Study, ***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*, Structural Color Production in Melanin-based Disordered Colloidal Nanoparticle Assemblies in Spherical Confinement, ***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
98. U. Kapoor#, A. Kulshreshtha#, A. Jayaraman*, Understanding the Effect of Heterogeneous Particle Functionalization on Graft-Matrix Wetting and Structure in Polymer Nanocomposites Containing Grafted Nanoparticles Using Multiscale Modeling and Simulation, ***ACS Applied Polymer Materials*** (2021) 3 (11), 5642–5655
97. Z. Ye, Z. Wu, A. Jayaraman*,Computational Reverse-Engineering Analysis for Scattering Experiments CREASE) on Vesicles Assembled from Amphiphilic Macromolecular Solutions, ***JACS Au*** (2021) 1 (11), 1925–1936
96. C. M. Heil, A. Jayaraman*, Computational reverse-engineering analysis for scattering experiments of assembled binary mixture of nanoparticles ***ACS Materials Au*** (2021) 1 (2), 140–156
95. M. G. Wessels, A. Jayaraman*, Machine Learning Enhanced Computational Reverse Engineering Analysis for Scattering Experiments (CREASE) to Determine Structures in Amphiphilic Polymer Solutions, ***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*, Anisotropic Synthetic Allomelanin Materials via Solid State Polymerization of Self-Assembled 1, 8-Dihydroxynaphthalene Dimers , ***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*, Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod Fillers ***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, Open-Source Molecular Modeling Software in Chemical Engineering Focusing on the Molecular Simulation Design Framework, ***AIChE Journal*** (2021) 67, 3, e17206
90. A. M. Hilderbrand, P. A. Taylor, F. Stanzione, M. LaRue, C. Guo, A. Jayaraman*, A. M. Kloxin*, Combining simulations and experiments for the molecular engineering of multifunctional collagen mimetic peptide-based materials, ***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*, Unraveling the Structure and Function of Melanin Through Synthesis, ***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*, Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments ***Macromolecules*** (2020) 54, 2, 797-811
87. M. Wessels, A. Jayaraman*, Computational Reverse Engineering Analysis of Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions: Cylindrical and Fibrillar Assembly ***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
85. J. L. Young, Y. Song, M. Wessels, A. Jayaraman*, K. Wooley*, D. Pochan*, Hierarchical Self-assembly of Poly(D-glucose carbonate) Amphiphilic Block Copolymers in Mixed Solvents, ***Macromolecules,*** (2020) 53, 19, 8581–8591
84. 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
83. 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
75. 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†, 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†, A. Jayaraman*, Impact of hydrogen bonding interactions on graft-matrix wetting and structure in polymer nanocomposites, ***Macromolecules,*** (2019) 52, 2725–2735
68. A. Prhashanna, P. A. Taylor, J. Qin#, K. L. Kiick*, A. Jayaraman*, 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
67. 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 Listed in the Top 10 Most Read Article in Macromolecules 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
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63. D. J. Beltran-Villegas#, I. Lyubimov#, A. Jayaraman*, 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
62. 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
59. 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† #, T. B. Martin#, A. Jayaraman*, 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#, T. B. Martin#, A. Jayaraman*, 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
53. 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
50. 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
48. 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
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41. 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
39. 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
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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
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32. 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

31. 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
30. 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
29. E. Jankowski[#], H. S. Marsh[#], A. Jayaraman*, 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[†], A. Jayaraman*, 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[†], A. Jayaraman*, 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[†], A. Jayaraman*, Effect of monomer sequences and particle monomer interactions on assembly of copolymer grafted nanoparticles' ***Soft Matter*** (2013) 9, 155-169
23. 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
21. 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
19. P. Dodd[†] and A. Jayaraman*, 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
18. 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
16. T. B. Martin[†#], A. Seifpour[#], A. Jayaraman*, Assembly of copolymer functionalized nanoparticles: A Monte Carlo simulation study, ***Soft Matter****,* (2011) 7, 5952-5964
15. 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
14. 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
13. A. Seifpour, P. Spicer[†], N. Nair, A. Jayaraman*, 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

