

# Rajeev Kumar

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## 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

## Professional Experience

- **Research Scientist** October 2020 -Present  
Center for Nanophase Materials Sciences (CNMS),  
Oak Ridge National Laboratory (ORNL), Oak Ridge, TN
- **Research Scientist** December 2012 -2020  
Computational Sciences and Engineering Division (CSED),  
Center for Nanophase Materials Sciences (CNMS),  
Oak Ridge National Laboratory (ORNL), Oak Ridge, TN
- **Adjunct Assistant Professor** October 2014 -Present  
Department of Mathematics,  
University of Tennessee, Knoxville, TN
- **American Recovery and Reinvestment Act Fellow** July 2010-December 2012  
Advisors: Dr. Bobby G. Sumpter and Dr. Ricky Kendall  
National Center for Computational Sciences,  
Oak Ridge National Laboratory, Oak Ridge, TN
- **Post-doctoral Research Associate** September 2008-June 2010  
Advisor: Prof. Glenn H. Fredrickson  
Materials Research Laboratory,  
University of California, Santa Barbara, CA

## Academic Honors/Activities

- Theme leader for the theme Harnessing Complex Macromolecular Conformations at the CNMS 2020-Present
- Member of Publicity Committee for the American Physical Society Division of Polymer Physics 2020-Present
- Mentored four post-docs, two graduate and four undergraduate students 2012-Present

- Organized three focus sessions: 1) Electric polarization and polymer physics; 2) Molecular and ion transport in polymers; and 3) Topological effects in soft matter, *the American Physical Society March Meeting*, Nashville, TN 2021
- Nominated for the American Physical Society John H. Dillon medal 2019
- Organized a workshop, "Understanding effects of electrostatics in macromolecular media," *the CNMS User Meeting*, ORNL, Oak Ridge, TN 2018
- Reviewer for research grant proposals submitted to the National Science Foundation and the US-Israel Binational Science Foundation 2014-Present
- Member of the American Physical Society and the American Chemical Society
- Reviewer for *The Journal of Chemical Physics*, *New Journal of Physics*, *Macromolecules*, *European Polymer Journal*, *Materials Chemistry and Physics*, *Advanced Energy Materials*, *Soft Matter*, *Langmuir*, *ACS Applied Materials and Interfaces*, *Chemistry and Physics of Lipids* 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. S. Zhang and **R. Kumar**, "Effects of local order parameter dependent transport coefficient in diblock copolymers under applied electric fields," *J. Chem. Phys.* **156**, 174903 (2022).
2. Z. Zhou, V. Bocharova, **R. Kumar**, A-C. Genix, B. Carroll, S. Samanta, I. Popov, A. Young-Gonzales, A. Kisliuk, S.P. Jeong, J. Ilavsky, and A.P. Sokolov, "Tuning the properties of nanocomposites by trapping them in deep metastable states," *ACS Applied Polymer Materials* **4**, 3174 (2022).
3. B. Hu, J-M. Carrillo, L. Collins, K.S. Silmore, J. Keum, P.V. Bonnesen, Y. Wang, S. Retterer, **R. Kumar**, and B.S. Lokitz, "Modular approach for the synthesis of bottlebrush diblock copolymers from poly(glycidyl vethacrylate)-block-poly(vinyldimethylazlactone) backbones," *Macromolecules* **55**, 488 (2022).
4. H. Mei, J.P. Mahalik, D. Lee, T.S. Laws, T. Terlier, G.E. Stein, **R. Kumar**, and R. Verduzco, "Understanding interfacial segregation in polymer blend films with random and mixed side chain bottlebrush copolymer additives," *Soft Matter* **17**, 9028 (2021).
5. K.S. Silmore and **R. Kumar**, "Dynamics of a single polyampholyte chain," *J. Chem. Phys.* **155**, 214903 (2021).
6. T. Herschberg, J-M. Y. Carrillo, B.G. Sumpter, E. Panagiotou, and **R. Kumar**, "Topological effects near order-disorder transitions in symmetric diblock copolymer melts," *Macromolecules* **54**, 7492 (2021).
7. **R. Kumar**, Z. Liu, B. Lokitz, J. Chen, J-M Carrillo, J. Jakowski, C.P. Collier, S. Retterer, and R. Advincula, "Harnessing autocatalytic reactions in polymerization and depolymerization," *MRS Communications* **11**, 377 (2021).
8. S.P. Jeong, **R. Kumar**, A-C. Genix, I. Popov, C. Li, S.M. Mahurin, X. Hu, W. Bras, I. Popovs, A.P. Sokolov, and V. Bocharova, "Improving gas selectivity in membranes using polymer-grafted silica nanoparticles," *ACS Applied Nano Materials* **4**, 5895 (2021).

