

ARTHI JAYARAMAN

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 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

Centennial Term Professor for Excellence in Research and Teaching	09/2020- 08/2023
Director, NSF-funded NRT graduate traineeship on <i>Computing and Data Science Training for Materials Innovation, Discovery, and Analytics</i>	09/2021 - present
Full Professor with Tenure Department of Chemical and Biomolecular Engineering & Department of Materials Science and Engineering University of Delaware, Newark	09/2019- present
Deputy Editor, ACS Polymers Au	01/2021-present
Associate Editor, Macromolecules	08/2019- present
Faculty Council, Data Science Institute University of Delaware, Newark	04/2020 - present
Graduate Program Director 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 Engineering University 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	08/2008 - 07/2014

III. HONORS/AWARDS

Professional Society

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

Lectureship/Federal Grant Agency Career Award

- 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*
- Featured as an Emerging Investigator in *Journal of Polymer Science B: Polymer Physics*

University Research & Teaching Awards

- 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
- 2006 Edward M. Schoenborn Award for Outstanding Graduate Research, Dept. of Chemical Engineering, NC State University
- 2000 Monali Dey Award for Outstanding Undergraduate Student, Dept. of Chemical Engineering, Birla Institute of Technology and Science, Pilani

IV. RESEARCH EXPERTISE

My research group develops and uses molecular models, theory, simulations, and machine learning to design macromolecular materials from the molecular level to achieve optimal materials for a variety of applications. Currently, we are focused on the following research thrusts:

1. Polymer Functionalized Nanoparticles
2. Polymer Blends, Solutions, and Nanocomposites
3. Peptides and Nucleic Acid based Biomaterials
4. Self-assembly in Colloidal Soft Materials
5. Machine Learning Enabled Analysis of Soft Materials Characterization

V. PEER-REVIEWED RESEARCH PUBLICATIONS

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

As Principal Investigator (Link to my [google scholar](#))

101. P. A. Taylor, A. 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 (submitted)
100. 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 (submitted)
99. Patil #, C. M. Heil #, B. Vanthournout, M. Bleuel, S. Singla, Z. Hu, 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* (accepted)
98. 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
97. 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
96. 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
95. C. Heil, A. Jayaraman*, Computational reverse-engineering analysis for scattering experiments of assembled binary mixture of nanoparticles *ACS Materials Au* (2021) 1 (2), 140–156
94. 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
93. 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* 60, 32, 17464-17471 (2021)
92. S. Lu #, Z. Wu#, **A. Jayaraman***, Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod Fillers *J. Phys Chem B*. 125, 9, 2435–2449 (2021)
91. P. Cummings*, C. McCabe*, C. Iacovella, A. Ledeczki, 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* 67, 3, e17206 (2021)
90. W. Cao, X. Zhou, N. C. McCallum, Z. Hu, Q. Z. Ni, U. Kapoor, C. M. Heil, K. S. Cay, T. Zand, A. Mantanona, **A. Jayaraman**, A. Dhinojwala, D. Deheyn, M. D. Shawkey, M. D. Burkart, J. D. Rinehart, N. C. Gianneschi*, Unraveling the Structure and Function of Melanin through Synthesis. *J. Am. Chem. Soc.* 143, 7, 2622-2637 (2021)
89. A. Hilderbrand, P. Taylor, F. Stanzione, M. LaRue, G. Chen, **A. Jayaraman***, A. Kloxin*, Combining simulations and experiments for the molecular engineering of multifunctional collagen mimetic peptide-based materials, *Soft Matter*, 17, 1985-1998 (2021)
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***, and R. J. Composto*, Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments, *Macromolecules*, 54, 2, 797-811 (2021)
87. M. G. Wessels, **A. Jayaraman***, Computational Reverse-Engineering Analysis of Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions: Cylindrical and Fibrillar, *Macromolecules*, 54, 2, 783–796 (2021)
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*, 12, 11, 2764 (2020)

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*, 53, 19, 8581–8591 (2020)
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*, 5, 1239-1254 (2020)
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*, 16, 7, 4599–4614 (2020)
82. P. A. Taylor, **A. Jayaraman***, Molecular modeling and simulations of peptide-polymer conjugates, *Annu. Rev. Chem. Biomol. Eng.*, 11, 257-276 (2020)
81. **A. Jayaraman***, Modeling and simulation of macromolecules with hydrogen bonds: Challenges, successes and opportunities, an invited viewpoint in *ACS Macro Letters*, 9, 656–665 (2020)
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*, 5, 864-875 (2020)
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.*, 124, 2702-2714 (2020)
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*, 53, 1302-1313 (2020)
77. M. Wessels, **A. Jayaraman***, Self-assembly of amphiphilic polymers of varying architectures near attractive surfaces, *Soft Matter*, 16, 623-633 (2020) [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*, 11, 19850-19861 (2019)
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.*, 141, 14916-14930 (2019)
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* 52, 4579-4589 (2019)
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* 5, 9, eaax1254 (2019)
72. D. J. Beltran-Villegas, D. Intriago†, K. Kim, N. Behaupt, J. D. Londono, **A. Jayaraman***, Coarse-grained molecular dynamics simulations of α -1,3-glucan, *Soft Matter*, 15, 4669-4681 (2019)
71. M. Wessels, **A. Jayaraman***, Molecular dynamics simulation study of linear, bottlebrush, and star-like amphiphilic block polymer assembly in solution, *Soft Matter*, 15, 3987-3998 (2019)
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*, 13, 5147-5162 (2019)
69. A. Kulshreshtha, K. Modica†, **A. Jayaraman***, Impact of hydrogen bonding interactions on graft-matrix wetting and structure in polymer nanocomposites, *Macromolecules*, 52, 2725–2735 (2019)
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*, 20, 1178–1189 (2019)
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*, 57, 1196–1208 (2019)
66. T. E. Gartner, III, **A. Jayaraman***, Modeling and Simulations of Polymers: A Roadmap, an invited perspective article for *Macromolecules*, 52, 755–786 (2019) [Listed in the Top 10 Most Read Article in Macromolecules](#)
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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*, 51 (19), 7586–7599 (2018)
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*, 51 (8), 2906–2922 (2018)

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*, Special Issue on Machine Learning and Data Science in Materials Design, 3, 453-472 (2018)
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.*, 122 (6), 1929–1939 (2018)
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*, 63 (7), 2351–2367 (2018)
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*, 14, 411-423 (2018)
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*, 7,13, 6770-6783 (2017)
58. I. Lyubimow, D. Beltran-Villegas, **A. Jayaraman***, PRISM theory study of amphiphilic block copolymer solutions with varying copolymer sequence and composition *Macromolecules*, 50 (18), 7419–7431 (2017)
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*, 50 (12),4854 (2017)
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*, 13, 2907-2918, (2017) [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*, 49 (24), 9684–9692, (2016)
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*, 12 (11), 5501–5510 (2016)
53. A. Ghobadi, **A. Jayaraman***, Effects of Polymer Conjugation on Hybridization Thermodynamics of Oligonucleic Acids, *J. Phys. Chem. B.* 120 (36), 9788 (2016)
52. F. Stanzione, **A. Jayaraman***, Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene glycol (PEG) in Explicit Water, *J. Phys. Chem. B* 120, 4160–4173 (2016)
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**, 3, 034001 (2016)
50. A. Ghobadi, **A. Jayaraman***, Effect of Backbone Chemistry on Hybridization Thermodynamics of Oligonucleic Acids: A Coarse-Grained Molecular Dynamics Simulation Study, *Soft Matter*, 12, 2276-2287 (2016)
49. A. Ghobadi, R. Letteri, T. Emrick*, **A. Jayaraman*** Dispersing zwitterions within comb polymers for non-viral transfection: Experiments and molecular simulations, *Biomacromolecules*, 17(2), 546-57 (2016)
48. H. S. Marsh, **A. Jayaraman*** Effect of side chain length on the morphology of blends of 2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) oligomers and fullerene derivatives, *J. Polymer Science B: Polymer Physics*, 54,1, 89-97 (2016)
47. F. Stanzione, **A. Jayaraman***, Computational design of oligopeptide containing poly(ethylene glycol) brushes for stimuli-responsive drug delivery, *J. Phys. Chem B.*, 119 (42), 13309-13320 (2015)
46. T. B. Martin[#], K. I. Mongcopa[#], R. Ashkar, P. Butler, R. Krishnamoorti*, **A. Jayaraman***, Wetting-Dewetting and Dispersion-Aggregation Transitions are Distinct in Mixtures of Polymer Grafted Nanoparticles and a Chemically Dissimilar Polymer Matrix, *J. Am. Chem. Soc.*, 137 (33), 10624–10631 (2015)
45. R. M. Elder, J. Pfaendtner, **A. Jayaraman***, Effect of hydrophobic and hydrophilic surfaces on the stability of double-stranded DNA, *Biomacromolecules*, 16 (6), 1862–1869 (2015)
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.*, 53, 1046-1057 (2015)
43. C. E. Estridge, **A. Jayaraman***, Diblock copolymer grafted particles as compatibilizers for immiscible homopolymer blends, *ACS Macro Letters*, 4, 155–159, (2015)
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.*, 136 (52), 18120-18130 (2014)

