

**ARTHI JAYARAMAN**

Department of Chemical and Biological Engineering  
 University of Colorado  
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**EDUCATION**

Birla Institute of Technology and Science (BITS), Pilani India  
 B. E. (Honors) Chemical Engineering 08/1996 - 07/2000

North Carolina State University, Raleigh NC  
 M.S. Chemical and Biomolecular Engineering 08/2000 - 12/2002  
 Ph.D. Chemical and Biomolecular Engineering 12/2002 – 05/2006

University of Illinois, Urbana-Champaign  
 Postdoctoral Research, Material Science and Engineering 06/2006 – 08/2008

**PROFESSIONAL EXPERIENCE**

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

**Postdoctoral Research Associate** 06/2006 – 08/2008  
 Department of Material Science and Engineering  
 University of Illinois, Urbana-Champaign  
 (*Advisor:* Dr. Kenneth Schweizer)

**Graduate Research Assistant** 01/2001 – 05/2006  
 Department of Chemical and Biomolecular Engineering  
 North Carolina State University  
 (*Advisors:* Dr. Carol Hall and Dr. Jan Genzer)

**HONORS/AWARDS**

- CU College of Engineering *Dean's Faculty Fellowship* 2011-12
- CU *Outstanding Faculty Undergraduate Teaching Award* in Dept. of Chemical Engineering 2010–11
- Department of Energy (DOE) *Early Career Research Award* 2010
- ACS Women Chemist Committee Lectureship Award 2010
- Elected *Liaison Director* COMSEF division of AIChE 2010-12
- Elected *Member-Elect* Area 1a AIChE Annual Meeting 2010-12
- Invited participant at NSF Workshop -computational energy research, Palm Desert CA April 2010
- Renewable and Sustainable Energy Initiative (RASEI) *Seed Grant Award* 2010
- University of Colorado Innovative *Seed Grant Award* 2009
- *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

## 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 four main research thrusts:

1. Functionalized Nanoparticles for Improved Polymer Nanocomposites and Metamaterials
2. Molecular Design of Organic Polymeric Photovoltaic Materials
3. Recognition and Repair of DNA base damage and Anticancer Drug-DNA Adducts
4. Molecular Design of Ligands and Polycations for Non-viral Gene Delivery

## PEER-REVIEWED PUBLICATIONS (\* corresponding author, † undergraduate)

### *Manuscripts Under Review*

1. 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' (submitted)
2. 'R. Elder, T. Emrick, and **A. Jayaraman\*** 'Understanding the effect of polylysine architecture on DNA binding and non-viral gene delivery ' (submitted)

### *Manuscripts Published*

1. T. B. Martin<sup>†</sup>#, A. Seifpour<sup>#</sup>, **A. Jayaraman\***, Assembly of copolymer functionalized nanoparticles: A Monte Carlo simulation study' *Soft Matter* 2011, **7**, 5952-5964 (# equal contributions) Impact Factor: 4.45
2. N. Nair, N. Wentzel and **A. Jayaraman\***, 'Effects of polydispersity in grafted chains on Potential of Mean Force between Functionalized Nanoparticles in a Homopolymer Matrix: Self-Consistent PRISM Theory-Monte Carlo Simulation Study ' *J. Chem Phys* 134, 194906 (2011) Impact Factor 3.01
3. N. Nair and **A. Jayaraman\***, 'Self-Consistent PRISM Theory-Monte Carlo Simulation Studies of Potential of Mean Force between Functionalized Nanoparticles in a Homopolymer Matrix' *Macromolecules* 43 (19), pp 8251–8263 (2010) Impact Factor: 4.84
4. A. Seifpour, P. Spicer<sup>†</sup>, N. Nair, **A. Jayaraman\***, 'Effect of monomer sequences on conformations of copolymers grafted on spherical nanoparticles: A lattice Monte Carlo simulation study' *J. Chem. Phys.* 131, 164901 (2010) Impact Factor: 3.01 (Selected to appear in *Virtual Journal of Biological Physics*)
5. 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) Impact factor 4.385
6. **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 article in Frontiers of Molecular Simulation, special issue) *Molecular Simulation* 35, 835-848 (2009) Impact Factor 1.32
7. **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) Impact Factor: 4.84
8. **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) Impact Factor: 4.84

9. **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) Impact Factor: 4.27
10. **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*) Impact Factor: 3.01
11. **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*) Impact Factor: 2.5
12. **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*) Impact Factor: 3.2
13. **A. Jayaraman**, C. K. Hall\* and J. Genzer, 'Computer simulation study of molecular recognition in model DNA microarrays' *Biophys. J.*, 91, 2227 (2006) Impact Factor: 4.7
14. 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*) Impact Factor: 3.01
15. **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) Impact Factor: 3.01
16. **A. Jayaraman**, C. K. Hall\* and J. Genzer, 'Designing pattern-recognition surfaces for selective adsorption of copolymer sequences using lattice Monte Carlo simulation', *Phys. Rev. Lett.*, 94, 078103 (2005) (Selected to appear in *Virtual Journal of Biological Physics*) Impact Factor: 7.6

