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

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 2020-2022
- Mentored seven post-docs, two graduate and five undergraduate students 2012-Present
- Organized a workshop, “Understanding structure and dynamics of charged polymers,” *the CNMS User Meeting*,ORNL, Oak Ridge, TN 2023.

- Organized a focus session, "Ion and thermal transport in polymers," *the American Physical Society March Meeting*, Chicago, IL 2022 (virtual).
- 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
- 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, the US-Israel Binational Science Foundation, and the Irish Research Council 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 E, 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. J-M. Carrillo, Y. Wang, **R. Kumar**, and B.G. Sumpter, "Coarse-grained explicit-solvent molecular dynamics simulations of semidilute unentangled polyelectrolyte solutions," *The European Physical Journal E* **46**, 92 (2023).
2. C. Gainaru, **R. Kumar**, I. Popov, Md A. Rahman, M. Lehmann, E. Stacy, V. Bocharova, B.G. Sumpter, T. Saito, K.S. Schweizer, and A.P. Sokolov, "Mechanisms controlling the energy barrier for ion hopping in polymer electrolytes," *Macromolecules* **56**, 6051 (2023).
3. Z. Liu, J.K. Keum, T. Li, J. Chen, K. Hong, Y. Wang, B.G. Sumpter, R. Advincula, and **R. Kumar**, "Anti-polyelectrolyte and polyelectrolyte effects on conformations of polyzwitterionic chains in dilute aqueous solutions," *PNAS Nexus* **2**, pgad204 (2023).
4. D. Eby, M. Jakowski, V. Lauter, M. Doucet, P. Ganesh, M. Fuentes-Cabrera, and **R. Kumar**, "Extraction of interaction parameters from specular neutron reflectivities in thin films of diblock copolymers: an "Inverse Problem"," *Nanoscale* **15**, 7280 (2023).
5. P.P. Angelopoulou, L.T. Kearney, J.K. Keum, L. Collins,**R. Kumar**, G. Sakellariou, R.C. Advincula, J.W. Mays, and K. Hong, "High-χ diblock copolymers containing poly(vinylpyridine-N-oxide) segments," *J. Mater. Chem. A***11**, 9846 (2023).
6. 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).
7. 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).
8. 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 di-

block copolymers from poly(glycidyl vethacrylate)-block-poly(vinyldimethylazlactone) backbones," *Macromolecules* **55**, 488 (2022).

9. 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).
10. K.S. Silmore and **R. Kumar**, "Dynamics of a single polyampholyte chain," *J. Chem. Phys.* **155**, 214903 (2021).
11. 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).
12. **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).
13. 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).
14. 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).
15. 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).
16. 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).
17. **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).
18. **R. Kumar** and M. Muthukumar, "Surface Tension of Dielectric–Air Interfaces," *J. Phys. Chem. B* **124**, 5265 (2020).
19. 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).
20. 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).
21. **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).
22. 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).

23. A.H. Mah, T.S. Laws, W. Li, H. Mei, C.C. Brown, A. Ievlev, **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).
24. **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).
25. 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).
26. 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).
27. 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).
28. 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).
29. 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 counteranions on ion conduction and polymerization kinetics," *J. Polym. Sci. Part A: Polym. Chem.* **56**, 1346 (2018).
30. 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).
31. 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).
32. 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).
33. 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).
34. 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).
35. 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).

36. J.P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Attraction between opposing planar dipolar polymer brushes," *Langmuir* **33**, 9231 (2017).
37. 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).
38. 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).
39. 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).
40. **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).
41. J.P. Mahalik, B.G. Sumpter, and **R. Kumar**, "Vertical phase segregation induced by dipolar interactions in planar brushes," *Macromolecules* **49**, 7096 (2016).
42. 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).
43. 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).
44. 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).
45. 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).
46. 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).
47. 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).
48. 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).
49. 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).

50. **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).
51. 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).
52. 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).
53. **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).
54. **R. Kumar**, B. G. Sumpter, and M. Muthukumar, "Enhanced phase segregation induced by dipolar interactions in polymer blends," *Macromolecules* **47**, 6491 (2014).
55. 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).
56. 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).
57. 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).
58. **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).
59. 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).
60. **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).
61. **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).
62. 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).