1. 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
2. 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,
3. 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
    - Inaugural Editorial for *ACS Polymers Au*, *ACS Polymers Au* 1, 1, 4-6 (2021)
    - *ACS Polymers Au*'s First Issue, *ACS Polymers Au* 1,1, 1-3 (2021)
    - Publishing in and reviewing for *ACS Polymers Au*, *ACS Polymers Au* 1,3, 131-133 (2021)
    - *ACS Polymers Au* recognizes Rising Stars in Polymers in 2021, *ACS Polymers Au* 2, 1, (2022)
    - *ACS Polymers Au*'s Most Viewed Papers in 2021, *ACS Polymers Au* 2,1, (2022)
    - *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)
    - *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. Invited Lecture, Indian Institute of Sciences (IISc), Chemical Engineering, "R Kumar Distinguished Visitor", August 2025
2. ACS POLY/PMSE Student Chapter Invited talk, ACS Fall Meeting 2025, August 2025
3. Invited Talk, Telluride Science Workshop on Molecular Engineering of Materials, June 2025
4. Plenary lecture, European Polymer Congress, Groningen, Netherlands, June 2025
5. Seminar, Dept of Chemical Engineering, Princeton University, April 2025
6. Invited Talk, Institut Laue-Langevin (ILL), Grenoble, France, April 2025
7. Seminar, Dept. of Chemical Engineering, University of Kentucky, April 2025
8. Invited Talk, ACS Spring Meeting COLL: Colloidal and Soft Metamaterials, March 2025
9. Invited Talk, ACS Spring Meeting COMP: Using Artificial Intelligence & Advanced Computing-enabled Tools to Study Biomolecular Assembly, March 2025
10. Invited Talk, ACS Spring Meeting PMSE: Advancing Polymer Science: Integrating High Throughput Techniques and Digital Technologies for Sustainability and More, March 2025
11. Seminar, Dept. of Chemical Engineering, University of Rochester, February 2025
12. Seminar, Dept. of Polymer Science and Engineering, University of Southern Mississippi Feb 2025
13. Technical Talk and Diversity Asia Network Lecturer, Dow Chemical, Collegeville, PA, January 2025
14. Invited talk, Small-Angle Scattering conference, Taipei Taiwan, November 2024

15. Invited talk, Small-Angle Scattering satellite meeting in Kitakyushu, Fukuoka, Japan, October 2024
16. Seminar, Macromolecules Innovation Institute, Virginia Tech October 2024
17. BASF Distinguished Lecture, Wayne State University, September 2024
18. Invited Talk, 'Advances in Machine Learning and Physics-based Modeling for Colloidal Materials', ACS Fall Meeting, Denver, August 2024
19. Invited Talk, 'Navigating the Nanoscale: Innovations in Molecular Dynamics Simulations and Machine Learning for Polymeric Materials', ACS Fall Meeting Denver August 2024.
20. Speaker, Gordon Research Conference, Organic Electronic Materials, Lucca Italy July 2024
21. Keynote speaker, PolyChar 2024, Madrid Spain, May 2024
22. Seminar, Dept. of Macromolecular Science and Engineering, Case Western Reserve University, April 2024
23. Seminar, 100th year celebration, Dept. of Chemical and Biological Engineering, NC State University, April 2024
24. Invited Talk, ACS Spring Meeting: PMSE Centennial: Celebration of Success and New Frontiers in Polymeric Materials Science and Engineering, New Orleans, March 2024
25. Invited Talk "Interactive Materials Talks - Simulation and Data Driven Material Design" Symposium in Aachen, Germany, March 2024
26. Invited Talk, APS March Meeting 2023, 'Computational Design, Understanding, and Discovery of Novel Materials' session, Minneapolis, March 2024
27. Seminar, AI+Science Schmidt Fellows Speaker Series at University of Chicago, February 2024
28. Panelist, Gordon Research Seminar, Colloidal and Macromolecular Materials, February 2024
29. Seminar, Dept. of Chemical Engineering, University of Texas in Austin, January 2024
30. Invited talk, AICHE Annual Meeting 2023, Session in honor of Juan De Pablo, November 2023
31. Invited talk, AICHE Annual Meeting 2023, *Polymer Thermodynamics and Self Assembly*. November 2023
32. Seminar, Dept. of Materials Science and Engineering, Cornell University, October 19th, 2023
33. Seminar, Dept. of Chemical Engineering, NYU, October 13th, 2023
34. Seminar, UConn Polymer Program, Institute of Materials Science, September 29th, 2023
35. Invited talk, Bayreuth Polymer Symposium, Germany September 17-19th 2023
36. 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
37. Invited talk at the symposium *Hybrid Functional Materials of Polymers for Inorganic Nanoparticles* (sponsored by PMSE) ACS Fall Meeting, San Francisco, CA, August 2023
38. Invited talk, 2023 American Crystallography Association, *Small Angle Scattering To Characterize Structurally Complex Materials*, Baltimore, June 2023
39. Invited talk, 2023 ACS Colloids and Surface Science meeting, *Artificial Intelligence in Colloids and Surface Science*, Raleigh NC, June 2023
40. Invited talk, 2023 International Polymer Colloid Group conference, June 19-23, 2023, Queen's University, Kingston/Canada
41. Invited Talk, Polymers in Water, High Polymer Research Group meeting, Pott Shirgley, UK April 23 – 27, 2023
42. Keynote lecture, NanoBioNYC NRT Launch event, City University of New York (CUNY) April 18 2023
43. Seminar, Department of Materials Science and Engineering, University of Virginia, April 10-11, 2023
44. Invited talk, Symposium on *Advances in Coarse-Graining and Multiscale Modeling*, ACS (COMP) Spring Meeting, March 26 – 30 2023 Indianapolis, IN,
45. 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)
46. Invited talk, Designing soft matter in and out of equilibrium, Lorentz Center, Oort in Leiden, The Netherlands, Jan 30 – Feb 3, 2023
47. Seminar, Department of Materials Science and Engineering, Carnegie Mellon University, January 20, 2023
48. Plenary Lecture. Equifase 2022 XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, Brazil, October 24-27, 2022
49. Invited talk, Digitization Track 2: *Artificial Intelligence for Materials Discovery*, Innovation Day 2022, Science History Institute, Philadelphia, PA September 13, 2022
50. Seminar (virtual), Department of Civil Engineering, Carnegie Mellon University September 23, 2022

