# ARTHI JAYARAMAN

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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	
Patten Assistant Professor Department of Chemical and Biological Engineering University of Colorado (CU), Boulder	11/2011 - present
Fellow Materials Science and Engineering Program University of Colorado (CU), Boulder	11/2012 - present
Assistant Professor Department of Chemical and Biological Engineering University of Colorado (CU), Boulder	08/2008 - present
Postdoctoral Research Associate Department of Material Science and Engineering University of Illinois, Urbana-Champaign (Advisor: Dr. Kenneth Schweizer)	06/2006 – 08/2008
Graduate Research Assistant Department of Chemical and Biomolecular Engineering North Carolina State University (Advisors: Dr. Carol Hall and Dr. Jan Genzer)	01/2001 - 05/2006

## III. HONORS/AWARDS

- ACS Polymeric Materials Science and Engineering (PMSE) Young Investigator 2014
- Provost Faculty Achievement Award 2013
- AIChE Computational Molecular Science and Engineering Forum (COMSEF) Young Investigator Award 2013
- Featured in Soft Matter's Emerging Investigators Issue 2013
- Featured in Journal of Polymer Science B: Polymer Physics Young Investigators Issue 2013
- Patten Faculty Fellow, University of Colorado (2011-15)
- University of Colorado College of Engineering Dean's Faculty Fellowship 2011-12
- Department of Energy (DOE) Early CAREER Research Award 2010
- Outstanding Faculty Undergraduate Teaching Award in Dept. of Chemical Engineering CU Boulder 2010–11

- ACS Women Chemist Committee Lectureship Award 2010
- Edward M. Schoenborn Award for outstanding graduate research, Department of Chemical Engineering, NC State University, 2006
- Richard D. Gilbert Award for Best Poster, ACS Polymer Discussion Group, NC section, 2004
- Monali Dey Award for outstanding undergraduate student Chemical Engineering department, Birla Institute of Technology and Science, Pilani, 2000

#### IV. RESEARCH INTERESTS

The overarching goal of my group's research is to elucidate molecular-level phenomena governing macroscopic events/properties in complex materials and biological systems using theoretical and simulation techniques. My group currently focuses on the following main research thrusts:

- 1. Polymer Functionalized Nanoparticles And Polymer Nanocomposites
- 2. Molecular Design of Conjugated Polymers for Organic Electronic Materials
- 3. Molecular Simulations of Macromolecular Binding and Recognition in Nucleic Acid Systems

## V. PEER-REVIEWED PUBLICATIONS

(\* denotes corresponding author, † denotes undergraduate)

### Under review:

J.J. Roberts, R.Elder, **A. Jayaraman**, S.J. Bryant\*. Characterization of Matrix Retaining Hydrogels Containing Hyaluronan Binding Peptides. *Biomacromolecules* (under review)

### Published/Accepted:

- 1. 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* (accepted) **DOI:** 10.1021/ma401763y
- 2. 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* (accepted and in press)
- 3. A. Seifpour, S. Dahl, **A. Jayaraman\***, Molecular simulation studies of assembly of DNA-grafted particles-Effect of bidispersity in DNA strand length. *Molecular Simulation* (published online)
- **4.** 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)
- 5. 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)
- E. Jankowski<sup>#</sup>, H. S. Marsh<sup>#</sup>, A. Jayaraman<sup>\*</sup>, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology *Macromolecules* 2013 (# equal contribution) 46 (14) 5775-5785 (2013) (This was one of 20 most downloaded articles from Macromolecules in July 2013)

- 7. 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 9 (29), 6876 – 6889 (2013)
- **8.** A. Seifpour, S. Dahl, B. Lin<sup>†</sup>, **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
- 9. 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)
- 10. T. Martin, P. Dodd<sup>†,</sup> **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)
- 11. T. Martin, C. McKinney<sup>†</sup>, **A. Jayaraman\***, Effect of monomer sequences and particle monomer interactions on assembly of copolymer grafted nanoparticles' *Soft Matter* **9**, 155-169 (2013)
- 12. 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)
- 13. R. Elder, **A. Jayaraman\***, "Coarse-grained simulation studies of effects of polycation architecture on structure of the polycation and polycation-polyanion complexes" *Macromolecules* (19), pp 8083-8096 (2012)
- 14. R. Elder, **A. Jayaraman\***, 'Sequence specific recognition of cancer drug-DNA adducts by HMGB1a repair protein', *Biophysical Journal* Volume 102, Issue 10, Pages 2331–2338, (2012)
- 15. **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" in *Molecular Simulation* 38, Issue 8-9, pages 751-761, (2012)
- 16. 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* Volume 50, Issue 10, pages 694–705, (2012)
- 17. 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* Volume 38, Issue 10, pages 793-808 (2012)
- 18. 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)
- 19. T. B. Martin<sup>†#</sup>, A. Seifpou<sup>r#</sup>, **A. Jayaraman\***, Assembly of copolymer functionalized nanoparticles: A Monte Carlo simulation study' *Soft Matter* **7**, 5952-5964 (# equal contributions, † undergraduate) (2011)
- 20. 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)
- 21. N. Nair and **A. Jayaraman\***, 'Self-Consistent PRISM Theory-Monte Carlo Simulation Studies of Copolymer Grafted Nanoparticles in a Homopolymer Matrix' *Macromolecules* 43 (19), pp 8251–8263 (2010)

