

# Rajeev Kumar

---

Center for Nanophase Materials Sciences,  
M-364, Oak Ridge National Laboratory,  
Oak Ridge, TN 37831

E-mail: kumarr@ornl.gov  
Phone: +1-413-335-3626

## Professional Experience

- **Soft Nanomaterials Theory and Simulation Research Scientist** December 2012 -  
Computer Science and Mathematics Division (CSMD),  
Oak Ridge National Laboratory, Oak Ridge, TN
- **American Recovery and Reinvestment Act Fellow** July 2010-December 2012  
Advisors: Bobby G. Sumpter and Ricky Kendall  
National Center for Computational Sciences (NCCS),  
Oak Ridge National Laboratory, Oak Ridge, TN
- **Post-doctoral Research Associate** September 2008-June 2010  
Advisor: Prof. Glenn H. Fredrickson  
Materials Research Laboratory (MRL),  
University of California, Santa Barbara, CA
- **Lecturer (Mathematics)** 2002-2003  
Career Point Inc., Kota, India
- **Intern** May-July 2001  
Jagatjeet Cotton Textile (JCT) Ltd., India

## Education

- **Ph.D. in Polymer Science & Engineering** 2004 -2008  
Dissertation Title: Self-consistent field theory for polyelectrolytes and its applications  
Advisor: Prof. M. Muthukumar  
University of Massachusetts, Amherst, MA
- **M.S. in Polymer Science & Engineering** 2003-2004  
University of Massachusetts, Amherst, MA
- **B.Tech. in Textile Technology** 1998-2002  
Indian Institute of Technology, Delhi, India

## Academic Honors/Activities

- Member of American Physical Society 2006-Present
- Reviewer for The Journal of Chemical Physics, New Journal of Physics, Macromolecules  
and European Polymer Journal E 2006-Present
- Jawahar Gajree Memorial Scholarship 2000-2001
- Award for social services from the National Service Scheme 1999-2000
- State Merit Scholarship from the Haryana Board of School Education 1994-1995

## Publications : Refereed Articles

1. J.Y. Carrillo, **R. Kumar**, M. Goswami, B.G. Sumpter and W.M. Brown, "New insights into dynamics and morphology of P3HT:PCBM active layers in bulk heterojunctions," *Phys. Chem. Chem. Phys. in press*.
2. C. Dyer, P. Driva, S.W. Sides, B.G. Sumpter, J. W. Mays, J. Chen, **R. Kumar**, M. Goswami and M. Dadmun, "Effect of macromolecular architecture on the morphology of polystyrene - polyisoprene block copolymers," *Macromolecules* **46**,2023 (2013).
3. **R. Kumar**, M. Goswami, B.G. Sumpter, V. Novikov and A.P. Sokolov, "Effects of backbone rigidity on the local structure and dynamics in polymer melts and glasses," *Phys. Chem. Chem. Phys.* **15**, 4604 (2013).
4. K. Misichronis, S. Rangou, E. Ashcraft, **R. Kumar**, M. Dadmun, B.G. Sumpter, N.E. Zafeiropoulos, J.W. Mays and A.T. Avgeropoulos, "Synthesis, characterization (molecular-morphological) and theoretical morphology predictions of linear triblock terpolymers containing poly(cyclohexadiene)," *Polymer* **54**, 1480 (2013).
5. **R. Kumar**, S.W. Sides, M. Goswami, B.G. Sumpter, K. Hong, X. Wu, T.P. Russell, S.P. Gido, K. Misichronis, S. Rangou, A.T. Avgeropoulos, T. Tsoukatos, N. Hadjichristidis, F. Beyer and J.W. Mays, "Morphologies of ABC triblock terpolymer melts containing poly(cyclohexadiene) : effects of conformational asymmetry," *Langmuir* **29**, 1995 (2013).
6. **R. Kumar**, Y. Li, S.W. Sides, J. Mays and B.G. Sumpter, "Morphology diagrams for A<sub>2</sub>B copolymer melts: real-space self-consistent field theory," *J. Phys.: Conf. Ser.* **402**, 012042 (2012).
7. J. Mays, **R. Kumar**, S.W. Sides, M. Goswami, B.G. Sumpter, K. Hong, X. Wu, T. P Russell, S.P. Gido, A. Avgeropoulos, T. Tsoukatos, N. Hadjichristidis and F. L. Beyer, "Morphologies of poly(cyclohexadiene) diblock copolymers: effect of conformational asymmetry," *Polymer* **53**, 5155 (2012).
8. **R. Kumar**, B.G. Sumpter and S.M. Kilbey, "Charge regulation and local dielectric function in planar polyelectrolyte brushes," *J. Chem. Phys.* **136**, 234901 (2012).
9. X. Wang, M. Goswami, **R. Kumar**, B.G. Sumpter and J. Mays, "Morphologies of block copolymers composed of charged and neutral blocks," *Soft Matter* **8**, 3036 (2012) (cover page).
10. R.A. Riggleman, **R. Kumar** and G.H. Fredrickson, "Investigation of the interfacial tension of complex coacervates using field-theoretic simulations," *J. Chem. Phys.* **136**, 024903 (2012).
11. M. Goswami, **R. Kumar**, B.G. Sumpter and J.W. Mays, "Breakdown of inverse morphologies in charged diblock copolymers," *J. Phys. Chem. B.* **115**, 3330 (2011).
12. **R. Kumar**, D. Audus and G.H. Fredrickson, "Phase separation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *J. Phys. Chem. B.* **114**, 9956 (2010).
13. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *J. Chem. Phys.* **131**, 194903 (2009).
14. **R. Kumar** and G.H. Fredrickson, "Theory of polyzwitterion conformations," *J. Chem. Phys.* **131**, 104901 (2009).
15. **R. Kumar**, A. Kundagrami and M. Muthukumar, "Counterion adsorption on flexible polyelectrolytes : comparison of theories," *Macromolecules* **42**, 1370 (2009).

16. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *J. Chem. Phys.* **128**, 184902 (2008).
17. **R. Kumar** and M. Muthukumar, "Microphase separation in polyelectrolytic diblock copolymer melt : Weak segregation limit," *J. Chem. Phys.* **126**, 214902 (2007).

### Conference Proceedings

18. **R. Kumar** and B.G. Sumpter, "Quantitative analysis of chain packing in polymer melts using large scale molecular dynamics simulations," in Proc. SciDAC 2011, Denver, CO, July 10-14, 2011, <http://press.mcs.anl.gov/scidac2011/>
19. M. Jassal, V. Raj, **R. Kumar**, N.S. Save, and A.K. Agrawal, "Synthesis of stimuli-sensitive polymers based on N-substituted acrylamides," *Proceedings of International Seminar on Frontiers of Polymer Science and Engineering*, MACRO , IIT Kharagpur, December 2002, 09.4.

### Book Chapter : Invited Contribution

20. A. Kundagrami, **R. Kumar**, and M. Muthukumar. "Simulations and Theories of Single Polyelectrolyte Chains" in "Modeling and Simulation in Polymers," edited by P.D. Gujrati and A.I. Leonov, WILEY-VCH Verlag, Weinheim, Germany, 2010.

### Conference Presentations : Invited

1. **R. Kumar**, B.G. Sumpter and S.M. Kilbey, "Local dielectric function in inhomogeneous polymeric media," *American Chemical Society Meeting*, Indianapolis, IN, September 2013 (talk).
2. **R. Kumar**, "Polymers near interfaces: field theory and neutron reflectivity experiments," *SNS-HIFR-CNMS User Workshop*, Oak Ridge National Laboratory, Oak Ridge, TN, August 2013 (talk).
3. S.W. Sides and **R. Kumar**, "Simulation of polymers in complex formulations: progress on developing numerical self-consistent field theory (SCFT)," *Proctor & Gamble/ORNL/TechX Corp. Reconnect*, Oak Ridge National Laboratory, Oak Ridge, TN, May 2012 (talk).
4. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Physics Department, University of Tennessee*, Knoxville, TN, April 2012 (talk).
5. **R. Kumar** and B.G. Sumpter, "Quantitative analysis of chain packing in polymer melts using large scale molecular dynamics simulations," *Scientific Discovery through Advanced Computing (SciDAC) Conference*, Denver, CO, July 2011 (poster).
6. **R. Kumar**, "Local dielectric function and its effects on planar polyelectrolyte brushes: field theoretical study," *Proctor & Gamble /ORNL /TechX Corp. Reconnect*, Oak Ridge National Laboratory, Oak Ridge, TN, June 2011 (talk).
7. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Department of Chemistry, University of Tennessee*, Knoxville, TN, March 2011 (talk).
8. **R. Kumar** and B.G. Sumpter, "Insights obtained from coarse-grained modeling of charged polymers," *66<sup>th</sup> Southwest and 62<sup>nd</sup> Southeastern Regional Meeting of the American Chemical Society*, New Orleans, LA, December 2010 (talk).
9. **R. Kumar**, "Modeling charged polymers using field-theoretic methods," *Center for Functional Nanomaterials, Brookhaven National Lab*, NY, March 2010 (talk).