### ***Manuscripts in preparation***

17. D. Zhang, C. Starbird, H. Marsh, **A. Jayaraman** \*, Dynamics of liquid crystalline transition and microphase separation in lamella forming rod coil diblock copolymers with spherical nanoadditives, *in preparation*

### **INVITED PRESENTATIONS**

#### **After joining University of Colorado**

1. DOE - SciDAC meeting, 'Theory and Simulation Studies of Macromolecular Materials for Metamaterials and Organic Photovoltaics (poster)' July 2011
2. "Young Investigators in Materials Research" UMass Amherst Materials Research Science & Engineering Center (MRSEC) May 2011
3. Seminar, Dept. of Chemical Engineering, Rice University, March 2011
4. Seminar, Dept. of Chemical Engineering, Texas A&M University, February 2011
5. Seminar, Dept. of Materials Science and Engineering, University of Illinois at Urbana, February 2011
6. Seminar, Dept of Chemical Engineering, Vanderbilt University, November 2010
7. Seminar, Dept. of Applied Math, University of Colorado Boulder, November 2010
8. Interfacial Phenomena in Nanostructured Materials and Devices, Telluride Workshop February 2010
9. Seminar, Dept. of Chemical Engineering, Colorado State University, October 2009
10. Condensed matter lunch seminar, Dept. of Physics, University of Colorado, Boulder, September 2008

#### **Before joining University of Colorado**

11. Seminar Dept. of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, April 2008
12. Seminar Dept. of Energy, Environmental and Chemical Engineering, WU St. Louis, March 2008

13. Seminar Dept. of Chemical and Biological Engineering, University of Colorado, Boulder, March 2008
14. Seminar Molecular Foundry, Lawrence Berkeley National Laboratories, February 2008
15. Seminar Dept. of Chemical Engineering, Lehigh University, February 2008
16. Seminar Dept. of Chemical and Biomolecular Engineering, Clemson University, February 2008
17. Seminar Dept. of Chemical Engineering, University of South Carolina, February 2008
18. Seminar Dept. of Chemical and Petroleum Engineering, University of Pittsburgh, January 2008
19. Seminar Dept. of Chemical and Biomolecular Engineering, Ohio State University, January 2008
20. Seminar Dept. of Chemical Engineering, University of California, Berkeley, March 2006
21. Seminar The Center for Engineering in Medicine, Harvard Medical School, February 2006

## CONTRIBUTED PRESENTATIONS (\*presenter)

### *With A. Jayaraman as Principal Investigator*

1. 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
2. A. Seifpour\*, A. Jayaraman, “Monte Carlo Simulations of the Assembly of Copolymer Functionalized Nanoparticles”, (talk) AIChE Annual Meeting, October 2011
3. A. Jayaraman\*, R. Elder, “Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery”, (talk) AIChE Annual Meeting, October 2011
4. A. Jayaraman\*, Theory and molecular simulations of functionalized nanoparticles in polymer nanocomposites, ACS National Meeting, August 2011
5. R. Elder\*, A. Jayaraman “Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors” (talk) ACS National Meeting, August 2011
6. R. Elder\*, A. Jayaraman “Molecular Dynamics Simulations for Recognition of Anticancer-Drug induced DNA damage by Repair Proteins” (poster) ACS National Meeting, August 2011
7. A. Jayaraman\*, R. Elder, “Molecular Simulations of Macromolecular Materials for Non-Viral Gene Delivery”, (talk) IUPAC World Chemistry Congress, August 2011
8. 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
9. R. Elder\*, A. Jayaraman “Molecular Dynamics Simulations for Designing Non-Viral Gene Delivery Vectors” (poster) Gordon Research Conference Macromolecular Materials, January 2011
10. 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
11. A. Jayaraman\*, Nitish Nair “Self-Consistent PRISM Theory-Monte Carlo Simulation of Functionalized Nanoparticles in a Polymer Matrix” (talk) AIChE Annual Meeting, November 2010

12. A. Seifpour\*, A. Jayaraman, "Monte Carlo Simulations of Assembly of Copolymer Functionalized Spherical Nanoparticles", (talk) AIChE Annual Meeting, November 2010
13. A. Jayaraman\*, R. Elder, M. Seyam "Molecular Dynamics Simulation Study of DNA Damage Recognition" (talk) AIChE Annual Meeting, November 2010
14. R. Elder\*, A. Jayaraman, "Molecular Dynamics Simulation Studies of Polycation-DNA Binding for Gene Delivery", (poster) AIChE Annual Meeting, November 2010
15. 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
16. A. Seifpour\*, Nitish Nair, A. Jayaraman "Functionalized nanoparticles in polymer nanocomposites" (poster) Energy Institute Student Poster Session, Boulder CO April 2010
17. 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
18. 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
19. 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
20. 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***

21. 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
22. 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
23. 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
24. 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
25. 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
26. A. Jayaraman\*, 'Computational and Theoretical Studies of Soft Materials and Biological Systems' poster presentation AIChE Annual Meeting, Salt Lake City, UT November 2007
27. 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
28. 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.