22. A. Seifpour, P. Spicer<sup>†</sup>, 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*) († undergraduate)

## Papers from A. Jayaraman's Doctoral and Postdoctoral Work

- 23. 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
- **24. A. Jayaraman\*** and K. S. Schweizer, 'Liquid state theory of the structure and phase behaviour of polymertethered nanoparticles in dense suspensions, melts and nanocomposites' invited review article in Frontiers of Molecular Simulation, special issue) Molecular Simulation 35, 835-848 (2009)
- 25. **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)
- 26. **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)
- **27. 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)
- 28. **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) (Selected to appear in *Virtual Journal of Nanoscale Science & Technology* and *Virtual Journal of Biological Physics*)
- 29. **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) (Selected to appear in *Virtual Journal of Biological Physics*)
- 30. **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) (Selected to appear in *Virtual Journal of Biological Physics*)
- 31. **A. Jayaraman**, C. K. Hall\* and J. Genzer, 'Computer simulation study of molecular recognition in model DNA microarrays' *Biophys. J.*, 91, 2227 (2006)
- **32.** 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) (Selected to appear in *Virtual Journal of Biological Physics*)
- 33. 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)
- 34. 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) (Selected to appear in *Virtual Journal of Biological Physics*)

## VI. INVITED TALKS (by A. Jayaraman)

#### After joining University of Colorado Boulder

- 1. ACS Spring Meeting 2014, Structure for Function: Rational design of new functional polymeric materials March 2014
- 2. ACS Spring Meeting 2014, PMSE Young Investigators Symposium, March 2014
- 3. AICHE Annual Meeting 2013, Modeling and Simulation of Polymers session, November 2013
- 4. AIChE Annual Meeting 2013, COMSEF Plenary Session, November 2013
- 5. APS meeting, Four Corners section, October 2013
- 6. Tulane University, Department of Chemical Engineering, September 2013
- 7. ACS Fall Meeting, Indianapolis, September 2013
- 8. APS March Meeting in 'Directed Assembly of Hybrid Materials' session March 2013
- 9. Army Research Laboratory, Aberdeen Proving Ground, Maryland, March 2013
- 10. Gordon Research Conference Macromolecular Materials, January 2013
- 11. Seminar, Department of Material Science and Engineering, University of Delaware, December 2012
- 12. AICHE Annual Meeting 2012, invited talk in Thermodynamics of Polymers' session
- 13. AICHE Annual Meeting 2012, invited talk in Emerging Areas in Polymer Science and Engineering session
- 14. AICHE Annual Meeting 2012, invited talk in Multiscale Modeling and Simulation for Renewable Energy session
- 15. Seminar, Department of Chemical Engineering, University of Washington, October 2012
- 16. Seminar, Chemistry Department, Colorado State University, September 2012
- 17. Seminar, Chancellor's Invitation to present to CU Alumni and friends, September 2012
- 18. Seminar, Molecular Biophysics Seminar Series, Institute of Computational Engineering and Sciences, University of Texas at Austin, April 2012
- 19. ACS Spring National Meeting COMP division Integration of Computer Simulation with Experiments (talk) March 2012
- 20. Seminar, Department of Chemical Engineering, Colorado School of Mines, January 2012
- 21. Seminar, Liquid Crystal Materials Research Center, CU Boulder January 2012
- 22. Seminar, Department of Polymer Engineering, University of Akron, Ohio, November 2011
- 23. "Young Investigators in Materials Research" UMass Amherst Materials Research Science & Engineering Center (MRSEC) May 2011
- 24. Seminar, Dept. of Chemical Engineering, Rice University, March 2011
- 25. Seminar, Dept. of Chemical Engineering, Texas A&M University, February 2011
- 26. Seminar, Dept. of Materials Science and Engineering, University of Illinois at Urbana, February 2011
- 27. Seminar, Dept of Chemical Engineering, Vanderbilt University, November 2010
- 28. Seminar, Dept. of Applied Math, University of Colorado Boulder, November 2010
- 29. Interfacial Phenomena in Nanostructured Materials and Devices, Telluride Workshop February 2010
- 30. Seminar, Dept. of Chemical Engineering, Colorado State University, October 2009
- 31. Condensed matter lunch seminar, Dept. of Physics, University of Colorado, Boulder, September 2008