9. J.P. Mahalik, W. Li, A.T. Savici, S. Hahn, H. Lauter, H. Ambaye, B.G. Sumpter, V. Lauter, and **R. Kumar**, "Dispersity-driven stabilization of coexisting morphologies in asymmetric diblock copolymer thin films," *Macromolecules* **54**, 450 (2021).
10. P.J. Scott, G.A. Spiering, Y. Wang, Z.D. Seibers, R.B. Moore, **R. Kumar**, B.S. Lokitz, and T.E. Long, "Phosphonium-based polyzwitterions: Influence of ionic structure and association on mechanical properties," *Macromolecules* **53**, 11009 (2020).
11. W. Li, J-M Y. Carrillo, B.G. Sumpter, and **R. Kumar**, "Modulating microphase separation of lamellae-forming diblock copolymers via ionic junctions," *ACS Macro Letters* **9**, 1667 (2020).
12. **R. Kumar**, J.P. Mahalik, K.S. Silmore, Z. Wojnarowska, A. Erwin, J.F. Ankner, A.P. Sokolov, B.G. Sumpter, and V. Bocharova, "Capacitance of thin films containing polymerized ionic liquids," *Science Advances* **6**, eaba7952 (2020).
13. **R. Kumar** and M. Muthukumar, "Surface Tension of Dielectric–Air Interfaces," *J. Phys. Chem. B* **124**, 5265 (2020).
14. V. Bocharova, A.C. Genix, J.M.Y. Carrillo, **R. Kumar**, B. Carroll, A. Erwin, D. Voylov, A. Kisliuk, Y. Wang, B.G. Sumpter, and A.P. Sokolov, "Addition of short polymer chains mechanically reinforces glassy poly(2-vinylpyridine)–silica nanoparticle nanocomposites," *ACS Appl. Nano Mater.* **3**, 3427 (2020).
15. H. Mei, T.S. Laws, J.P. Mahalik, J. Li, A.H. Mah, T. Terlier, P. Bonnesen, D. Uhrig, **R. Kumar**, G.E. Stein, and R. Verduzco, "Entropy and enthalpy mediated segregation of bottlebrush copolymers to interfaces," *Macromolecules* **52**, 8910 (2019).
16. **R. Kumar**, W. Li, B.G. Sumpter, and M. Muthukumar, "Understanding the effects of dipolar interactions on the thermodynamics of diblock copolymer melts," *J. Chem. Phys.* **151**, 054902 (2019).
17. W. Li, J.M.Y. Carrillo, J. Katsaras, B.G. Sumpter, R. Ashkar, and **R. Kumar**, "The influence of curvature on domain distribution in binary mixture membranes," *Soft Matter* **15**, 6642 (2019).
18. A.H. Mah, T.S. Laws, W. Li, H. Mei, C.C. Brown, A. Ilevlev, **R. Kumar**, R. Verduzco, and G.E. Stein, "Entropic and Enthalpic Effects in Thin Film Blends of Homopolymers and Bottlebrush Polymers," *Macromolecules* **52**, 1526 (2019).
19. **R. Kumar**, B. Lokitz, T.E. Long, and B.G. Sumpter, "Enhanced scattering induced by electrostatic correlations in concentrated solutions of salt-free dipolar and ionic polymers," *J. Chem. Phys.* **149**, 163336 (2018).
20. H. Kim, M.M.L. Arras, J.P. Mahalik, W. Wang, D.M. Yu, S. Chernyy, M. Goswami, **R. Kumar**, B.G. Sumpter, K. Hong, G.S. Smith, and T.P. Russell, "Studies on the 3-lamellar morphology of miktoarm terpolymers," *Macromolecules* **51**, 7491 (2018).
21. J.W. Dugger, W. Li, M. Chen, T.E. Long, R.J. L. Welbourn, M.W. A. Skoda, J.F. Browning, **R. Kumar**, and B.S. Lokitz, "Nanoscale resolution of electric-field induced motion in ionic diblock copolymer thin films," *ACS Appl. Mater. Interfaces* **10**, 32678 (2018).
22. S. Chernyy, J.P. Mahalik, **R. Kumar**, J.J.K. Kirkensgaard, M.M.L. Arras, H. Kim, L. Schulte, S. Ndoni, G.S. Smith, K. Mortensen, B.G. Sumpter, T.P. Russell, and K. Almdal, "On the morphological behavior of ABC miktoarm stars containing poly(cis 1,4-isoprene), poly(styrene), and poly(2-vinylpyridine)," *J. Polym. Sci. Part B: Polym. Phys.* **56**, 1491 (2018).