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

89. Seminar, Department of Chemical Engineering, Columbia, February 2020
90. Invited talk, MRS Fall Meeting 2019, Boston December 2019
91. Seminar, Department of Chemical Engineering, Univ. of Buffalo, November 2020
92. Invited talk, New Frontiers in Molecular Thermodynamics, AICHE Annual Meeting 2019
93. Invited talk, Area 8A (Polymers) Plenary Session, AICHE Annual Meeting 2019
94. Invited talk, ARL's Strategic Materials, Temple University, August 2019
95. Invited talk, Gordon Research Conference, Polymers, June 2019
96. Invited lecture, PPEPPD 2019, Canada, May 2019
97. Seminar, School of Polymer Science and Engineering, University of Southern Mississippi, May 2019
98. Invited talk, "Multicomponent Block Polymer Systems" session at ACS Spring Meeting, April 2019
99. Invited talk, "Using Polymer Sequence to Control Material Properties" session at APS March Meeting, March 2019
100. Invited talk, AICHE Annual Meeting Thermodynamics at the nanoscale, Pittsburgh, Oct-Nov 2018
101. Invited talk, Frontiers in Molecular Engineering, Chicago Sept 2018
102. Invited talk, ACS Fall Meeting, Boston, August 2018
103. Plenary lecture, FOMMS 2018 Innovations for Complex Systems, July 2018
104. Invited talk, 4th Functional Polymeric Materials Conference, Bahamas, June 2018
105. Invited talk, 30th anniversary of the Midwest Thermodynamics and Statistical Mechanics (MTSM) conference June 2018
106. Invited talk, Polymer Nanocomposites Workshop, iPRIME meeting, University of Minnesota, May 2018
107. Invited talk, STM Global Publishing Conference, Philadelphia, April 2018
108. Seminar, Department of Chemical Engineering, BYU April 2018
109. Invited talk, ACS Spring Meeting, Polymers with Complex Architecture: From Synthesis to Self-Assembly, March 2018
110. Seminar, Department of Chemistry, University of Minnesota, February 2018
111. Keynote address, NCSU Department of Chemical and Biomolecular Engineering, Schoenborn Graduate Student Symposium, January 2018
112. Seminar, Dept. of Chemical Engineering (*students-nominated speaker*) Cornell University, Sept 2017
113. Invited talk, Telluride Science Workshop on *Molecular Engineering in Soft Matter* June 2017
114. Invited talk, Mid-Atlantic Soft Matter Meeting University of Pennsylvania, May 2017
115. Invited talk, Argonne Research Lab, Center for Nanostructured Materials, May 2017
116. Invited talk, Pan-American Polymer Science Conference (ACS) in Brazil, Invited Speaker March 2017
117. Seminar, Macromolecular Science and Engineering, Case Western Reserve University, March 2017
118. Invited talk, Experimental Station Dupont, January 2017
119. Invited talk, AICHE Annual Meeting, Invited-only session to honor Carol Hall, November 2016
120. Seminar, University of Pennsylvania, PICS Seminar Series, October 2016
121. Seminar, University of Florida, Physical Chemistry Seminar Series, October 2016
122. Seminar, University of Akron, Physics Club, October 2016
123. Invited talk, ACS Fall Meeting, Philadelphia, August 2016
124. Invited speaker, Gordon Research Conference, Polymer Physics July 2016
125. Keynote Lecture, PPG-Pitt Innovations in Materials Symposium, May 2016
126. Seminar, Dept. of Chemical Engineering, University of Akron, March 2016
127. Invited talk, PittConn Meeting, March 2016
128. Saville Lecture, Department of Chemical Engineering, Princeton University, March 2016
129. ACS Southeast Regional meeting, Multiscale modeling and simulations, November 2015
130. Seminar, Nanotechnology Seminar Series, Stevens Institute of Tech, October 2015
131. Seminar, Biomedical and Chemical Engg. Syracuse University, September 2015
132. Seminar, Chemical Engineering, URhode Island, September 2015
133. Invited talk, ACS Fall Meeting, *Functional Polymers: Connecting Modeling and Experiment,* August 2015
134. Invited talk, SPIE Meeting, Physical Chemistry of Interfaces and Nanomaterials, August 2015
135. Invited talk, Functional Polymeric Material Conference, Ascot UK 2015