### Prior to joining University of Colorado Boulder

- 32. Seminar Dept. of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, April 2008
- 33. Seminar Dept. of Energy, Environmental and Chemical Engineering, WU St. Louis, March 2008
- 34. Seminar Dept. of Chemical and Biological Engineering, University of Colorado, Boulder, March 2008
- 35. Seminar Molecular Foundry, Lawrence Berkeley National Laboratories, February 2008
- 36. Seminar Dept. of Chemical Engineering, Lehigh University, February 2008
- 37. Seminar Dept. of Chemical and Biomolecular Engineering, Clemson University, February 2008
- 38. Seminar Dept. of Chemical Engineering, University of South Carolina, February 2008
- 39. Seminar Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, January 2008
- 40. Seminar Dept. of Chemical and Biomolecular Engineering, Ohio State University, January 2008
- 41. Seminar Dept. of Chemical Engineering, University of California, Berkeley, March 2006
- 42. Seminar The Center for Engineering in Medicine, Harvard Medical School, February 2006

## VII. CONTRIBUTED PRESENTATIONS (\*presenter)

### With A. Jayaraman as Principal Investigator

- 1. 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
- 2. H. Marsh\*, A. Jayaraman, Computationally linking molecular features of conjugated polymers and fullerene derivatives to bulk heterojunction morphology (talk) MRS Fall meeting 2013
- 3. 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
- 4. 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
- 5. R.Elder\*, A. Jayaraman, Nanoscale behavior of DNA oligomers near hydrophobic and hydrophilic functionalized surfaces. (talk) AICHE Annual Meeting 2013
- 6. T. Martin\*, A. Jayaraman, Molecular Simulations Studies of Polydispersity Effects on The Morphology of Polymer Nanocomposites (talk), AICHE Annual Meeting 2013
- 7. R. Elder \*, A. Jayaraman, DNA at the Nanoscale: Interactions with Proteins, Polycations and Surfaces (poster) AICHE Annual Meeting 2013
- 8. A. Jayaraman\*, T. Martin, Theory and Simulations of Polymer Functionalized Nanoparticles (poster), PPEPPD 2013 Iguazu Argentina
- 9. A .Jayaraman\*, R. Elder, Thernodynamics guided design of vectors for DNA delivery (talk), ACS Spring Meeting 2013
- 10. E. Jankowski\*, H. Marsh, A. Jayaraman, Molecular Simulation Studies of Morphology in Conjugated polymer Acceptor Blends (talk), APS march Meeting 2013,
- 11. T. Martin\* and A. Jayaraman, Using Polydispersity in Polymer Grafted Particles to Tune Morphology in Polymer Nanocomposites (talk), APS March meeting 2013
- 12. 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
- 13. 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
- 14. T. Martin\* and A. Jayaraman," Theory and simulation studies of polymer functionalized nanoparticles with heterogeneity in polymer grafts." (poster) Gordon Conference Macromolecular Materials 2013
- 15. A. Jayaraman\*, T. Martin, A. Seifpour, Effect of Monomer Sequence on Assembly of Copolymer Functionalized Nanoparticles: A Computational Study, (talk) MRS Fall Meeting 2012
- 16. R. Elder\* and A. Jayaraman "Sequence Specific Recognition of Cancer Drug-DNA Adducts by HMGB1a Repair Protein" (talk) AICHE Annual Meeting 2012
- 17. 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
- 18. 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
- 19. 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
- 20. A. Jayaraman\*," Theory and simulation studies of polymer functionalized nanoparticles with heterogeneity in polymer grafts." (poster) Gordon Conference Polymer Physics July 2012
- 21. 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
- 22. 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
- 23. 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
- 24. C. Starbird\*, D. Zhang, A. Jayaraman, "Dissipative particle dynamics studies of rod-coil polymer nanocomposites" (talk) APS march meeting March 2012
- 25. P. Dodd\*, A. Jayaraman, "Polydispersity effects on scaling behavior of polymers grafted on surfaces with varying curvature", (poster) APS march meeting, March 2012