23. J.P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Understanding the effects of symmetric salt on the structure of a planar dipolar polymer brush," *J. Chem. Phys.* **149**, 163334 (2018).
24. M. Chen, J.W. Dugger, X. Li, Y. Wang, **R. Kumar**, K.M. Meek, D.W. Uhrig, J.F. Browning, L.A. Madsen, T.E. Long, and B.S. Lokitz, "Polymerized ionic liquids: Effects of counter-anions on ion conduction and polymerization kinetics," *J. Polym. Sci. Part A: Polym. Chem.* **56**, 1346 (2018).
25. J.P. Mahalik, J.W. Dugger, S.W. Sides, B.G. Sumpter, V. Lauter, and **R. Kumar**, "Interpreting neutron reflectivity profiles of diblock copolymer nanocomposite thin films using hybrid particle-field simulations," *Macromolecules* **51**, 3116(2018).
26. J. Cummings, J.S. Lowengrub, B.G. Sumpter, S.M. Wise, and **R. Kumar**, "Modeling solvent evaporation during thin film formation in phase separating polymer mixtures," *Soft Matter* **14**, 1833 (2018).
27. S. Chernyy, J.J.K. Kirkensgaard, J.P. Mahalik, H. Kim, M.M.L. Arras, **R. Kumar**, B.G. Sumpter, G.S. Smith, K. Mortensen, T.P. Russell, and K. Almdal, "Bulk and surface morphologies of ABC miktoarm star terpolymers composed of PDMS, PI, and PMMA arms," *Macromolecules* **51**, 1041 (2018).
28. V. Bocharova, Z. Wojnarowska, P-F. Cao, Y. Fu, **R. Kumar**, B. Li, V.N. Novikov, S. Zhao, A.M. Kisliuk, T. Saito, J.W. Mays, B.G. Sumpter, and A.P. Sokolov, "The influence of chain rigidity and dielectric constant on the glass transition temperature in polymerized ionic liquids," *J. Phys. Chem. B* **121**, 11511 (2017).
29. Y. Fu, V. Bocharova, M. Ma, A.P. Sokolov, B.G. Sumpter, and **R. Kumar**, "Effects of counterion size and backbone rigidity on the dynamics of ionic polymer melts and glasses," *Phys. Chem. Chem. Phys.* **19**, 27442 (2017).
30. Z. Wojnarowska, H. Feng, Y. Fu, S. Cheng, B. Carroll, **R. Kumar**, V.N. Novikov, A.M. Kisliuk, T. Saito, N-G. Kang, J.W. Mays, A.P. Sokolov, and V. Bocharova, "Effect of chain rigidity on the decoupling of ion motion from segmental relaxation in polymerized ionic liquids: ambient and elevated pressure studies," *Macromolecules* **50**, 6710 (2017).
31. J.P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Attraction between opposing planar dipolar polymer brushes," *Langmuir* **33**, 9231 (2017).
32. E.S. Muckley, C.B. Jacobs, K. Vidal, J.P. Mahalik, **R. Kumar**, B.G. Sumpter, and I. Ivanov, "New insights on electro-optical response of poly (3, 4-ethylenedioxythiophene): poly (styrenesulfonate) film to humidity," *ACS Appl. Mater. Interfaces* **9**, 15880 (2017).
33. S.M. Yang, A.N. Morozovska, **R. Kumar**, E.A. Eliseev, Y. Cao, L. Mazet, N. Balke, S. Jesse, R.K. Vasudevan, C. Dubourdieu, and S.V. Kalinin, "Mixed electrochemical-ferroelectric states in nanoscale ferroelectrics," *Nature Physics* **13**, 812 (2017).
34. K. Misichronis, J. Chen, A. Imel, **R. Kumar**, J. Thostenson, K. Hong, M. Dadmun, B. G. Sumpter, J. G. Kennemur, N. Hadjichristidis, J. W. Mays, and A. Avgeropoulos, "Investigation on the phase diagram and interaction parameter of poly(styrene-b-1,3-cyclohexadiene) diblock copolymers," *Macromolecules* **50**, 2354 (2017).
35. **R. Kumar**, J.P. Mahalik, V. Bocharova, E.W. Stacy, C. Gainary, T. Saito, M. P. Gobet, S. Greenbaum, B.G. Sumpter, and A.P. Sokolov, "A Rayleighian approach for modeling kinetics of ionic transport in polymeric media," *J. Chem. Phys.* **146**, 064902 (2017).
36. J.P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Vertical phase segregation induced by dipolar interactions in planar brushes," *Macromolecules* **49**, 7096 (2016).

