# Rajeev Kumar

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# **Professional Experience**

Soft Nanomaterials Theory and Simulation Research Scientist
 Center for Nanophase Materials Sciences (CNMS),
 Computer Science and Mathematics Division (CSMD),
 Oak Ridge National Laboratory, Oak Ridge, TN

American Recovery and Reinvestment Act Fellow
 Advisors: Bobby G. Sumpter and Ricky Kendall
 National Center for Computational Sciences (NCCS),
 Oak Ridge National Laboratory, Oak Ridge, TN

September 2008-June 2010

2004 - 2008

 Post-doctoral Research Associate 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

Jagatjeet Cotton Textile (JCT) Ltd., India

May-July 2001

# **Education**

Ph.D. in Polymer Science & Engineering

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
University of Massachusetts, Amherst, MA

• B.Tech. in Textile Technology
Indian Institute of Technology, Delhi, India

#### **Academic Honors/Activities**

 Reviewer for research grant proposal submitted to the National Science Foundation (NSF) and the US-Israel Binational Science Foundation (BSF)
 2014-Present

Member of American Physical Society
 2006-Present

 Reviewer for The Journal of Chemical Physics, New Journal of Physics, Macromolecules, European Polymer Journal E, Materials Chemistry and Physics, Advanced Energy Materials
 2006-Present

• Jawahar Gajree Memorial Scholarship 2000-2001

Award for social services from the National Service Scheme
 1999-2000

#### **Publications: Refereed Articles**

- 1. N. Herath, S. Das, J. K. Keum, J. Zhu, **R. Kumar**, I. N. Ivanov, B. G. Sumpter, J. F. Browning, K. Xiao, G. Gu, P. Joshi, and V. Lauter, "Peculiarity of two thermodynamically-stable morphologies and their impact on the efficiency of small molecule bulk heterojunction solar cells," *Scientific Reports*, (in press).
- 2. J. Zhu, Y. Han, **R. Kumar**, Y. He, K. Hong, B. G. Sumpter, S. Smith, I. Ivanov and C. Do, "Controlling assembly of a water-soluble conjugated polymer," *Nanoscale*, (2015) DOI: 10.1039/C5NR02037A.
- 3. J.Y. Carrillo, S. Cheng, **R. Kumar**, M. Goswami, A. P. Sokolov, and B. G. Sumpter, "Untangling the effects of chain rigidity on the structure and dynamics of stronly adsorbed polymer melts," *Macromolecules* **48**, 4207 (2015).
- 4. **R. Kumar**, B. S. Lokitz, S. W. Sides, J. Chen, W. Heller, J. F. Ankner, J. Browning, S. M. Kilbey II, and B. G. Sumpter, "Microphase separation in thin films of lamellar forming polydisperse di-block copolymers," *RSC Advances* **5**, 21336 (2015).
- 5. E. Strelcov, **R. Kumar**, V. Bocharova, B. G. Sumpter, A. Tselev, and S. V. Kalinin, "Nanoscale lubrication of ionic surfaces controlled via strong electric field," *Scientific Reports* **5**, 8049 (2015).
- V. Bocharova, A. L. Agapov, A. Tselev, L. Collins, R. Kumar, S. Berdzinski, V. Strehmel, A. Kisliuk, I. I. Kravchenko, B. G. Sumpter, A. P. Sokolov, S. V. Kalinin, and E. Strelcov, "Controlled nanopatterning of a polymerized ionic liquid in a strong electric field," *Adv. Func. Mat.* 25, 805 (2015).
- R. Kumar, V. Bocharova, E. Strelcov, A. Tselev, I. I. Kravchenko, S. Berdzinski, V. Strehmel, O. S. Ovchinnikova, J. A. Minutolo, J. R. Sangoro, A. L. Agapov, A. P. Sokolov, S. V. Kalinin, and B. G. Sumpter, "Ion transport and softening in a polymerized ionic liquid," *Nanoscale* 7, 947 (2015).
- 8. **R. Kumar**, B. G. Sumpter, and M. Muthukumar, "Enhanced phase segregation induced by dipolar interactions in polymer blends," *Macromolecules* **47**, 6491 (2014).
- M. Shao, J. K. Keum, R. Kumar, J. Chen, J. F. Browning, S. Das, W. Chen, J. Hou, C. Do, K. C. Littrell, A. Rondinone, D. B. Geohegan, B. G. Sumpter, and K. Xiao, "Understanding how processing additives tune the nanoscale morphology of high efficiency organic photovoltaic blends: From casting solution to spun-cast thin film," *Adv. Func. Mat.* 24, 6647 (2014).
- 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.* 15, 17873 (2013).
- 11. 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).
- 12. **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).