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*, 53, 76-88 (2015) [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*, 3, 628–632 (2014)
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”) 52, 1661-1668 (2014)
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)
37. 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* 47 (8), 2736–2747 (2014) (This was one of 20 most downloaded articles from Macromolecules in May 2014)
35. J.J. Roberts, R.Elder, **A. Jayaraman**, S.J. Bryant*, Characterization of Matrix Retaining Hydrogels Containing Hyaluronan Binding Peptides, *Biomacromolecules*, 15 (4), 1132–1141 (2014)
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*, **10**, 13-38 (2014)
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*, 40, 1085-1098 (2013)
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*, 46 (22), 9144–9150 (2013)
31. R. Elder, **A. Jayaraman*** Structure and thermodynamics of ssDNA Oligomers near hydrophobic and hydrophilic Surfaces: A molecular simulation study, *Soft Matter* **9**, 11521-11533 (2013)
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.*, 117 (40), 11988–11999 (2013)
29. E. Jankowski#, H. S. Marsh#, **A. Jayaraman***, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology, *Macromolecules*, 46 (14) 5775-5785 (2013) (This was one of 20 most downloaded articles from Macromolecules in July 2013)
28. T. Martin, **A. Jayaraman***, Polydisperse Polymer Grafts for Stabilizing Dispersion of Homopolymer Grafted Nanoparticles in Chemically Identical Homopolymer Matrix, Peer-reviewed article for special issue on ‘*Emerging Investigators in Soft Matter*’ in *Soft Matter*, 9 (29), 6876 – 6889 (2013)
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*, 39(9)741-753 (2013)
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* 51(7), 524–534 (2013) (This was the fourth most downloaded article in the Journal in February 2013)
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* 110, 018301 (2013)
24. T. Martin, C. McKinney†, **A. Jayaraman***, Effect of monomer sequences and particle monomer interactions on assembly of copolymer grafted nanoparticles’ *Soft Matter* **9**, 155-169 (2013)
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*, 51 (1), 64-77 (2013)
22. R. Elder, **A. Jayaraman***, Coarse-grained simulation studies of effects of polycation architecture on structure of the polycation and polycation-polyanion complexes, *Macromolecules* (19), 8083-8096 (2012)
21. R. Elder, **A. Jayaraman***, Sequence specific recognition of cancer drug-DNA adducts by HMGB1a repair protein, *Biophysical Journal*, 102, 10, 2331–2338, (2012)

20. A. Jayaraman* and N. Nair, Integrating PRISM theory and Monte Carlo simulation to study polymer functionalized particles and polymer nanocomposites', for a special issue "New developments in Molecular Simulations" *Molecular Simulation*, 38, 8-9, 751-761, (2012)
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*, 50, 10, 694–705, (2012)
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*, 38, 10, 793-808 (2012)
17. R. Elder, T. Emrick, and A. Jayaraman* Understanding the effect of polylysine architecture on DNA binding using molecular dynamics simulations, *Biomacromolecules*, 12(11), 3870-9 (2011)
16. T. B. Martin‡, A. Seifpou‡, A. Jayaraman*, Assembly of copolymer functionalized nanoparticles: A Monte Carlo simulation study, *Soft Matter*, 7, 5952-5964 (2011)
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*, 134, 194906 (2011)
14. N. Nair and A. Jayaraman*, Self-Consistent PRISM Theory-Monte Carlo Simulation Studies of Copolymer Grafted Nanoparticles in a Homopolymer Matrix, *Macromolecules*, 43 (19), 8251–8263 (2010)
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.*, 131, 164901 (2010) (Selected to appear in *Virtual Journal of Biological Physics*)

Doctoral and Postdoctoral Work

12. L. M. Hall, A. Jayaraman, K. S. Schweizer*, Molecular theories of polymer nanocomposites, invited article to *Current Opinion in Solid State & Materials Science*, 14, 38-48 (2010) *** Listed as one of the top cited articles published in *Current Opinion in Solid State & Materials Science* from 2007
11. A. Jayaraman* and K. S. Schweizer, Liquid state theory of the structure and phase behaviour of polymer-tethered nanoparticles in dense suspensions, melts and nanocomposites, invited review article in Frontiers of Molecular Simulation, special issue) *Molecular Simulation*, 35, 835-848 (2009)
10. A. Jayaraman and K. S. Schweizer*, Effective Interactions and Self Assembly of Hybrid Polymer Grafted Nanoparticles in a Homopolymer Matrix, *Macromolecules*, 42,8423-8434 (2009)
9. A. Jayaraman and K. S. Schweizer*, Effective interactions, structure and phase behavior of lightly tethered nanoparticles in polymer melt, *Macromolecules*, 41 (23), 9430–9438 (2008)
8. A. Jayaraman and K. S. Schweizer*, Effect of number and placement of polymer tethers on the structure of concentrated solutions and melts of hybrid nanoparticles, *Langmuir*, 24(19) 11119-11130 (2008)
7. A. Jayaraman and K. S. Schweizer*, Structure and phase behavior of dense solutions and melts of single polymer tethered nanoparticles, *J. Chem. Phys.*, 128, 164904 (2008)
6. A. Jayaraman, E. E. Santiso, C. K. Hall* and J. Genzer, Theoretical study of zipping phenomena in biomimetic polymers' *Phys. Rev. E.*, 76 (1), 011915 (2007)
5. A. Jayaraman, C. K. Hall* and J. Genzer, Computer simulation study to understand the effect of surface density on hybridization in model DNA microarrays *J Chem. Phys.*, 127, 144912 (2007)
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3. A. Striolo, A. Jayaraman, C. K. Hall*, and J. Genzer, Adsorption of comb copolymers on weakly-attractive solid surfaces, *J. Chem. Phys.*, 123, 064710 (2005)
2. A. Jayaraman, C. K. Hall* and J. Genzer, Computer simulation study of pattern transfer in AB diblock copolymer film adsorbed on a heterogeneous surface, *J. Chem. Phys.*, 123, 124702 (2005)
1. A. Jayaraman, C. K. Hall* and J. Genzer, Designing pattern-recognition surfaces for selective adsorption of copolymer sequences using lattice Monte Carlo simulation, *Physical. Review. Letters.*, 94, 078103 (2005)

VI. PROCEEDINGS/BOOK CHAPTERS

1. 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,
2. 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. A. Jayaraman, H-A. Klok, Inaugural **Editorial** for ACS Polymers Au, *ACS Polymers Au* 1, 1, 4-6 (2021)
3. A. Jayaraman, H-A. Klok, ACS Polymers Au; First Issue, *ACS Polymers Au* 1,1, 1-3 (2021)
4. A. Jayaraman, H-A. Klok, Publishing in and Reviewing for ACS Polymers Au, *ACS Polymers Au* 1,3, 131-133 (2021)
5. A. Jayaraman, H-A. Klok, ACS Polymers Au recognizes Rising Stars in Polymers in 2021, *ACS Polymers Au* 2,1, (2022)
6. A. Jayaraman, H-A. Klok, ACS Polymers Au's Most Viewed Papers in 2021, *ACS Polymers Au* 2,1, (2022)

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

With A. Jayaraman as Principal Investigator

1. Plenary Lecture. Equifase 2022 XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, Brazil, from October 2022
2. Plenary Lecture, Division of Condensed Matter and Materials Physics, 2022 Canadian Association of Physicists (CAP) Congress, June 2022
3. Invited talk, ACS Mid-Atlantic Regional Meeting, Session on *Simulation and Machine Learning of Soft Materials* June 2022
4. Invited talk, ACS Mid-Atlantic Regional Meeting, Session on *Industrial Applications of Molecular simulations* June 2022
5. 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
6. Seminar, Dept. of Polymer Engineering, Uakron, April 2022
7. Seminar, Dept. of Materials Science and Engineering, UIUC, April 2022
8. Invited talk, APS March Meeting DPOLY session on *Polymer Nanocomposites*, March 2022
9. Seminar, Dept. of Chemistry, Stony Brook University, February 2022
10. Seminar, Mechanical Engineering and Chemical Engineering, IIT Madras, January 2022
11. Plenary Lecture, AIChE Annual Meeting, COMSEF Plenary Session, Boston, MA, November 2021
12. Seminar, Dept. of Chemical Engineering, Georgia Tech, November 2021
13. Invited talk, TechConnect, Washington DC, October 2021
14. Seminar, Dept. of Chemical Engineering, University of Notre Dame, October 2021
15. Invited talk, Computing in Engineering forum, University of Wisconsin-Madison, September 2021
16. Invited talk, ACS SCIENCE TALKS series featuring editors talking about their science, India, September 2021
17. Invited talk, Telluride Science Workshop on *Polymer Physics*, Telluride CO, June-July 2021
18. 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
19. Seminar, Dept. of Chemical Engineering, UMass-Amherst, April 2021
20. Seminar, Dept. of Chemistry, University of Delaware, March 2021
21. Short course invited lecture, 2021 APS March meeting DPOLY short course on 'Macromolecular Engineering of Formulations', March 2021