37. N. Herath, S. Das, J. Zhu, **R. Kumar**, J. Chen, K. Xiao, G. Gu, J.F. Browning, B.G. Sumpter, I.N. Ivanov, and V. Lauter, "Unraveling the fundamental mechanisms of solvent-additive-induced optimization of power conversion efficiencies in organic photovoltaic devices," *ACS Appl. Mater. Interfaces* **8**, 20220 (2016).
38. J.Y. Carrillo, Z. Seibers, **R. Kumar**, M.A. Matheson, J.F. Ankner, M. Goswami, K. Bhaskaran-Nair, W.A. Shelton, B.G. Sumpter, and S.M. Kilbey, "Petascale simulations of the morphology and the molecular interface of bulk heterojunctions," *ACS Nano* **10**, 7008 (2016).
39. A.P. Holt, V. Bocharova, S. Cheng, A.M. Kisliuk, B.T. White, T. Saito, D. Uhrig, J.P. Mahalik, **R. Kumar**, A.E. Imel, T. Etampawala, H. Martin, N. Sikes, B.G. Sumpter, M.D. Dadmun, and A.P. Sokolov, "Controlling interfacial dynamics: covalent bonding versus physical adsorption in polymer nanocomposites," *ACS Nano* **10**, 6843 (2016).
40. E. Muckley, J. Lynch, **R. Kumar**, B.G. Sumpter, and I.N. Ivanov, "PEDOT:PSS/QCM-based multimodal humidity and pressure sensor," *Sensors and Actuators B: Chemical* **236**, 91 (2016).
41. J. P. Mahalik, Y. Yang, C. Deodhar, J. F. Ankner, B. S. Lokitz, S. M. Kilbey, B. G. Sumpter, and **R. Kumar**, "Monomer volume fraction profiles in pH responsive planar polyelectrolyte brushes," *Journal of Polymer Science Part B: Polymer Physics* **54**, 956 (2016).
42. 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 strongly adsorbed polymer melts," *Macromolecules* **48**, 4207 (2015).
43. 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* **5**, 13407 (2015).
44. 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* **7**, 15134 (2015).
45. **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).
46. 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).
47. 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).
48. **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).
49. **R. Kumar**, B. G. Sumpter, and M. Muthukumar, "Enhanced phase segregation induced by dipolar interactions in polymer blends," *Macromolecules* **47**, 6491 (2014).
50. 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).