29. 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
30. A. Jayaraman\*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' AIChE Conference, October 30, 2005, Cincinnati, OH
31. A. Jayaraman\*, C. K. Hall and J. Genzer, 'Computer Simulation Studies of Pattern Recognition in Biomimetic Polymers' (poster) Thermo 2005, College Park, MD
32. 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
33. 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.
34. 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.
35. 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.

#### PERSONNEL SUPERVISED (Fall 2008 – present)

<u>Name</u>	<u>Department</u>	<u>Title/Position</u>	<u>Period</u>
Arezou Seifpour	ChBE	PhD student	06/2009- current
Robert Elder	ChBE	PhD student	01/2010- current
Hilary Marsh	ChBE	PhD student	01/2011- current
Charles Starbird	ChBE	PhD student	01/2011- current
Dr. Dongsheng Zhang	ChBE	Postdoc	06/2010- current
Paul Dodd	ChBE	Undergrad Senior Thesis	08/2010- current
Xiao Ba	ChBE	Undergrad Senior Thesis	06/2011-current
Brandon Lin	ChBE	Undergrad Senior Thesis	08/2011-current
Chris Mckinney	Clarkson Univ.	Undergraduate REU student	06/2011-current
Mohamed Seyam	ChBE	MS student	08/2008-06/2011
Dr. Nathaniel Wentzel	ChBE	Postdoc	07/2010-05/2011
Dr. Steven Dahl	ChBE	Postdoc (50% appointment)	01/2010-03/2011
Tyler Martin	Clarkson Univ.	Undergraduate REU student	06/2010-08/2010
Philip Spicer	ChBE	Undergraduate Research Asst.	04/2009-12/2009
Owen Lewis	Mathematics	Undergraduate Research Asst	05/2009-08/2009
Audrey Schaiberger	ChBE	Undergraduate Independent study	08/2008-12/2008
Dr. Nitish Nair	ChBE	Postdoc	06/2009-12/2010

#### TEACHING

- **Fall 2008** Materials and Energy Balances CHEN2120 (48 students) – 3 credits
  - Instructor rating 4.7/6.0 (Department average: 4.4/6.0)
  - Use of active learning techniques 5.3/6.0 Intellectual challenge of the course 5.5/6.0
- **Spring 2009** Process Control CHEN4570 (64 students) - 4 credits
  - Instructor rating 4.7/6.0 (Department average: 4.8/6.0)
  - Use of active learning techniques 4.8/6.0 Intellectual challenge of the course 5.5/6.0

- **Spring 2010** Process Control CHEN4570 (1 section of lecture, 2 sections of lab) (69 students) – 4 credits
  - Instructor rating 4.3/6.0 (Department average: 4.8/6.0)
  - Use of active learning techniques 4.6/6.0 Intellectual challenge of the course 5.0/6.0
- **Spring 2011** Process Control CHEN4570-1 (1 section lecture, 1.5 sections of lab) (~49 students) – 4 credits
  - Instructor rating 4.5/6.0 (Department average: 4.9/6.0)
  - Use of active learning techniques 4.3/6.0 Intellectual challenge of the course 5.1/6.0
- **Spring 2011** Process Control CHEN4570-2 (1 section lecture, 1.5 sections of lab) (~47 students) – 4 credits
  - Instructor rating 5.0/6.0 (Department average: 4.9/6.0)
  - Use of active learning techniques 4.4/6.0 Intellectual challenge of the course 5.3/6.0

## SERVICE ACTIVITIES

- **Professional meetings, workshops and conferences**
  - 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, 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), 2 panels for CBET (2010), 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
  
- **University Services**
  - Member of College of Engineering Diversity Action Committee (2009- )
  - Member of CU- Materials Science and Engineering Program Task Force (2010-)
  - Member of CU- Materials Science and Engineering Program Faculty Search Committee (2010-)
  
- **Department Services**
  - Member of Department Leadership Committee (2011-12)
  - 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- ), Josh McCall (2009- ), and Lauren Andrews (2009- ) Sean Ryland (2010- )
  - Undergraduate Freshman Advisor (2008-2009 ) Undergraduate Sophomore Advisor (2009-2010), Undergraduate Junior Advisor (2010-2011)