22. Seminar, Dept. of Chemical Engineering, Mississippi State University, March 2021
23. Invited Lecture, AICTE short term course - advances in biomaterials and tissue engineering, IIT Madras, India, January 2021
24. Invited Talk, International Conference on New Trends in Applied Chemistry, Sacred Heart College, India, December 2020
25. Invited talk, MRS Fall/Spring virtual Meeting CT04: Tailored Interphases for High Strength and Functional Composites" 2020
26. Invited talk, MRS Fall/Spring virtual Meeting MT04: Materials Theory, Characterization and Data Science, 2020
27. Invited talk, One of three speakers highlighted in "100 Years of Polymer Science" virtual symposium organized by Wiley, October 2020
28. Virtual Seminar, Department of Chemical Engineering, UIUC, October 2020
29. Invited talk, Frontiers in Chemical Engineering – Virtual Symposium, Caltech, October 2020
30. Invited talk, ACS Fall meeting, COMP division *Multiscale Modeling of Protein and Nucleic Acid Therapeutics* August 2020
31. Invited talk, ACS Fall meeting, POLY/PMSE division, *Advances in the synthesis, characterization, modeling and application of bottlebrush polymers*, August 2020
32. Invited talk, Next Generation Synchrotron X-ray Needs in Soft Matter Science, Argonne National Lab, May 2020 *Cancelled due to COVID*
33. Seminar, Department of Chemical Engineering, Caltech May 2020 *Cancelled due to COVID*
34. Invited talk, BASF, April 2020 *Virtual seminar*
35. Invited talk, MRS Spring Meeting 2020, Phoenix, April 2020 *Cancelled due to COVID*
36. Seminar, Department of Chemical Engineering, UMass Amherst, April 2020 *Cancelled due to COVID*
37. Invited talk, ACS Spring Meeting, Philadelphia, March 2020 *Cancelled due to COVID*
38. Invited talk, US-France Polymer Nanocomposites Workshop, Columbia University, March 2020 *Cancelled due to COVID*
39. Seminar, Department of Chemical Engineering, Columbia, February 2020
40. Invited talk, MRS Fall Meeting 2019, Boston December 2019
41. Seminar, Department of Chemical Engineering, Univ. of Buffalo, November 2020
42. Invited talk, New Frontiers in Molecular Thermodynamics, AIChE Annual Meeting 2019
43. Invited talk, Area 8A (Polymers) Plenary Session, AIChE Annual Meeting 2019
44. Invited talk, ARL's Strategic Materials, Temple University, August 2019
45. Invited talk, Gordon Research Conference, Polymers, June 2019
46. Invited lecture, PPEPPD 2019, Canada, May 2019
47. Seminar, School of Polymer Science and Engineering, University of Southern Mississippi, May 2019
48. Invited talk, "Multicomponent Block Polymer Systems" session at ACS Spring Meeting, April 2019
49. Invited talk, "Using Polymer Sequence to Control Material Properties" session at APS March Meeting, March 2019
50. Invited talk, AIChE Annual Meeting Thermodynamics at the nanoscale, Pittsburgh, Oct-Nov 2018
51. Invited talk, Frontiers in Molecular Engineering, Chicago Sept 2018
52. Invited talk, ACS Fall Meeting, Boston, August 2018
53. Plenary lecture, FOMMS 2018 Innovations for Complex Systems, July 2018
54. Invited talk, 4th Functional Polymeric Materials Conference, Bahamas, June 2018
55. Invited talk, 30th anniversary of the Midwest Thermodynamics and Statistical Mechanics (MTSM) conference June 2018
56. Invited talk, Polymer Nanocomposites Workshop, iPRIME meeting, University of Minnesota, May 2018
57. Invited talk, STM Global Publishing Conference, Philadelphia, April 2018
58. Seminar, Department of Chemical Engineering, BYU April 2018
59. Invited talk, ACS Spring Meeting, Polymers with Complex Architecture: From Synthesis to Self-Assembly, March 2018
60. Seminar, Department of Chemistry, University of Minnesota, February 2018
61. Keynote address, NCSU Department of Chemical and Biomolecular Engineering, Schoenborn Graduate Student Symposium, January 2018
62. Seminar, Dept. of Chemical Engineering (*students-nominated speaker*) Cornell University, Sept 2017

63. Invited talk, Telluride Science Workshop on *Molecular Engineering in Soft Matter* June 2017
64. Invited talk, Mid-Atlantic Soft Matter Meeting University of Pennsylvania, May 2017
65. Invited talk, Argonne Research Lab, Center for Nanostructured Materials, May 2017
66. Invited talk, Pan-American Polymer Science Conference (ACS) in Brazil, Invited Speaker March 2017
67. Seminar, Macromolecular Science and Engineering, Case Western Reserve University, March 2017
68. Invited talk, Experimental Station Dupont, January 2017
69. Invited talk, AIChE Annual Meeting, Invited-only session to honor Carol Hall, November 2016
70. Seminar, University of Pennsylvania, PICS Seminar Series, October 2016
71. Seminar, University of Florida, Physical Chemistry Seminar Series, October 2016
72. Seminar, University of Akron, Physics Club, October 2016
73. Invited talk, ACS Fall Meeting, Philadelphia, August 2016
74. Invited speaker, Gordon Research Conference, Polymer Physics July 2016
75. Keynote Lecture, PPG-Pitt Innovations in Materials Symposium, May 2016
76. Seminar, Dept. of Chemical Engineering, University of Akron, March 2016
77. Invited talk, PittConn Meeting, March 2016
78. Saville Lecture, Department of Chemical Engineering, Princeton University, March 2016
79. ACS Southeast Regional meeting, Multiscale modeling and simulations, November 2015
80. Seminar, Nanotechnology Seminar Series, Stevens Institute of Tech, October 2015
81. Seminar, Biomedical and Chemical Engg. Syracuse University, September 2015
82. Seminar, Chemical Engineering, URhode Island, September 2015
83. Invited talk, ACS Fall Meeting, *Functional Polymers: Connecting Modeling and Experiment*, August 2015
84. Invited talk, SPIE Meeting, Physical Chemistry of Interfaces and Nanomaterials, August 2015
85. Invited talk, Functional Polymeric Material Conference, Ascot UK 2015
86. Invited talk, Telluride workshop on *Multiscale modeling in organic electronic materials*, July 2015
87. Invited talk, Telluride workshop on *Polymer Physics*, June 2015
88. Seminar, Dept. of Chemical Engineering, UC Santa Barbara, April 2015
89. Invited talk, ACS Spring Meeting 2015 *Design principles for functional macromolecular materials* March 2015
90. Invited talk, ACS Spring Meeting 2015 *Polymer Modeling: Structure, Function, Properties* March 2015
91. Invited talk, APS March Meeting San Antonio March 2015
92. Invited talk, XPV- Excitonic Photovoltaics –Telluride science workshop August 2014
93. Invited talk NSF-US-Poland Workshop on Thermodynamics of Complex Fluids and Interfaces June 2014
94. Invited talk, ACS Spring Meeting 2014, *Structure for Function: Rational design of new functional polymeric materials* March 2014
95. Invited talk, ACS Spring Meeting 2014, *PMSE Young Investigators Symposium*, March 2014
96. Seminar, Dept. of Materials Engineering, Purdue University, February 2014
97. Seminar, Center for Molecular Engineering and Thermodynamics, University of Delaware, Jan 2014
98. Invited talk, AIChE Annual Meeting 2013, *Modeling and Simulation of Polymers* session, November 2013
99. Invited award talk, AIChE Annual Meeting 2013, *COMSEF Plenary Session*, November 2013
100. Invited talk, APS meeting, Four Corners section, October 2013
101. Seminar, Tulane University, Department of Chemical Engineering, September 2013
102. Invited talk, ACS Fall Meeting, Indianapolis, September 2013
103. Invited talk, APS March Meeting in ‘*Directed Assembly of Hybrid Materials*’ session March 2013
104. Invited talk, Army Research Laboratory, Aberdeen Proving Ground, Maryland, March 2013
105. Invited speaker, Gordon Research Conference Macromolecular Materials, January 2013
106. Seminar, Department of Material Science and Engineering, University of Delaware, December 2012
107. Invited talk, AIChE Annual Meeting 2012, invited talk in *Thermodynamics of Polymers*’ session
108. Invited talk, AIChE Annual Meeting 2012, invited talk in *Emerging Areas in Polymer Science and Engineering* session
109. Invited talk, AIChE Annual Meeting 2012, invited talk in *Multiscale Modeling and Simulation for Renewable Energy* session
110. Seminar, Department of Chemical Engineering, University of Washington, October 2012
111. Seminar, Chemistry Department, Colorado State University, September 2012
112. Seminar, Chancellor’s Invitation to present to CU Alumni and friends, September 2012