51. 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).
52. 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).
53. **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).
54. 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).
55. **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).
56. **R. Kumar**, Y. Li, S.W. Sides, J.W. Mays, and B.G. Sumpter, “Morphology diagrams for  $A_2B$  copolymer melts: real-space self-consistent field theory,” *J. Phys.: Conf. Ser.* **402**, 012042 (2012).
57. 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).
58. **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).
59. 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).
60. 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).
61. 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).
62. **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).
63. **R. Kumar** and M. Muthukumar, “Origin of translocation barriers for polyelectrolyte chains,” *J. Chem. Phys.* **131**, 194903 (2009).
64. **R. Kumar** and G.H. Fredrickson, “Theory of polyzwitterion conformations,” *J. Chem. Phys.* **131**, 104901 (2009).

65. **R. Kumar**, A. Kundagrami, and M. Muthukumar, "Counterion adsorption on flexible polyelectrolytes : comparison of theories," *Macromolecules* **42**, 1370 (2009).
66. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *J. Chem. Phys.* **128**, 184902 (2008).
67. **R. Kumar** and M. Muthukumar, "Microphase separation in polyelectrolytic diblock copolymer melt : Weak segregation limit," *J. Chem. Phys.* **126**, 214902 (2007).

### Conference Proceedings

68. J.W. Dugger, M. Chen, J. Mahalik, W. Li, T.E. Long, A. Ievlev, O. Ovchinnikova, D. Uhrig, P. Bonnesen, **R. Kumar**, J. Browning, and B.S. Lokitz, "Investigating the electromechanical response mechanism of ionic block copolymers," *TechConnect Briefs*, Vol 1, Materials for Energy, Efficiency and Sustainability : TechConnect Briefs, 258-261, Washington, Virginia, May 2017.
69. **R. Kumar**, V. Bocharova, E. Strelcov, A. Tselev, L. Collins, I.I. Kravchenko, S. Berdzinski, V. Strehmel, O.S. Ovchinnikova, J.A. Minutolo, J.R. Sangoro, A.L. Agapov, A. Kisliuk, A.P. Sokolov, S.V. Kalinin, and B.G. Sumpter, "Polymerized ionic liquid films in strong electric fields: ion transport and nanopatterning," *TechConnect Briefs, Materials for Energy, Efficiency and Sustainability*, Vol 1, Advanced Materials : TechConnect Briefs, 514-517, Washington, Virginia, June 2015.
70. **R. Kumar** and B.G. Sumpter, "Quantitative analysis of chain packing in polymer melts using large scale molecular dynamics simulations," *Proc. SciDAC 2011*, Denver, CO, July 10-14, 2011, <http://press.mcs.anl.gov/scidac2011/>
71. 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 Chapters : Invited Contributions

72. **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.
73. 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.

### Presentations : Invited

1. **R. Kumar**, "Spatiotemporal changes in thin films of ionic polymers due to electric field and thermal effects," Basic Energy Science Slam on Energy Storage, August 2022 (webinar).
2. **R. Kumar**, "Modeling charge and mass transport in polymeric media," Material Science and Technology Division Journal Club, Oak Ridge, TN, April 2022 (talk).
3. **R. Kumar**, "Generating knotted configurations in polymers using field theory approach," *Novel Mathematical Methods in Material Science: Applications to Biomaterials*, Banff International Research Station (BIRS) for Mathematical Innovation and Discovery, Canada (virtual), June 2021 (talk).