136.Invited talk, Telluride workshop on *Multiscale modeling in organic electronic materials*, July 2015
137.Invited talk, Telluride workshop on *Polymer Physics*, June 2015
138.Seminar, Dept. of Chemical Engineering, UC Santa Barbara, April 2015
139.Invited talk, ACS Spring Meeting 2015 *Design principles for functional macromolecular materials* March 2015
140.Invited talk, ACS Spring Meeting 2015 *Polymer Modeling: Structure, Function, Properties* March 2015
141.Invited talk, APS March Meeting San Antonio March 2015
142.Invited talk, XPV- Excitonic Photovoltaics –Telluride science workshop August 2014
143.Invited talk NSF-US-Poland Workshop on Thermodynamics of Complex Fluids and Interfaces June 2014
144.Invited talk, ACS Spring Meeting 2014, *Structure for Function: Rational design of new functional polymeric materials* March 2014
145.Invited talk, ACS Spring Meeting 2014, *PMSE Young Investigators Symposium*, March 2014
146.Seminar, Dept. of Materials Engineering, Purdue University, February 2014
147.Seminar, Center for Molecular Engineering and Thermodynamics, University of Delaware, Jan 2014
148.Invited talk, AICHE Annual Meeting 2013, *Modeling and Simulation of Polymers* session, November 2013
149.Invited award talk, AIChE Annual Meeting 2013, *COMSEF Plenary Session*, November 2013
150.Invited talk, APS meeting, Four Corners section, October 2013
151.Seminar, Tulane University, Department of Chemical Engineering, September 2013
152.Invited talk, ACS Fall Meeting, Indianapolis, September 2013
153.Invited talk, APS March Meeting in '*Directed Assembly of Hybrid Materials*' session March 2013
154.Invited talk, Army Research Laboratory, Aberdeen Proving Ground, Maryland, March 2013
155.Invited speaker, Gordon Research Conference Macromolecular Materials, January 2013
156.Seminar, Department of Material Science and Engineering, University of Delaware, December 2012
157.Invited talk, AICHE Annual Meeting 2012, invited talk in *Thermodynamics of Polymers'* session
158.Invited talk, AICHE Annual Meeting 2012, invited talk on *Emerging Areas in Polymer Science and Engineering* session
159.Invited talk, AICHE Annual Meeting 2012, invited talk in *Multiscale Modeling and Simulation for Renewable Energy* session
160.Seminar, Department of Chemical Engineering, University of Washington, October 2012
161.Seminar, Chemistry Department, Colorado State University, September 2012
162.Seminar, Chancellor's Invitation to present to CU Alumni and friends, September 2012
163.Seminar, Molecular Biophysics Seminar Series, Institute of Computational Engineering and Sciences, University of Texas at Austin, April 2012
164.Invited talk, ACS Spring National Meeting COMP division *Integration of Computer Simulation with Experiments* March 2012
165.Seminar, Department of Chemical Engineering, Colorado School of Mines, January 2012
166.Seminar, Liquid Crystal Materials Research Center, CU Boulder January 2012
167.Seminar, Department of Polymer Engineering, University of Akron, Ohio, November 2011
168.Seminar, "Young Investigators in Materials Research" UMass Amherst Materials Research Science & Engineering Center (MRSEC) May 2011
169.Seminar, Dept. of Chemical Engineering, Rice University, March 2011
170.Seminar, Dept. of Chemical Engineering, Texas A&M University, February 2011
171.Seminar, Dept. of Materials Science and Engineering, University of Illinois at Urbana, February 2011
172.Seminar, Dept of Chemical Engineering, Vanderbilt University, November 2010
173.Seminar, Dept. of Applied Math, University of Colorado Boulder, November 2010
174.Invited talk, Interfacial Phenomena in Nanostructured Materials and Devices, Telluride Workshop February 2010
175.Seminar, Dept. of Chemical Engineering, Colorado State University, October 2009
176.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)
- **Spring 2025** Computing and Data Science for Soft Materials Innovation and Design CHEG/CISC/ECEG/MSEG 848 (total 15 students including 1 student from 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 CHEN4570-0**2** (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 CHEN4570-0**2** (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)