- 113.Seminar, Molecular Biophysics Seminar Series, Institute of Computational Engineering and Sciences, University of Texas at Austin, April 2012
- 114.Invited talk, ACS Spring National Meeting COMP division *Integration of Computer Simulation with Experiments* March 2012
- 115.Seminar, Department of Chemical Engineering, Colorado School of Mines, January 2012
- 116.Seminar, Liquid Crystal Materials Research Center, CU Boulder January 2012
- 117.Seminar, Department of Polymer Engineering, University of Akron, Ohio, November 2011
- 118.Seminar, “Young Investigators in Materials Research” UMass Amherst Materials Research Science & Engineering Center (MRSEC) May 2011
- 119.Seminar, Dept. of Chemical Engineering, Rice University, March 2011
- 120.Seminar, Dept. of Chemical Engineering, Texas A&M University, February 2011
- 121.Seminar, Dept. of Materials Science and Engineering, University of Illinois at Urbana, February 2011
- 122.Seminar, Dept of Chemical Engineering, Vanderbilt University, November 2010
- 123.Seminar, Dept. of Applied Math, University of Colorado Boulder, November 2010
- 124.Invited talk, Interfacial Phenomena in Nanostructured Materials and Devices, Telluride Workshop February 2010
- 125.Seminar, Dept. of Chemical Engineering, Colorado State University, October 2009
- 126.Seminar, Condensed Matter Lunch, Dept. of Physics, University of Colorado, Boulder, September 2008

From Doctoral and Postdoctoral Work

- 127.Seminar Dept. of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, April 2008
- 128.Seminar Dept. of Energy, Environmental and Chemical Engineering, Wash U St. Louis, March 2008
- 129.Seminar Dept. of Chemical and Biological Engineering, University of Colorado, Boulder, March 2008
- 130.Seminar Molecular Foundry, Lawrence Berkeley National Laboratories, February 2008
- 131.Seminar Dept. of Chemical Engineering, Lehigh University, February 2008
- 132.Seminar Dept. of Chemical and Biomolecular Engineering, Clemson University, February 2008
- 133.Seminar Dept. of Chemical Engineering, University of South Carolina, February 2008
- 134.Seminar Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, January 2008
- 135.Seminar Dept. of Chemical and Biomolecular Engineering, Ohio State University, January 2008
- 136.Seminar Dept. of Chemical Engineering, University of California, Berkeley, March 2006
- 137.Seminar Center for Engineering in Medicine, Harvard Medical School, February 2006

IX. CONTRIBUTED RESEARCH PRESENTATIONS (*presenter)

With A. Jayaraman as Principal Investigator

1. P. A. Taylor*, A.M. Kloxin, A. Jayaraman, Impact of collagen-like peptide (CLP) triple helix design on CLP melting transition and assembly, Talk, ACS Spring Meeting (2022)
2. S. Lu*, A. Jayaraman, Effect of nanorod physical roughness on the aggregation and percolation of nanorods in polymer nanocomposites, Talk, APS March Meeting (2022)
3. C. Heil*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments of Assembled Mixtures of Nanoparticles, Talk, APS March Meeting (2022)
4. C. Heil*, A. Patil, A. Dhinojwala, A. Jayaraman, Structural Color Production in Melanin-based Disordered Colloidal Nanoparticle Assemblies in Spherical Confinement, Poster, APS March Meeting (2022)
5. Z. Wu*, J.-W. Wu, Q. Michaudel, A. Jayaraman, Computational Study Linking Polysulfamide Chain Design to the Hydrogen Bonding Induced Chain Aggregation, Talk, APS March Meeting (2022)
6. Z. Wu*, A. Jayaraman, Computational reverse-engineering analysis for scattering experiments (CREASE) on thermoresponsive assembly of methylcellulose in aqueous solutions, Poster, APS March Meeting (2022)
7. A. Kulshreshtha*, R. Hayward, A. Jayaraman, Impact of placement and composition of hydrogen bonding groups along polymer chains on blend morphology using coarse-grained molecular dynamics simulations, Talk, APS March Meeting (2022)
8. P. A. Taylor*, A. M. Kloxin, A. Jayaraman, Award Session: Impact of Collagen-like-Peptide (CLP) Triple Helix Design on CLP Melting Transition and Assembly: A Coarse-Grained Molecular Dynamics Simulation Study, Talk, AIChE Annual Meeting (2021)

9. P. A. Taylor*, A. M. Kloxin, A.M., A. Jayaraman, Impact of Collagen-like-Peptide (CLP) Triple Helix Design on CLP Melting Transition and Assembly: A Coarse-Grained Molecular Dynamics Simulation Study, Talk, AIChE Annual Meeting (2021)
10. P. A. Taylor*, A. M. Kloxin, A. Jayaraman, Computational Studies of the Phase Transitions and Self-Assembly of Thermoresponsive Peptide-Based Biomaterials, Poster, AIChE Annual Meeting (2021)
11. A. Kulshreshtha*, R. Hayward, A. Jayaraman, Tuning Structure and Thermodynamics in Polymer Blends Containing Hydrogen Bonding Polymers: A Coarse-Grained Molecular Dynamics Simulation Study, Talk, AIChE Annual Meeting (2021)
12. A. Kulshreshtha*, A. Jayaraman, Theory and Simulation Studies of Structure and Thermodynamics in Polymer Blends and Polymer Nanocomposites with Directional Interactions, Poster, AIChE Annual Meeting (2021)
13. U. Kapoor*, A. Jayaraman, Atomistic Simulation Studies of Synthetic Melanin Particles in Aqueous Solutions with Poly (ethylene glycol), Talk, Virtual MRS Spring Meeting (2021)
14. P. A. Taylor*, A. M. Kloxin, A. Jayaraman, Understanding the impact of sequence length, composition, and dispersity on the melting transition and assembly of collagen-like-peptide (CLP) triple helices, Talk, Virtual MRS Spring Meeting (2021)
15. Z. Wu*, A. Jayaraman, Development of a Coarse-Grained Model to Simulate Assembly within Solutions of Cellulose and Cellulose Derivatives, Talk, Virtual MRS Spring Meeting (2021)
16. Z. Ye*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on the Self-Assembly of Amphiphilic Polymer-peptide Conjugates, Talk Virtual MRS Spring Meeting (2021)
17. A. Kulshreshtha*, R. Hayward, A. Jayaraman, Coarse-grained molecular dynamics simulation study of structure and thermodynamics in blends with hydrogen bonding polymers, Talk, APS March Meeting (2021)
18. C. Heil*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments of Assembled Binary Colloidal Particle Mixtures, Talk, APS March Meeting (2021)
19. M. Wessels*, A. Jayaraman, Computational Reverse Engineering Analysis of Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions, Talk, APS March Meeting (2021)
20. S. Lu*, Z. Wu, A. Jayaraman, Coarse-grained models for predicting the morphology of polymer nanocomposites containing nanorod fillers, Talk, APS March Meeting (2021)
21. J. Kim*, A. Faraone, N. Wagner, A. Jayaraman, Microscopic Structure and Dynamics of Attractive Polymer Nanocomposites, APS March Meeting (2021)
22. Z. Ye*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on the Self-Assembly of Amphiphilic Polymer-peptide Conjugates, Talk, APS March Meeting (2021) C. Heil*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments of Assembled Binary Colloidal Particle Mixtures, AIChE Annual Meeting (2020)
23. M. Wessels*, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions, AIChE Annual Meeting (2020)
24. P. Taylor*, A. Kloxin, A. Jayaraman, Understanding the Impact of Sequence Length, Composition, and Dispersity on the Melting Transitions and Gelation of Collagen-like-Peptides (CLPs), AIChE Annual Meeting (2020)
25. P. Taylor*, K. Kiick, A. Jayaraman Tuning the LCST-like Transition of Elastin-like-Peptide (ELP) and Conjugates of ELP to Collagen-like-Peptide (CLP) Using ELP Sequence and Composition, AIChE Annual Meeting (2020)
26. U. Kapoor*, A. Jayaraman, Understanding the Self-Assembly of Allomelanin Dimers and the Impact of Poly (ethylene glycol) on the Assembly Using Atomistic Simulations, AIChE Annual Meeting (2020)
27. Z. Wu*, A. Jayaraman, A Coarse-Grained Model Capturing Hydrogen Bonding Effect in Cellulose and Its Derivatives, AIChE Annual Meeting (2020)
28. M. Wessels*, C. Johnson, A. Jayaraman, Self-Assembly of Bottlebrush Amphiphilic Polymers Near/on Surfaces: Coarse-Grained Molecular Dynamics Simulation Study, AIChE Annual Meeting (2020)
29. A. Kulshreshtha*, A. Jayaraman, Development of Coarse-Grained Models to Capture Specific and Directional Interactions in Macromolecular Materials, AIChE Annual Meeting (2020)
30. U. Kapoor*, A. Kulshreshtha, A. Jayaraman, Development of Coarse-Grained Polymer Models for Chemistries with Hydrogen Bonding Capability, AIChE Annual Meeting (2020)