4. **R. Kumar**, "Counter-intuitive effects of electrostatics in charged polymers," *Department of Chemistry, Clemson University, SC* (virtual), April 2021 (talk).
5. **R. Kumar**, "Modeling structure and ionic transport in polymer electrolytes," *DOE CABLE Workshop* (virtual), April 2021 (talk).
6. **R. Kumar**, "Modeling electrostatic effects in charged polymers," *Energy and Soft Matter over Tea*, Oak Ridge, TN (virtual), March 2021 (talk).
7. **R. Kumar**, "Topological effects in polymers," *American Mathematical Society: Applied Knot Theory Workshop* (virtual), October 2020 (talk).
8. **R. Kumar**, "Surface induced segregation in bottlebrushes," *American Chemical Society Meeting* (virtual), August 2020 (talk).
9. **R. Kumar**, "Effects of polydispersity on microphase separation in thin films of diblock copolymers: Theories, simulations, and experiments," *American Chemical Society Meeting*, Orlando, FL, April 2019 (talk).
10. **R. Kumar**, "Undulated films of conformationally asymmetric binary lipids and polymer blends," *American Chemical Society Meeting*, Orlando, FL, March 2019 (talk).
11. **R. Kumar**, "Fundamental role of electric polarization in polymer physics," *CNMS Seminar Series*, Oak Ridge, TN, August 2018 (talk).
12. **R. Kumar**, "Applied Mathematics and Polymer Physics," *Department of Mathematics, University of Tennessee*, Knoxville, TN, August 2018 (talk).
13. **R. Kumar**, "Insights obtained from theories and simulations of charged polymers," *Polymer Day*, Oak Ridge, TN, May 2018 (talk).
14. **R. Kumar**, "A Rayleighian approach for modeling kinetics of ionic transport in polymeric media," *American Chemical Society Meeting*, San Francisco, CA, April 2017 (talk).
15. **R. Kumar**, "Effects of dipolar interactions in polymer brushes," *American Physical Society Meeting*, Baltimore, MD, March 2016 (talk).
16. **R. Kumar**, "Polymerized ionic liquid films in strong electric fields: ion transport and nanopatterning," *TechConnect World Innovation Conference*, Washington, DC, June 2015 (talk).
17. **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).
18. **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).
19. **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).
20. **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).
21. **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).



22. 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).
23. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Physics Department, University of Tennessee, Knoxville, TN, April 2012* (talk).
24. **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).
25. **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).
26. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Department of Chemistry, University of Tennessee, Knoxville, TN, March 2011* (talk).
27. **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).
28. **R. Kumar**, "Modeling charged polymers using field-theoretic methods," *Center for Functional Nanomaterials, Brookhaven National Lab, NY, March 2010* (talk).

#### Other Presentations

29. **R. Kumar**, "Non-equilibrium thermodynamics of ion transport in polymeric media," *Workshop on Resolving the Dynamics in Soft Materials, Oak Ridge, TN, Sep 2022* (poster).
30. **R. Kumar**, "Non-equilibrium thermodynamics of ion transport in polymeric media," *Gordon Research Conference: Polymer Physics, Mount Holyoke, MA, July 2022* (poster).
31. **R. Kumar**, "Modeling knotted topological configurations in confined polymers using a field theoretic approach," *APS March Meeting, Chicago, IL, March 2022* (talk).
32. **R. Kumar**, E. Panagiotou and L. Kauffman, "Discovering topological invariants in inhomogeneous polymeric systems," *APS March Meeting, Nashville, TN, March 2021* (talk).
33. **R. Kumar**, "Rayleighian approach for modeling dynamics of charged polymers in external electric fields," *CNMS User Meeting* (virtual), August 2020 (poster).
34. **R. Kumar**, W. Li, B.G. Sumpter, and M. Muthukumar, "Microphase separation in dipolar diblock copolymer melts," *APS March Meeting, Boston, MA, March 2019* (talk).
35. J. Mahalik, H. Kim, M.M.L. Arras, W. Wang, S. Chernyy, K. Hong, G.S. Smith, B.G. Sumpter, T.P. Russell, and **R. Kumar**, "Interpreting the hierarchical morphology of ABC miktoarm terpolymers using self-consistent field theory," *APS March Meeting, Boston, MA, March 2019* (talk).
36. H. Mei, A. Mah, T. Laws, W. Li, T. Terlier, **R. Kumar**, G.E. Stein, and R. Verduzco, "Three-dimensional morphological analysis of polymer blends through combined ToF-SIMS/AFM," *APS March Meeting, Boston, MA, March 2019* (talk).
37. **R. Kumar**, B. Lokitz, B.G. Sumpter, and T.E. Long, "Dipolar interactions as the origin of excess scattering in concentrated solutions and melts of ionic polymers," *APS March Meeting, Los Angeles, CA, March 2018* (talk).