## Other Presentations

10. J.Y. Carrillo, **R. Kumar**, M. Goswami, B.G. Sumpter and W.M. Brown, "Coarse-grained molecular dynamics simulations of thermal annealing of P3HT:PCBM bulk heterojunctions for organic photovoltaic applications," *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA, November 2013 (talk).
11. **R. Kumar**, B.G. Sumpter and S.M. Kilbey, "Charge regulation and local dielectric function in planar polyelectrolyte brushes," *American Physical Society*, Baltimore, MD, March 2013 (talk).
12. S.W. Sides, **R. Kumar**, B. Jamroz, R. Crockett and A. Pletzer, "Using adaptive-mesh refinement in SCFT simulations of surfactant adsorption," *American Physical Society*, Baltimore, MD, March 2013 (talk).
13. A.P. Sokolov, J.W. Mays, T. Zawodzinski, A. Kisliuk, K. Hong and **R. Kumar**, "Fundamentals of ionic conductivity in polymeric materials for energy storage applications," *Laboratory Directed Research and Development (LDRD) renewal*, Oak Ridge National Laboratory, Oak Ridge, TN, June 2011 (talk).
14. **R. Kumar**, S.W. Sides and B.G. Sumpter, "Local dielectric constant and its effects on the microphase separation in charged-neutral diblock copolymer melts," *American Physical Society*, Dallas, TX, March 2011 (talk).
15. **R. Kumar**, B.G. Sumpter and S.M. Kilbey, "Charge regulation and local dielectric function in planar polyelectrolyte brushes," *Center for Nanophase Materials Sciences User Meeting*, Oak Ridge National Laboratory, Oak Ridge, TN, September 2012 (poster).
16. A.P. Sokolov, J.W. Mays, T. Zawodzinski, A. Kisliuk, K. Hong and **R. Kumar**, "Fundamentals of ionic conductivity in polymeric materials for energy storage applications," *Laboratory Directed Research and Development (LDRD) renewal*, Oak Ridge National Laboratory, Oak Ridge, TN, June 2011 (talk).
17. **R. Kumar**, S.W. Sides and B.G. Sumpter, "Local dielectric constant and its effects on the microphase separation in charged-neutral diblock copolymer melts," *American Physical Society*, Dallas, TX, March 2011 (talk).
18. A. Sokolov, J.W. Mays, T. Zawodzinski, A. Kisliuk, K. Hong and **R. Kumar**, "Fundamentals of ionic conductivity in polymeric materials for energy storage applications," *Laboratory Directed Research and Development (LDRD) proposal*, Oak Ridge National Laboratory, Oak Ridge, TN, August 2010 (talk).
19. **R. Kumar** and G.H. Fredrickson, "Coacervation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *American Physical Society*, Portland, OR, March 2010 (talk).
20. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *American Physical Society*, Portland, OR, March 2010 (poster).
21. **R. Kumar**, D. Audus and G.H. Fredrickson "Theoretical investigations of complex coacervates for biosensor technology," *Institute for Collaborative Biotechnologies Army-Industry Collaboration Conference*, Santa Barbara, CA, March 2010 (poster).
22. **R. Kumar** and G.H. Fredrickson, "Coacervation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *Complex Fluids Design Consortium*, Santa Barbara, CA, February 2010 (talk).

23. **R. Kumar** and G.H. Fredrickson, "Theory of polyelectrolytic solutions," *American Physical Society*, Pittsburgh, PA, March 2009 (talk).
24. D. Audus, **R. Kumar** and G.H. Fredrickson, "Theoretical investigations of polyelectrolyte complexes for biosensors," *Institute for Collaborative Biotechnologies Army-Industry Collaboration Conference*, Santa Barbara, CA, March 2009 (poster).
25. **R. Kumar** and G.H. Fredrickson, "Conformational characteristics of a single polyelectrolytic chain: effect of salt," *Complex Fluids Design Consortium*, Santa Barbara, CA, Feb. 2009 (talk).
26. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *American Physical Society*, New Orleans, LA, March 2008 (talk).
27. **R. Kumar** and M. Muthukumar, "Confinement effects on flexible polyelectrolytic systems," *Modeling and Computation in Physics, Mathematics and Biology, University of Massachusetts, Amherst /University of Heidelberg Workshop*, Amherst, MA, May 2007 (poster).
28. **R. Kumar** and M. Muthukumar, "Morphology diagrams for polyelectrolytic diblock copolymers," *American Physical Society*, Baltimore, MD, March 2006 (talk).
29. **R. Kumar** and M. Muthukumar, "Morphology diagrams for polyelectrolytic diblock copolymers," *6<sup>th</sup> National Graduate Research Conference, University of Massachusetts*, Amherst, MA, June 2005 (talk).