31. S. Lu*, Z. Wu, A. Jayaraman, Coarse-Grained Models for Predicting the Morphology of Polymer Nanocomposites Containing Nanorod Fillers, AIChE Annual Meeting (2020)
32. A. Kulshreshtha*, A. Jayaraman, Effect of Attractive Graft-Matrix Interactions on the Dispersion and Aggregation of Polymer Grafted Particles in Polymer Nanocomposites- a Theory and Simulation Study, AIChE Annual Meeting (2020)
33. A. Kulshreshtha*, A. Jayaraman, Molecular engineering of graft and matrix polymers for tuning grafted particle dispersion in polymer nanocomposites: A theory and simulation study, GRS Virtual Polymer Physics Symposium July 2020
34. U. Kapoor*, A. Jayaraman, Unraveling the Morphology of Melanin Nanoparticles Using Atomistic Molecular Dynamics Simulations (Talk), AIChE Annual Meeting 2019
35. Z. Wu*, A. Jayaraman, Development of a New Coarse-Grained Model Capturing Hydrogen Bonding Effects in Polysaccharides (Talk), AIChE Annual Meeting 2019
36. P.A. Taylor*, April. M. Kloxin, A. Jayaraman, Understanding the Impact of Non-Natural Amino Acid Incorporation on the Assembly of Multifunctional Collagen Mimetic Peptides: Simulations and Experiments (Poster), AIChE Annual Meeting 2019
37. P.A. Taylor*, A. Jayaraman, Atomistic and Coarse-Grained Molecular Dynamics Simulations of Elastin-like Peptides and Collagen-like Peptides (Talk), AIChE Annual Meeting 2019
38. J. Young Lee*, D. Pochan, A. Jayaraman, K. Wooley, Self-Assembly of poly(D-glucose carbonate) Amphiphilic Block copolymers in Solution (Talk), APS March Meeting 2019
39. P. Taylor*, A. Prhashanna, A. Jayaraman, Atomistic and Coarse-grained Simulations of Thermoresponsive Biopolymers (Talk), APS March Meeting 2019
40. A. Prhashanna*, A. Jayaraman, Coarse-grained molecular simulation studies of effect of solvent quality on melting thermodynamics of oligonucleic acids (ONA) and ONA-polymer conjugates (Talk), APS March Meeting 2019
41. T. E. Gartner III, M. Hore, A. Jayaraman, Solvent quality and polymer concentration effects in linear and cyclic polymer solutions (Talk), APS March Meeting 2019
42. A. Jayaraman*, Coarse-Grained Models for Predicting Structure and Thermodynamics in Polymer Systems with Specific and Directional Intermolecular Interactions (Talk), APS March Meeting 2019
43. A. Kulshreshtha*, A. Jayaraman, Impact of hydrogen bonding interactions on graft-matrix wetting and structure in polymer nanocomposites Surface segregation of binary particles in photonic colloidal assemblies (Talk), APS March Meeting 2019
44. M. Wessels*, A. Jayaraman, Self-assembly of Bottlebrush Block Polymers at Surfaces using Coarse-grained Molecular Dynamics Simulations (Talk), APS March Meeting 2019
45. T.E. Gartner, III,* A. Jayaraman, Understanding the interplay between polymer architecture and solvent quality through coarse-grained molecular simulation and liquid state theory (Talk), AIChE Annual Meeting 2018
46. T.E. Gartner, III,* A. Jayaraman, Combining Molecular Simulation, Liquid State Theory, and Gibbs Ensemble Techniques to Study the Structure, Thermodynamics, and Phase Behavior of Polymer-Solvent Mixtures (Poster), AIChE Annual Meeting 2018
47. A. Prhashanna*, A. Jayaraman, Coarse-Grained Molecular Simulation Studies of Melting Thermodynamics of Oligonucleic Acids Conjugated with Polymers (talk), AIChE Annual Meeting 2018
48. A. Prhashanna*, J. Condon, P. A. Taylor, A. Jayaraman, Multi-Scale Simulations of Biomacromolecules for Design of Biomaterials (poster), AIChE Annual Meeting 2018
49. A. Kulshreshtha*, A. Jayaraman, Theory and Simulation Studies of Structure and Thermodynamics in Polymer Nanocomposites Containing Grafted Nanoparticles (talk), AIChE October Meeting 2018
50. M. Wessels*, A. Jayaraman, Self-Assembly of Bottlebrush and Star-like Copolymer Architectures in Solution: A Coarse-Grained Molecular Simulation Study (talk), 2018 AIChE Annual Meeting
51. M. Wessels*, A. Jayaraman, Effects of Copolymer Architecture on the Structure and Thermodynamics of Self-Assembly in Block Copolymer Solutions: a Coarse-Grained Molecular Dynamics Study (talk), APS March Meeting 2018
52. T. E. Gartner*, A. Jayaraman, Understanding Linear and Cyclic Polymer Chain Conformations and Thermodynamics in Solution (talk), APS March Meeting 2018