GRADUATE STUDENTS

Name	Dept./Univ.	Title (Current Position)	Period
Emily Yao	CBE (UD)	PhD candidate	01/2025- current
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- 12/2024
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- 12/2024
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

Name	Department	Title	Period
Nina Borodin	CHEM (UD)	Undergraduate research	09/2023 -present
Kaveri Shrivatsava	CBE (UD)	Undergraduate research	08/2023-05/2024
Shivam Chauhan	CBE (UD)	Undergraduate research	01/2022-02/2022
Geoffrey Bonanzino	CBE (UD)	Undergraduate research	05/2020-05/2022
Ryan Tarr	CBE (UD)	Undergraduate research	01/2021-05/2021

Chandler Amato	CBE (UD)	Undergraduate research	06/2018-06/2020
Daniel Intriago	CBE (UD)	Undergraduate research	01/2017-05/2019
Christopher Johnson	CBE (UD)	Undergraduate research	06/2018-05/2020
Paul Blanchard	Penn State	REU Undergrad Research	06/2016-08/2016
Kevin Modica	CBE (UD)	Undergraduate research	06/2016-05/2019
Christopher Knieste	CBE (UD)	Undergraduate research	01/2015-12/2015
Sloane McNeill	AppMath (CU)	Undergraduate 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	Undergraduate 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	02/2022-01/2025
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 Mondelēz International)	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 Nxera Pharma)	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 Photovoltaics (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 1st 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.
- **Grant agencies**: 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) Computing and Data Science Training for Materials Innovation, Discovery, and Analytics
- 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:
    - Cohort 1: George Kramarenko (UD Biomedical Engineering, Emily Day primary advisor)
    - Cohort 1: Kayla Hapler (UD Materials Science and Engineering, Charles Dhong primary advisor)

- Cohort 1: Peter Osazuwa (UD Materials Science and Engineering, Laure Kayser, primary advisor)
- Cohort 2: Kelsey Koutsoukos (UD Materials Science and Engineering, Laure Kayser primary advisor)
- Cohort 2: Justin Lombard (UD Elec and Computer Engineering, Austin Brockmeier primary advisor)
- Cohort 3: Leonardo Pierre (DSU Applied Physics, Q. Lu primary advisor)
- Cohort 4: Rudi DiMuri (UD Materials Science and Engineering, Darrin Pochan primary advisor)
- Cohort 4: Dylan Trott (UD Materials Science and Engineering, Christian Pester primary advisor)
- Cohort 4: Alex Sawyers (UD Biomedical Engineering, Emily Day 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)

- Elected Member of Graduate College Council (AY 2022-present)
- Elected Member of Graduate College Council (AY 2019-2020)
- Member of the 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)