- 26. 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
- 27. A. Seifpour\*, A. Jayaraman, "Monte Carlo Simulations of the Assembly of Copolymer Functionalized Nanoparticles", (talk) AIChE Annual Meeting, October 2011
- 28. A. Jayaraman\*, R. Elder, "Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery", (talk) AIChE Annual Meeting, October 2011
- 29. 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
- 30. 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
- 31. 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
- 32. 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
- 33. A. Jayaraman\*, Theory and molecular simulations of functionalized nanoparticles in polymer nanocomposites (talk) ACS National Meeting, August 2011
- 34. R. Elder\*, A. Jayaraman "Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors" (talk) ACS National Meeting, August 2011
- 35. R. Elder\*, A. Jayaraman "Molecular Dynamics Simulations for Recognition of Anticancer-Drug induced DNA damage by Repair Proteins" (poster) ACS National Meeting, August 2011
- 36. A. Jayaraman\*, R. Elder, "Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery", (talk) IUPAC World Chemistry Congress, August 2011
- 37. 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
- 38. R. Elder\*, A. Jayaraman "Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors" (poster) Gordon Research Conference Macromolecular Materials, January 2011
- 39. 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
- 40. A. Jayaraman\*, Nitish Nair "Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix" (talk) AIChE Annual Meeting, November 2010
- 41. A. Seifpour\*, A. Jayaraman, "Monte Carlo Simulations of Assembly of Copolymer Functionalized Spherical Nanoparticles", (talk) AIChE Annual Meeting, November 2010
- 42. A. Jayaraman\*, R. Elder, M. Seyam "Molecular Dynamics Simulation Study of DNA Damage Recognition" (talk) AIChE Annual Meeting, November 2010
- 43. R. Elder\*, A. Jayaraman, "Molecular Dynamics Simulation Studies of Polycation-DNA Binding for Gene Delivery", (poster) AIChE Annual Meeting, November 2010
- 44. 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
- 45. A. Seifpour\*, Nitish Nair, A. Jayaraman "Functionalized nanoparticles in polymer nanocomposites" (poster) Energy Institute Student Poster Session, Boulder CO April 2010
- 46. 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
- 47. 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
- 48. 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

49. 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

- 50. 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
- 51. 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
- 52. 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
- 53. 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
- 54. 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
- 55. A. Jayaraman\*, 'Computational and Theoretical Studies of Soft Materials and Biological Systems' poster presentation AIChE Annual Meeting, Salt Lake City, UT November 2007
- 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
- 57. 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.
- 58. 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
- 59. A. Jayaraman\*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' AIChE Conference, October 30, 2005, Cincinnati, OH
- 60. A. Jayaraman\*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' (poster) Thermo 2005, College Park, MD
- 61. 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
- 62. 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.
- 63. 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.
- 64. 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.

## VIII. TEACHING (08/2008-present)

(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 Course Rating: 4.2 Instructor Rating: 4.7
- **Spring 2009** ProcessControl CHEN4570 (64 students) 4 credits Course Rating: 5.2 Instructor Rating: 4.7
- **Spring 2010** ProcessControl CHEN4570 (1 section of lecture, 2 sections of lab) (69 students) 4 credits Course Rating: 4.1 Instructor Rating: 4.3
- **Spring 2011** ProcessControl CHEN4570-01 (1 section lecture, 1.5 sections of lab) (49 students) 4 credits Course Rating: 4.2 Instructor Rating: 4.5
- **Spring 2011** ProcessControl CHEN4570-0**2** (1 section lecture, 1.5 sections of lab) (47 students) 4 credits Course Rating: 4.6 Instructor Rating: 5.0
- Spring 2012 ProcessControl CHEN4570-01 (1 section lecture, 1.5 sections of lab) (52 students) 4 credits Course Rating: 3.5 Instructor Rating: 3.3

- Spring 2012 ProcessControl CHEN4570-02 (1 section lecture, 1.5 sections of lab) (50 students) 4 credits Course Rating: 3.7 Instructor Rating: 3.7
- Fall 2012 CHEN5838 Molecular Modeling and Simulation of Materials and Biological Systems (15 students) 3 Credits

Course Rating: 5.6 Instructor Rating: 5.7

• **Spring 2013** ProcessControl CHEN4570 (1 section lecture, 2 sections of lab, 2 sections of recitation) (81 students) – 4 credits