53. I. Lyubimov*, A. Jayaraman, Integrating PRISM theory and molecular dynamics simulations for studying assembly in solutions of block copolymers with varying sequences and composition (talk), APS March Meeting 2018
54. T. B. Martin*, T. E. Gartner, R. Jones, C. Snyder, A. Jayaraman, typyPRISM: A Computational Tool for Liquid-State Theory Calculations of Macromolecular Materials (poster), APS March Meeting 2018
55. T. E. Gartner*, A. Jayaraman, Multiscale Simulation Study of Synthetic Melanin Nanoparticle Self-Assembly (poster), APS March Meeting 2018
56. D. Beltran-Villegas*, A. Jayaraman, Molecular simulations study of assembly in solutions of block copolymers and nanoparticles (talk), APS March Meeting 2018
57. J. Young Lee*, D. Pochan, A. Jayaraman, Self-Assembly of Computationally Designed Amphiphilic Block copolymers in Solution talk), APS March Meeting 2018
58. T. E. Gartner*, A. Jayaraman, Solvent Effects on the Structure and Thermodynamics of Polymer Blends with Varying Architectures, (Talk) 2017 AIChE Annual Meeting, October-November 2017
59. T. E. Gartner*, H. Kuang, E. Kokkoli, A. Jayaraman, Influence of Molecular Design on the Self-Assembly of Single-Stranded DNA Amphiphiles, (Poster) 2017 AIChE Annual Meeting, October-November 2017
60. I. Lyubimov*, D. J. Beltran-Villegas, A. Jayaraman, Comparison of PRISM Theory and Molecular Dynamics Simulations for Studying Assembly in Block Copolymer Solutions of Varying Sequences and Composition, (Poster) 2017 AIChE Annual Meeting, October-November 2017
61. D.J. Beltran-Villegas*, A. Jayaraman, Molecular Simulations Study of Solvophobicity Effects on Assembled Structure in Solutions of Amphiphilic Block Copolymers and Nanoparticles, (Talk) 2017 AIChE Annual Meeting, October-November 2017
62. T. E. Gartner*, A. Jayaraman, Gibbs ensemble-based molecular simulation methods for predicting structure and thermodynamics of polymer films during solvent vapor annealing, (Talk) ACS Fall 2017 Meeting, August 2017
63. D.J. Beltran-Villegas*, A. Jayaraman, Molecular Simulation Study of Assembly of Amphiphilic Copolymers and Nanoparticles: Effect of Copolymer Architecture On Assembled Structure and Thermodynamics, (Talk) ACS Fall Meeting, August 2017
64. I. Lyubimov*, D. Beltran-Villegas, A. Jayaraman, Evaluating PRISM Theory for Predicting Assembly Behaviour of Amphiphilic Copolymers, (Talk) Mid Atlantic Soft Matter Workshop (MASM18), May 2017
65. D.J. Beltran-Villegas*, A. Jayaraman, Molecular simulations study of changing solvophobicity on evolution of micelle structure in amphiphilic polymers, (Talk, sound bite) Mid Atlantic Soft Matter Workshop (MASM18), May 2017
66. T. E. Gartner*, T. H. Epps III, A. Jayaraman, Gibbs Ensemble Simulations of the Solvent Swelling of Polymer Films, (Poster) APS March Meeting 2017
67. T. E. Gartner*, C. K. Shelton, M. A. Morris, A. Jayaraman, T. H. Epps III, Salt Distribution, Domain Spacing, and Interfacial Characteristics in Lithium Ion-Doped Block Polymer Electrolyte Films, (Talk) APS March Meeting 2017
68. K. J. Modica*, T. B. Martin, A. Jayaraman, Effect of Graft Polymer Architecture on the Grafted Layer Structure in Polymer Functionalized Nanoparticles (Talk) APS March Meeting 2017
69. J. Condon*, A. Jayaraman, Molecular simulation studies of phase transitions in diblock polymer conjugates of elastin-like peptides and collagen mimicking peptide triple helices (Poster), ACS Fall Meeting 2016
70. T. Gartner III*, T. H. Epps, A. Jayaraman, Utilizing Gibbs ensemble molecular dynamics and hybrid Monte Carlo/molecular dynamics simulations for efficient study of polymer-solvent phase equilibria, Talk, ACS Fall Meeting 2016
71. A. Jayaraman*, Effect of oligonucleic acid (ONA) backbone design on the thermodynamics of ONA hybridization and melting, Talk, ACS Fall Meeting, August 2016
72. A. Ghobadi*, A. Jayaraman, Effect of Backbone Design on Hybridization Thermodynamics of Oligonucleic Acids: A Coarse-Grained Molecular Dynamics Simulation Study, Talk, APS March Meeting 2016
73. F. Stanzione*, A. Jayaraman, Using Atomistic Molecular Dynamics Simulations to Guide Development of Coarse-Grained Models of Polyethylene glycol (PEG), Elastic-like peptides (ELP) and Collagen-like peptides (CMP) For Biomaterial Design, Poster, APS March Meeting 2016
74. T. B. Martin*, A. Jayaraman, Dispersion-Aggregation and Wetting-Dewetting Phase Transitions in Mixtures of Polymer Grafted Nanoparticles and a Chemically Dissimilar Polymer Matrix Talk APS March Meeting 2016

75. T. Gartner III*, T. H. Epps, A. Jayaraman, Development of Simulation Methods in the Gibbs Ensemble to Predict Polymer-Solvent Phase Equilibria APS March Meeting 2016
76. T. Martin*, A. Jayaraman, Entropic and Enthalpic Driving Forces on Morphology in Polymer Grafted Particle Filled Nanocomposites: Integral Equation Theory and Molecular Simulations, AICHE Annual Meeting 2015
77. F. Stanzione*, A. Jayaraman, Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene Glycol (PEG) Chains in Explicit Water for Designing Peg Based Biomaterials, AICHE Annual Meeting 2015
78. T. Martin*, A. Jayaraman, Dispersion-Aggregation and Wetting-Dewetting Phase Transitions in Mixtures of Polymer Grafted Nanoparticles and a Chemically Dissimilar Polymer Matrix, AICHE Annual Meeting 2015
79. F. Stanzione*, A. Jayaraman, Computational Design of Peptide Containing Poly(ethylene glycol) Brushes for Stimuli Responsive Drug Delivery, AICHE Annual Meeting 2015
80. A. Jayaraman*, H. S. Marsh, Coarse-Grained Simulations and Experiments of 2,5-Bis(3-alkylthiophen-2-yl)Thieno[3,2-b]Thiophene (BTTT) Oligomer Morphology for Organic Electronics Applications, AICHE Annual Meeting 2015
81. A. Ghobadi*, A. Jayaraman, Design of Sulfobetaine-Lysine Copolymers for DNA Complexation and Delivery: Molecular Simulations and Experiments, AICHE Annual Meeting 2015
82. A. Ghobadi*, A. Jayaraman, Using Coarse-Grained Molecular Simulations to Understand Effects of Backbone Chemistry in Oligo-Nucleic Acids on the Thermodynamics of Melting/Hybridization, AICHE Annual Meeting 2015
83. F. Stanzione*, A. Jayaraman, Computational design of polyethylene glycol (PEG) brushes for display of biofunctional molecules for delivery applications. ACS Spring Meeting 2015
84. H. Marsh*, A. Jayaraman, Understanding the effects of physical and chemical features of solvent additives on the bulk heterojunction morphology of blends of conjugated polymers and fullerene derivatives using molecular simulations. ACS Spring Meeting 2015
85. C. Estridge*, A. Jayaraman Molecular dynamics simulations of structure and effective interactions of diblock copolymer grafted nanoparticles in a homopolymer blend matrix. ACS Spring Meeting 2015
86. A. Ghobadi*, A. Jayaraman, Coarse-grained Molecular Simulation Studies of Complexation of Sulfobetaine-Lysine Copolymer and DNA for Gene Delivery, APS March Meeting 2015
87. T. B. Martin*, A. Jayaraman, Theory and Simulation Studies of Effect of Entropic and Enthalpic Driving Forces on Morphology in Polymer Grafted Particle Filled Nanocomposites APS March Meeting 2015
88. T. B. Martin*, A. Jayaraman, Theory and Simulations of Macromolecular Materials, Gordon Research Conference Macromolecular Materials, January 2015 (poster)
89. H. S. Marsh*, A. Jayaraman, Understanding the Effects of Physical and Chemical Features of Additives on the Morphology of Blends of Conjugated Polymers and Fullerene Derivatives Using Molecular Simulations (talk) MRS Fall Meeting 2014
90. A. Jayaraman*, H.S. Marsh Understanding the Effects of Physical and Chemical Features of Additives on the Morphology of Blends of Conjugated Polymers and Fullerene Derivatives Using Molecular Simulations (talk) AICHE Annual Meeting 2014
91. R. Elder*, A. Jayaraman, Structure and Thermodynamics of Single- and Double-Stranded DNA Oligomers Near Hydrophilic and Hydrophobic Functionalized Surfaces (talk), AICHE Annual Meeting 2014
92. T. B. Martin*, A. Jayaraman, Decreasing Polymer Flexibility Improves Wetting and Dispersion of Polymer Grafted Particles in a Chemically Identical Polymer Matrix (poster), AICHE Annual Meeting 2014
93. T. B. Martin*, A. Jayaraman, Effect of Polydispersity in Grafts and Matrix on the Morphology of Polymer Grafted Nanoparticle Filled Polymer Nanocomposites (talk), AICHE Annual Meeting 2014
94. H. Marsh*, A. Jayaraman, G. Rumbles, Molecular simulations and experiments linking molecular features of conjugated polymers to morphology and charge carrier behavior, (poster) XPV Meeting 2014 (Won best poster award)
95. T. B. Martin*, A. Jayaraman, Theory and simulation studies of polymer grafted nanoparticles in polymer matrix: effect of polymer flexibility and polydispersity on particle dispersion, (poster) Gordon conference Polymer Physics 2014
96. T. B. Martin*, A. Jayaraman, Effect of Matrix Polydispersity on Morphology of Hybrid Materials Consisting of Homopolymer Grafted Nanoparticles in a Homopolymer Matrix (poster) APS March Meeting 2014