- 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).
- 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).
- 15. **R. Kumar**, Y. Li, S.W. Sides, J.W. 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).
- J.W. 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).
- 17. **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).
- X. Wang, M. Goswami, R. Kumar, B.G. Sumpter, and J.W. Mays, "Morphologies of block copolymers composed of charged and neutral blocks," *Soft Matter* 8, 3036 (2012) (cover page).
- 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).
- 20. M. Goswami, **R. Kumar**, B.G. Sumpter, and J.W. Mays, "Breakdown of inverse morphologies incharged diblock copolymers," *J. Phys. Chem. B.* **115**, 3330 (2011).
- 21. **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).
- 22. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *J. Chem. Phys.* **131**, 194903 (2009).
- 23. **R. Kumar** and G.H. Fredrickson, "Theory of polyzwitterion conformations," *J. Chem. Phys.* **131**, 104901 (2009).
- 24. **R. Kumar**, A. Kundagrami, and M. Muthukumar, "Counterion adsorption on flexible polyelectrolytes: comparison of theories," *Macromolecules* **42**, 1370 (2009).
- 25. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *J. Chem. Phys.* **128**, 184902 (2008).
- 26. **R. Kumar** and M. Muthukumar, "Microphase separation in polyelectrolytic diblock copolymer melt: Weak segregation limit," *J. Chem. Phys.* **126**, 214902 (2007).

## **Conference Proceedings**

27. **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/

28. 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 Contributions**

- 29. **R. Kumar**, J. Carrillo, M. Goswami, and B. G. Sumpter, "Insights obtained from modeling of organic photovoltaics: morphology, interfaces and coupling with charge transport," in "Organic Solar Cells: Materials, Devices, Interfaces, and Modeling," edited by Q. Qiao, CRC Press, Taylor and Francis Group, 2015.
- 30. 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**, "Polymerized ionic liquid films in strong electric fields: ion transport and nanopatterning," *TechConnect World Innovation Conference*, Washington, DC, June 2015 (talk).
- 2. **R. Kumar**, B.G. Sumpter, and M. Muthukumar, "Effects of dipolar interactions in polymeric media," *Energy Materials Nanotechnology (EMN) Meeting on Polymer*, Orlando, FL, Jan 2015 (talk).
- 3. **R. Kumar**, J. Carrillo, M. Goswami, and B.G. Sumpter, "Insights obtained from coarse-grained modeling of P3HT:PCBM active layers," *Energy Materials Nanotechnology (EMN) Summer Meeting*, Cancun, Mexico, June 2014 (talk).
- 4. **R. Kumar**, J. Carrillo, M. Goswami, and B.G. Sumpter, "Structure and dynamics of polymeric materials in complex solutions and thin films," *Physical Sciences Directorate (PSD) Advisory Committee Meeting*, Oak Ridge, TN, May 2014 (poster).
- 5. **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).
- 6. **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).
- 7. 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).
- 8. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Physics Department, University of Tennessee*, Knoxville, TN, April 2012 (talk).
- 9. **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).
- 10. **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).

- 11. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Department of Chemistry, University of Tennessee*, Knoxville, TN, March 2011 (talk).
- 12. **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).
- 13. **R. Kumar**, "Modeling charged polymers using field-theoretic methods," *Center for Functional Nanomaterials, Brookhaven National Lab*, NY, March 2010 (talk).

### **Other Presentations**

- 14. J. P. Mahalik, **R. Kumar**, and B.G. Sumpter, "Planar dipolar polymerr brush: field theoretical investigations," *American Physical Society Meeting*, San Antonio, TX, March 2015 (talk).
- R. Kumar, V. Bocharova, E. Strelcov, V. Strehmel, J. R. Sangoro, A. P. Sokolov, S. V. Kalinin, and B. G. Sumpter, "Ion transport and softening in a polymerized ionic liquid," American Physical Society Meeting, San Antonio, TX, March 2015 (talk).
- S. W. Sides, R. Kumar, L. Hall, J. Brown, "Self-consistent field theory simulations of block copolymer systems: Recent results using the PolySwift++ framework,", San Francisco, CA, August 2014 (talk).
- 17. J. Carrillo, **R. Kumar**, M. Goswami, S. M. Kilbey II, B. G. Sumpter, and W. M. Brown, "Petascale molecular dynamics simulations of thermal annealing of P3HT:PCBM active layers in bulk heterojunctions", *American Physical Society*, Denver, CO, March 2014 (talk).
- 18. **R. Kumar**, M. Muthukumar, and B. G. Sumpter, "Effects of dipolar interactions on thermodynamic stabilities of polymer blends and diblock copolymer melts", *American Physical Society*, Denver, CO, March 2014 (talk).
- 19. 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).
- 20. **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).
- 21. 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).
- 22. 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).
- 23. **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).
- 24. **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).

- 25. 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).
- 26. **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).
- 27. 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).
- 28. **R. Kumar** and G.H. Fredrickson, "Coacervation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *American Physical Society*, Portland, OR, March 2010 (talk).
- 29. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *American Physical Society*, Portland, OR, March 2010 (poster).
- 30. **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).
- 31. **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).
- 32. **R. Kumar** and G.H. Fredrickson, "Theory of polyzwitterionic solutions," *American Physical Society*, Pittsburgh, PA, March 2009 (talk).
- 33. 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).
- 34. **R. Kumar** and G.H. Fredrickson, "Conformational characteristics of a single polyzwitterionic chain: effect of salt," *Complex Fluids Design Consortium*, Santa Barbara, CA, Feb. 2009 (talk).
- 35. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *American Physical Society*, New Orleans, LA, March 2008 (talk).
- 36. **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).
- 37. **R. Kumar** and M. Muthukumar, "Morphology diagrams for polyelectrolytic diblock copolymers," *American Physical Society*, Baltimore, MD, March 2006 (talk).
- 38. **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).