Course Rating: 4.9 Instructor Rating: 5.4

• Fall 2013 Analytical Methods Chemical Engineering CHEN5740 (1 section lecture) (25 students)

## IX. PERSONNEL SUPERVISED (08/2008 – present)

### **GRADUATE STUDENTS**

<u>Name</u>	<b>Department</b>	Title (Current Position)	<b>Period</b>
Robert Elder	ChBE	5th year PhD student	01/2010- current
Hilary Marsh	ChBE	4 <sup>th</sup> year PhD student	01/2011- current
Tyler Martin	ChBE	3rd year PhD student	12/2011- current
Daniel Johnson	ChBE	2 <sup>nd</sup> year PhD student	12/2012- current
Carla Estridge	Chem	5th year PhD student	01/2013- current
Alex Van Fosson	ChBE	MS 2013	12/2011-06/2013
Arezou Seifpour	ChBE	PhD 2013 (currently at Intel)	06/2009-01/2013
Charles Starbird	ChBE	MS 2012 (currently at Eastman)	01/2011-06/2012
Mohamed Seyam	ChBE	MS 2011	08/2008-06/2011

### **UNDERGRADUATES**

<u>Name</u>	<b>Department</b>	Title (Current Position)	<b>Period</b>
Anna Mcleland	ChBE	Undergrad Senior Thesis	08/2013- current
Brandon Lin	ChBE	Undergrad Senior Thesis, MS thesis	08/2011- current
Melika Ashtiani	ChBE	Undergrad research	06/2013-current
Paul Dodd	ChBE	Undergrad Senior Thesis (UMich Grad)	08/2010-05/2012
Xiao Ba	ChBE	Undergrad Senior Thesis	06/2011-07/2012
Gilberto Haro	ChBE	Undergrad Independent study	01/2012-05/2012
Chris Mckinney	ClarksonU	Undergraduate REU student	06/2011-08/2011
Tyler Martin	ClarksonU	Undergraduate REU student (CU grad)	06/2010-08/2010
Philip Spicer	ChBE	Undergraduate Research Asst.	04/2009-12/2009
Owen Lewis	Mathematics	Undergraduate Research Asst (MIT grad)	05/2009-08/2009
Audrey Schaiberger	ChBE	Undergraduate Independent study	08/2008-12/2008

### **POSTDOCS**

<u>Name</u>	<u>Title (Current Position)</u>	<b>Period</b>
Renfeng Hu	Postdoc	09/2013- current
Eric Jankowski	Postdoc	08/2012- current
Dongsheng Zhang	Postdoc (currently at UT Dallas postdoc)	06/2010-09/2011
Nathaniel Wentzel	Postdoc (currently at Milligen as Instructor)	07/2010-05/2011
Steven Dahl	Postdoc @50% appointment (currently at BP)	01/2010-03/2011
Nitish Nair	Postdoc (currently at Shell)	06/2009-12/2010

### **COMPLETED DOCTORAL and MASTERS DEGREES**

Ms. Arezou Seifpour PhD 2013 – currently employed at Intel

Mr. Robert Elder expected to defend his PhD in Dec 2013 - next position Army Research Lab

Mr. Alex Van Fosson MS 2013

Mr. Charles Starbird MS 2012 - currently employed at Eastman

Mr. Mohamed Seyam MS 2011

#### X. SERVICE ACTIVITIES

### Professional meetings, workshops and conferences

- 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
- Elected Liason Director for COMSEF division of AICHE (2010-2012)
- Elected Member-Elect for Area 01a AICHE Annual meeting (2010)
- 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

#### • Reviewer for

- Journals: Journal of American Chemical Society (JACS), Biomacromolecules, ACS Nano, ACS Macroletters, 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
- Grant agencies: National Science Foundation (NSF)-1 panel for DMR (2010), 1 mail review for DMR (2011,2013), 2 panels for CBET (2010), 2 panels for CBET (2011), 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, Sigma Xi, International Institute of Complex Adaptive Matter
- Member of Brazil-USA Energy Workshop: Nanotechnology for Renewable and Sustainable Energy Materials

#### • University Services

- 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 Services

- 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- current), Aaron Murray (2011-2012), Blake Langdon (2011-current), Jon Monserud (2011-current), Blaine Carter (2011-current), Kyle Berger (2012- current)
- Undergraduate Freshman Advisor (2008-2009) Undergraduate Sophomore Advisor (2009-2010), Undergraduate Junior Advisor (2010-2011)