97. C. Estridge*, A. Jayaraman, Assembly of diblock copolymer grafted nanoparticles in a homopolymer blend matrix (talk) APS March Meeting 2014
98. A. McLelland*, D. Johnson, A. Jayaraman, Coarse-grained molecular dynamics simulations linking molecular features of polycations to polycation-polyanion complexation for gene delivery (poster) APS March Meeting 2014
99. H. Marsh*, E. Jankowski, A. Jayaraman, Using Molecular Simulations to Link Chemical and Physical Features of Conjugated Polymers and Fullerene Derivatives to Bulk Heterojunction Morphology for Organic Photovoltaics (talk) APS March Meeting 2014
100. A. Jayaraman*, Using theory and simulation to link molecular features of nanoscale fillers to morphology in polymer nanocomposites (talk) Dillon Medal Symposium ApS March Meeting 2014
101. T. Martin, A. Jayaraman*, Effects of Polydispersity in Graft and Matrix Polymer on the Morphology of Composites Comprising Polymer Grafted Nanoparticles in a Polymer Matrix: A Theory and Simulation Study (talk), MRS Fall Meeting 2013
102. H. Marsh*, A. Jayaraman, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology (talk) MRS Fall meeting 2013
103. A. Jayaraman*, Computational Design of Ligands to Graft on Nanoparticle Surfaces to Tailor Nanoparticle Dispersion or Assembly in a Medium (talk), Cabot Corporation, August 2013
104. E. Jankowski*, H. Marsh, A. Jayaraman, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology (talk) AIChE Annual meeting 2013
105. R. Elder*, A. Jayaraman, Nanoscale behavior of DNA oligomers near hydrophobic and hydrophilic functionalized surfaces. (talk) AIChE Annual Meeting 2013
106. R. Elder* and A. Jayaraman, Molecular Simulation Studies Relating Polycation Architecture to the Structure and Thermodynamics of Polycation-DNA Complexes (poster) GRC Macromolecular Materials 2013
107. R. Elder* and A. Jayaraman “Sequence Specific Recognition of Cancer Drug-DNA Adducts by HMGB1a Repair Protein” (talk) Gordon Research Seminar (Students) Macromolecular Materials 2013
108. T. Martin* and A. Jayaraman,” Theory and simulation studies of polymer functionalized nanoparticles with heterogeneity in polymer grafts.”(poster) Gordon Conference Macromolecular Materials 2013
109. A. Jayaraman*, T. Martin, A. Seifpour, Effect of Monomer Sequence on Assembly of Copolymer Functionalized Nanoparticles: A Computational Study, (talk) MRS Fall Meeting 2012
110. R. Elder* and A. Jayaraman “Sequence Specific Recognition of Cancer Drug-DNA Adducts by HMGB1a Repair Protein” (talk) AIChE Annual Meeting 2012
111. R. Elder* and A. Jayaraman, Molecular Simulation Studies Relating Polycation Architecture to the Structure and Thermodynamics of Polycation-DNA Complexes (poster) AIChE Annual Meeting 2012
112. A. Seifpour* and H. Marsh, Molecular Simulation Studies of Assembly of DNA-Grafted Nanoparticles: Effect of Grafted DNA Strand Sequence and Composition (poster) AIChE Annual Meeting 2012
113. H. Marsh* and A. Jayaraman, Molecular Simulations of Blends of Conjugated Polymers and Fullerene Derivatives for Bulk Heterojunction Organic Solar Cells (poster) AIChE Annual Meeting 2012
114. A. Jayaraman*,” Theory and simulation studies of polymer functionalized nanoparticles with heterogeneity in polymer grafts.”(poster) Gordon Conference Polymer Physics July 2012
115. Robert Elder* and A. Jayaraman,” Understanding the effect of polylysine architecture on DNA binding using molecular dynamics simulations”, (poster) Gordon Conference Polymer Physics July 2012
116. T. Martin*, A. Jayaraman, “Effect of competing monomer-monomer and monomer-particle interactions on the assembly of copolymer grafted nanoparticles”, (talk) APS March Meeting, March 2012
117. A. Jayaraman*, N. Nair, “Effect of bidispersity in grafted chain length on potential of mean force between polymer grafted nanoparticles in a homopolymer matrix”, (talk) APS march meeting , March 2012
118. C. Starbird*, D. Zhang, A. Jayaraman, “Dissipative particle dynamics studies of rod-coil polymer nanocomposites” (talk) APS march meeting March 2012
119. P. Dodd*, A. Jayaraman, “Polydispersity effects on scaling behavior of polymers grafted on surfaces with varying curvature”, (poster) APS march meeting, March 2012
120. A. Jayaraman*, N. Nair, “Integrated Theory and Simulation Approach for Studying Polymer Functionalized Nanoparticles In Polymer Nanocomposites”, (talk) COMSEF Plenary Session, AIChE Annual Meeting, October 2011
121. A. Seifpour*, A. Jayaraman, “Monte Carlo Simulations of the Assembly of Copolymer Functionalized Nanoparticles”, (talk) AIChE Annual Meeting, October 2011

- 122.A. Jayaraman*, R. Elder, “Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery”, (talk) AIChE Annual Meeting, October 2011
- 123.R. Elder*, A. Jayaraman, “Molecular dynamics simulation studies of recognition of anticancer drug-induced DNA damage by repair proteins” (poster) First Annual Front Range High Performance Computing Symposium, Golden CO September 2011
- 124.H. Marsh*, A. Jayaraman, “ Molecular Simulations of Conjugated Polymers and Fullerene Derivatives for Bulk Heterojunction Organic Solar Cells”, (poster) First Annual Front Range High Performance Computing Symposium, Golden CO September 2011
- 125.C. Starbird*, A. Jayaraman “ Dissipative Particle Dynamics Simulations of Morphology within Conjugated Block Copolymers” (poster) First Annual Front Range High Performance Computing Symposium, Golden CO September 2011
- 126.X. Ba*, A. Jayaraman “ Molecular Dynamics Simulation Studies of Polyamine-DNA Binding “(poster) First Annual Front Range High Performance Computing Symposium, Golden CO September 2011
- 127.A. Jayaraman*, Theory and molecular simulations of functionalized nanoparticles in polymer nanocomposites (talk) ACS National Meeting, August 2011
- 128.R. Elder*, A. Jayaraman “Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors” (talk) ACS National Meeting, August 2011
- 129.R. Elder*, A. Jayaraman “Molecular Dynamics Simulations for Recognition of Anticancer-Drug induced DNA damage by Repair Proteins” (poster) ACS National Meeting, August 2011
- 130.A. Jayaraman*, R. Elder, “Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery”, (talk) IUPAC World Chemistry Congress, August 2011
- 131.A. Jayaraman*, N. Nair, A. Seifpour, N. Wentzel, Designing Functionalized Nanoparticles for Controlled Assembly in Polymer Matrix: Self consistent PRISM Theory and Monte Carlo simulation Study’, (talk) American Physical Society March meeting, March 2011
- 132.R. Elder*, A. Jayaraman “Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors” (poster) Gordon Research Conference Macromolecular Materials, January 2011
- 133.A. Jayaraman*, N. Nair, “Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Nanocomposite” (poster) Gordon Research Conference Macromolecular Materials, January 2011
- 134.A. Jayaraman*, Nitish Nair “Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix” (talk) AIChE Annual Meeting, November 2010
- 135.A. Seifpour*, A. Jayaraman, “Monte Carlo Simulations of Assembly of Copolymer Functionalized Spherical Nanoparticles”, (talk) AIChE Annual Meeting, November 2010
- 136.A. Jayaraman*, R. Elder, M. Seyam “Molecular Dynamics Simulation Study of DNA Damage Recognition” (talk) AIChE Annual Meeting, November 2010
- 137.R. Elder*, A. Jayaraman, “Molecular Dynamics Simulation Studies of Polycation-DNA Binding for Gene Delivery”, (poster) AIChE Annual Meeting, November 2010
- 138.A. Jayaraman*, Nitish Nair “Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix” (poster) Gordon Research Conference Polymer Physics, June 2010
- 139.A. Seifpour*, Nitish Nair, A. Jayaraman “Functionalized nanoparticles in polymer nanocomposites” (poster) Energy Institute Student Poster Session, Boulder CO April 2010
- 140.A. Jayaraman*, Arezou Seifpour, Phil Spicer, Nitish Nair, “Theory and simulation of copolymer grafted nanoparticles in polymer nanocomposites” (talk) APS March Meeting, Portland OR, March 2010
- 141.Nitish Nair*, A. Jayaraman “Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix” (poster) APS March Meeting, Portland OR, March 2010
- 142.A. Jayaraman*, Arezou Seifpour, Phil Spicer, Nitish Nair, “Theory and simulation of copolymer grafted nanoparticles in polymer nanocomposites” (talk) AIChE Annual Meeting, Nashville, TN November 2009
- 143.A. Jayaraman* Arezou Seifpour, Phil Spicer, “Theory and simulation of copolymer grafted nanoparticles in polymer nanocomposites” (poster) Fundamentals of Molecular Modelling and Simulations, July 2009

From A. Jayaraman’s Graduate and Postdoctoral Research

1. A. Jayaraman* and K. S. Schweizer, “Theoretical study of polymer tethered nanoparticles as novel fillers in polymer nanocomposites’ (talk) APS March Meeting, Pittsburgh, PA March 2009