63. **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).
64. 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).
65. 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).
66. 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).
67. **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).
68. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *J. Chem. Phys.* **131**, 194903 (2009).
69. **R. Kumar** and G.H. Fredrickson, "Theory of polyzwitterion conformations," *J. Chem. Phys.* **131**, 104901 (2009).
70. **R. Kumar**, A. Kundagrami, and M. Muthukumar, "Counterion adsorption on flexible polyelectrolytes : comparison of theories," *Macromolecules* **42**, 1370 (2009).
71. **R. Kumar** and M. Muthukumar, "Confinement free energy of flexible polyelectrolytes in spherical cavities," *J. Chem. Phys.* **128**, 184902 (2008).
72. **R. Kumar** and M. Muthukumar, "Microphase separation in polyelectrolytic diblock copolymer melt : Weak segregation limit," *J. Chem. Phys.* **126**, 214902 (2007).

Conference Proceedings

73. 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.
74. **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.
75. **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/
76. 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

77. **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.
78. 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**, "Interpreting neutron reflectivity data from thin films of block copolymers using neural networks," ACS March Meeting, San Francisco CA, August 2023 (talk).
2. **R. Kumar**, "Theme Science Research: Harnessing Complex Macromolecular Conformations (HCMC)," CNMS User Meeting, Knoxville TN, August 2023 (talk).
3. **R. Kumar**, "Using statistical mechanics to understand the structure, dynamics, and conductivity in polymerized ionic liquids," EFRC All Hands Meeting, Oak Ridge, TN, May 2023 (talk).
4. **R. Kumar**, "Developing a theory of ion transport in solid polymer electrolytes," Mathematics in Computation Seminar, Oak Ridge, TN, March 2023 (talk).
5. **R. Kumar**, "Plasmon mode in semi-dilute polyelectrolyte solutions," ORNL Soft Matter Symposium, Oak Ridge, TN, October 2022 (talk).
6. **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).
7. **R. Kumar**,"Modeling charge and mass transport in polymeric media," Material Science and Technology Division Journal Club, Oak Ridge, TN, April 2022 (talk).
8. **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).
9. **R. Kumar**, "Counter-intuitive effects of electrostatics in charged polymers," *Department of Chemistry, Clemson University*, SC (virtual), April 2021 (talk).
10. **R. Kumar**, "Modeling structure and ionic transport in polymer electrolytes," *DOE CABLE Workshop* (virtual), April 2021 (talk).
11. **R. Kumar**, "Modeling electrostatic effects in charged polymers," *Energy and Soft Matter over Tea*, Oak Ridge, TN (virtual), March 2021 (talk).
12. **R. Kumar**, "Topological effects in polymers," *American Mathematical Society: Applied Knot Theory Workshop* (virtual), October 2020 (talk).
13. **R. Kumar**, "Surface induced segregation in bottlebrushes," *American Chemical Society Meeting* (virtual), August 2020 (talk).
14. **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).

15. **R. Kumar**, "Undulated films of conformationally asymmetric binary lipids and polymer blends," *American Chemical Society Meeting*, Orlando, FL, March 2019 (talk).
16. **R. Kumar**, "Fundamental role of electric polarization in polymer physics," *CNMS Seminar Series*, Oak Ridge, TN, August 2018 (talk).
17. **R. Kumar**, "Applied Mathematics and Polymer Physics," *Department of Mathematics, University of Tennessee*, Knoxville, TN, August 2018 (talk).
18. **R. Kumar**, "Insights obtained from theories and simulations of charged polymers," *Polymer Day*, Oak Ridge, TN, May 2018 (talk).
19. **R. Kumar**, "A Rayleighian approach for modeling kinetics of ionic transport in polymeric media," *American Chemical Society Meeting*, San Francisco, CA, April 2017 (talk).
20. **R. Kumar**, "Effects of dipolar interactions in polymer brushes," *American Physical Society Meeting*, Baltimore, MD, March 2016 (talk).
21. **R. Kumar**, "Polymerized ionic liquid films in strong electric fields: ion transport and nanopatterning," *TechConnect World Innovation Conference*, Washington, DC, June 2015 (talk).
22. **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).
23. **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).
24. **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).
25. **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).
26. **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).
27. 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).
28. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Physics Department, University of Tennessee*, Knoxville, TN, April 2012 (talk).
29. **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).
30. **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).
31. **R. Kumar**, "Theory and simulations of neutral and charged polymers," *Department of Chemistry, University of Tennessee*, Knoxville, TN, March 2011 (talk).