38. W. Li, B. Lokitz, B.G. Sumpter, and **R. Kumar**, "Molecular dynamics of ionic block copolymers in thin films under electric fields," *APS March Meeting*, Los Angeles, CA, March 2018 (talk).
39. J.W. Dugger, W. Li, M. Chem, T.E. Long, **R. Kumar**, J.F. Browning, and B.S. Lokitz, "Nanoscale resolution of electric-field induced motion in ionic copolymer films," *APS March Meeting*, Los Angeles, CA, March 2018 (talk).
40. B.S. Lokitz, J. Dugger, W. Li, **R. Kumar**, L. Collins, N. Balke, and J. Browning, "Nanoscale resolution of electric-field induced motion in ionic copolymer films," *ACS National Meeting*, Boston, MA, August 2018 (talk).
41. W. Li, B. Lokitz, B.G. Sumpter, and **R. Kumar**, "Effects of dipolar interactions on microphase separation in diblock copolymer melts," *APS March Meeting*, Los Angeles, CA, March 2018 (poster).
42. **R. Kumar**, "Polymerized ionic liquids (PolyILs) in electric fields," *CNMS Advisory Committee On-Site Meeting*, Oak Ridge, TN, April 2018 (poster).
43. **R. Kumar**, "Polymerized ionic liquids (PolyILs) in electric fields," *Gordon Research Conference-Polymer Physics*, South Hadley, MA, July 2018 (poster).
44. W. Li, J.M.Y. Carrillo, B.G. Sumpter, and **R. Kumar**, "Curvature-induced domain sorting in membranes of phase-separating binary mixtures," *Gordon Research Conference-Polymer Physics*, South Hadley, MA, July 2018 (poster).
45. J. Cummings, S. Wise, and **R. Kumar**, "Modeling and simulation of microstructural evolution in organic photovoltaic thin films," *41st SIAM Southeastern Atlantic Section Conference (SIAM-SEAS)*, Florida State University, FL, March 2017 (talk).
46. Y. Fu, M. Chen, T.E. Long, J. Dugger, J.F. Browning, B.G. Sumpter, B.S. Lokitz, and **R. Kumar**, "Probing electromechanical responses of ionic polymers in nanoscale thin films using molecular dynamics simulations," *CNMS User Meeting*, Oak Ridge, TN, August 2016 (poster).
47. J. P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Modeling helical polymer brushes using self-consistent field theory (SCFT)," *American Physical Society Meeting*, Baltimore, MD, March 2016 (talk).
48. B. Philip and **R. Kumar**, "Iterative methods for nonlinear systems arising in diblock copolymer systems," *American Mathematical Society Meeting*, Huntsville, AL, March 2015 (talk).
49. J. P. Mahalik, **R. Kumar**, and B.G. Sumpter, "Planar dipolar polymer brush: field theoretical investigations," *American Physical Society Meeting*, San Antonio, TX, March 2015 (talk).
50. **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).
51. 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).
52. 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).

53. **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).
54. 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).
55. **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).
56. 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).
57. 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).
58. **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).
59. **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).
60. 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).
61. **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).
62. 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).
63. **R. Kumar** and G.H. Fredrickson, "Coacervation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *American Physical Society*, Portland, OR, March 2010 (talk).
64. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *American Physical Society*, Portland, OR, March 2010 (poster).
65. **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).
66. **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).

67. **R. Kumar** and G.H. Fredrickson, "Theory of polyelectrolytic solutions," *American Physical Society*, Pittsburgh, PA, March 2009 (talk).
68. 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).
69. **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).
70. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *American Physical Society*, New Orleans, LA, March 2008 (talk).
71. **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).
72. **R. Kumar** and M. Muthukumar, "Morphology diagrams for polyelectrolytic diblock copolymers," *American Physical Society*, Baltimore, MD, March 2006 (talk).
73. **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).