2. A. Jayaraman* and K. S. Schweizer, 'Theoretical study of polymer tethered nanoparticles as novel fillers in polymer nanocomposites' (talk) AIChE Annual Meeting, Philadelphia, PA November 2008
3. A. Jayaraman* and K. S. Schweizer, 'Structure and phase behavior of melts and dense solutions of polymer tethered nanoparticles and colloids' APS March Meeting, New Orleans, LA March 2008
4. A. Jayaraman* and K. S. Schweizer, 'Structure and phase behavior of melts and dense solutions of polymer tethered nanoparticles and colloids' (talk) AIChE Annual Meeting, Salt Lake City, UT November 2007
5. A. Jayaraman* and K. S. Schweizer, 'Structure and phase behavior of melts and dense solutions of polymer tethered nanoparticles and colloids' (talk) 81st ACS Colloid and Surface Science Symposium, Newark, DE, June 25, 2007
6. A. Jayaraman*, 'Computational and Theoretical Studies of Soft Materials and Biological Systems' poster presentation AIChE Annual Meeting, Salt Lake City, UT November 2007
7. A. Jayaraman*, C. K. Hall and J. Genzer, 'A Computer Simulation and Theoretical Study of Molecular Recognition in Model DNA Microarrays' (talk) AIChE Conference, November 14, 2006, San Francisco, CA
8. A. Jayaraman*, C. K. Hall and J. Genzer, 'A Computer Simulation and Theoretical Study of Molecular Recognition in Model DNA Microarrays' (poster) Polymer Physics Gordon Conference, June 2006.
9. A. Jayaraman*, C. K. Hall and J. Genzer, 'A Computer Simulation and Theoretical Study of Molecular Recognition in Model DNA Microarrays' (talk) AIChE Conference, October 31, 2005, Cincinnati, OH
10. A. Jayaraman*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' AIChE Conference, October 30, 2005, Cincinnati, OH
11. A. Jayaraman*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' (poster) Thermo 2005, College Park, MD
12. A. Jayaraman*, C. K. Hall and J. Genzer, 'Designing pattern recognition surfaces for copolymers using computer simulation' (talk) AIChE Conference, November 10, 2004, Austin, TX
13. A. Jayaraman*, C. K. Hall and J. Genzer, 'Designing pattern recognition surfaces for copolymers using computer simulation' (poster) 10th PPEPPD Conference, May 18, 2004, Snowbird, UT.
14. A. Jayaraman*, C. K. Hall and J. Genzer, 'Designing pattern recognition surfaces for copolymers using computer simulation' (poster) Richard D. Gilbert Award Symposium, ACS Polymer Discussion Group, February 12, 2004, Raleigh, NC.
15. A. Jayaraman*, C. K. Hall and J. Genzer, 'Designing pattern recognition surfaces for copolymers using computer simulation' (talk) AIChE Conference, November 20, 2003, San Francisco, CA.

X. TEACHING

(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** UG and G Elective 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) co-taught with Prof. April Kloxin (Fermentation) and instructor Dr. Sunita Sadala (BioDiesel)
- **Spring 2022** Computing and Data Science for Soft Materials Innovation and Design CHEG 867-015 (15 students) co-taught with Prof. Sunita Chandrasekaran

(2008-2014) at UNIVERSITY OF COLORADO, BOULDER

(Course rating and Instructor rating on a scale from 1 (low) to 6 (high))

- **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)

GRADUATE STUDENTS

<u>Name</u>	<u>Dept./Univ.</u>	<u>Title (Current Position)</u>	<u>Period</u>
Stephen Kronenberger	CBE (UD)	1 st year PhD student	01/2022-current
Shizhao Lu	CBE (UD)	3 rd year PhD student	01/2020-current
Jihyuk Kim	CBE (UD)	3 rd year MS student (primary advisor: Norm Wagner)	01/2020- current
Christian Heil	CBE (UD)	4 th year PhD student	01/2019-current
Zijie Wu	CBE (UD)	4 th year PhD student	01/2019-current
Phillip Taylor	CBE (UD)	5 th year PhD student (secondary advisor: April Kloxin)	05/2018-current
Arjita Kulshreshta	CBE(UD)	5 th year PhD student	01/2018-current
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>	<u>Period</u>
Shivam Chauhan	CBE (UD)	Undergrad research	01/2022-current
Geoffrey Bonanzino	CBE (UD)	Undergrad research	05/2020-current
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

<u>Name</u>	<u>Title (Current Position)</u>	<u>Period</u>
Umashankar Erigi	Postdoc	12/2021-current
Ziyu Ye	Postdoc (unknown)	08/2020-08/2021
Utkarsh Kapoor	Postdoc (currently at Texas A&M)	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 (currently at DSL)	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 Assoc. 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 know BP)	01/2010-03/2011
Nitish Nair	Postdoc (currently at Shell)	06/2009-12/2010

COMPLETED DOCTORAL and MASTERS DEGREES (last known position)

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

XII. RESEARCH AWARDS TO GRADUATE STUDENTS MENTORED

Robert Elder	UColorado 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: Organic semiconducting materials)
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 Thomas E. Gartner	Best Poster Award, PMSE Division, ACS Fall Meeting 2016 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 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 poster award for MRS 2021 Spring meeting SM09: Peptide and Protein Design for Responsive Materials symposium 1 st place in ‘Outstanding Biomaterials Graduate Research’ Area 08B: AICHE Annual Meeting 2021

XIII. PROFESSIONAL SERVICE ACTIVITIES (2008—present)

Editorial Board/Editorial Advisory Boards

- Deputy Editor, ACS Polymers Au (2021 – present)
- Associate Editor, Macromolecules (2019 – present)
- Editorial Board, Polymer Theory and Simulation section, Polymers (2020 – present)
- Editorial Board, Theory and Simulation section, Current Opinion in Colloid and Interface Science (2020 – present)
- Editorial advisory board of Journal of Polymer Science B: Polymer Physics (August 2018 – present)
- Editorial advisory board of new RSC Journal Molecular Systems Design and Engineering (March 2017-present)
- Editorial Advisory Board of Macromolecules and ACS Macro Letters 01/2015- 01/2018

Meetings, conferences, workshops

- Main organizer of 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

- Serving on DPOLY Nomination Committee (2020 – present)
- Serving on Advisory Board for UPenn-Grenoble REACT center grant (2015- present)
- Elected “Member at Large” Division of Polymer Physics (DPOLY), Executive Committee, APS (2017-2020)
- 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. DEPARTMENT, COLLEGE, UNIVERSITY of DELAWARE SERVICE (2014-)

- **NRT Graduate Traineeship**
 - Director of NRT program (Fall 2021 – present)
 - Chair of NRT Program Coordinator 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)
 - Secondary Thesis Advisor for 2021 NRT trainees: George Kramerenko (BME, UD), Kayla Hapler (MSEG, UD), Peter Osazuwa (MSEG, UD), Ai Nin Nang (CHEM, UD)
- **Department of Chemical and Biological Engineering (University of Delaware)**
 - 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)
 - Member of PhD Thesis Committee (Melody Morris (2014-2019), Amber Hildebrand (2014-2019), Hao Wang (2015-2019), David Phan (2016-current), Glenn Ferriera (2016-2019), Josh Lansford (2016-2020), Priyanka Ketkar (2018-current), Jon Wilson (2018-current), Mukund Kabra (2018-current), Akash Vaidya (2019-current), Jingya Chen (MSE, 2017-2021), Jee Young (MSE, 2016-2021)
- **Department of Materials Science and Engineering (University of Delaware)**
 - Member of Chair search committee (Spring 2022)
 - Member of materials theory faculty search committee (2014-15)
 - Member of PhD Thesis Committee (Brian Sobieski (2015-17), Jee Young (2017-current), Jingya Qin (2018 – current)
- **College of Engineering (University of Delaware)**
 - Member of Diversity in Graduate Programs Committee, College of Engineering (2016-2017)

- **Data Science Institute (University of Delaware)**
 - Faculty council member (2020 – 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 2019-2020)
 - Member of search committee for Grants Facilitator, Research Office, University of Delaware

XV. DEPARTMENT, COLLEGE, UNIVERSITY of COLORADO SERVICE (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:
 - Ryan Crisman (2008-09), Brett Ludwig (2008-09), Brett Voss (2008-2011), Josh McCall (2009-2012), Lauren Andrews (2009-2013) Sean Ryland (2010-2012) Peter Mitrano (2011- 2014), Aaron Murray (2011-2012), Blake Langdon (2011-2014), Jon Monserud (2011-current), Blaine Carter (2011-2014), Kyle Berger (2012- 2014)
 - Undergraduate Freshman Advisor (2008-2009) Undergraduate Sophomore Advisor (2009-2010), Undergraduate Junior Advisor (2010-2011)