32. **R. Kumar** and B.G. Sumpter, "Insights obtained from coarse-grained modeling of charged polymers," *66th Southwest and 62nd Southeastern Regional Meeting of the American Chemical Society*, New Orleans, LA, December 2010 (talk).
33. **R. Kumar**, "Modeling charged polymers using field-theoretic methods," *Center for Functional Nanomaterials, Brookhaven National Lab*, NY, March 2010 (talk).

Other Presentations

34. **R. Kumar**, "Interpreting neutron reflectivity data from thin films of block copolymers using neural networks," APS March Meeting, Las Vegas NV, March 2023 (talk).
35. **R. Kumar**, "Polyelectrolyte and anti-polyelectrolyte effects on chain conformations of polyzwitterions," APS March Meeting, Las Vegas NV, March 2023 (talk).
36. **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).
37. **R. Kumar**, "Non-equilibrium thermodynamics of ion transport in polymeric media," *Gordon Research Conference: Polymer Physics*, Mount Holyoke, MA, July 2022 (poster).
38. **R. Kumar**, "Modeling knotted topological configurations in confined polymers using a field theoretic approach," *APS March Meeting*, Chicago, IL, March 2022 (talk).
39. **R. Kumar**, E. Panagiotou and L. Kauffman, "Discovering topological invariants in inhomogeneous polymeric systems," *APS March Meeting*, Nashville, TN, March 2021 (talk).
40. **R. Kumar**, "Rayleighian approach for modeling dynamics of charged polymers in external electric fields," *CNMS User Meeting* (virtual), August 2020 (poster).
41. **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).
42. 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).
43. 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).
44. **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).
45. 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).
46. 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).
47. 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).

48. 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).
49. **R. Kumar**, “Polymerized ionic liquids (PolyILs) in electric fields,” *CNMS Advisory Committee On-Site Meeting*, Oak Ridge, TN, April 2018 (poster).
50. **R. Kumar**, “Polymerized ionic liquids (PolyILs) in electric fields,” *Gordon Research Conference-Polymer Physics*, South Hadley, MA, July 2018 (poster).
51. 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).
52. 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).
53. 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).
54. 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).
55. B. Philip and **R. Kumar**,“Iterative methods for nonlinear systems arising in diblock copolymer systems,” *American Mathematical Society Meeting*, Huntsville, AL, March 2015 (talk).
56. 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).
57. **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).
58. 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).
59. 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).
60. **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).
61. 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).
62. **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).

63. 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).
64. 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).
65. **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).
66. **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).
67. 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).
68. **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).
69. 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).
70. **R. Kumar** and G.H. Fredrickson, "Coacervation in symmetric mixtures of oppositely charged rodlike polyelectrolytes," *American Physical Society*, Portland, OR, March 2010 (talk).
71. **R. Kumar** and M. Muthukumar, "Origin of translocation barriers for polyelectrolyte chains," *American Physical Society*, Portland, OR, March 2010 (poster).
72. **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).
73. **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).
74. **R. Kumar** and G.H. Fredrickson, "Theory of polyzwitterionic solutions," *American Physical Society*, Pittsburgh, PA, March 2009 (talk).
75. 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).
76. **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).

77. **R. Kumar** and M. Muthukumar, “Confinement free energy of flexible polyelectrolytes in spherical cavities,” *American Physical Society* , New Orleans, LA, March 2008 (talk).
78. **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).
79. **R. Kumar** and M. Muthukumar, “Morphology diagrams for polyelectrolytic diblock copolymers,” *American Physical Society* , Baltimore, MD, March 2006 (talk).
80. **R. Kumar** and M. Muthukumar, “Morphology diagrams for polyelectrolytic diblock copolymers,” 6^{th} *National Graduate Research Conference, University of Massachusetts*, Amherst, MA, June 2005 (talk).