Rajesh Khare

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Education

B.S., Chemical Engineering**,** Institute of Chemical Technology (formerly UDCT), Mumbai, India (1989).

Ph.D., Chemical Engineering (Advisor: Michael Paulaitis), University of Delaware (1994).

Post-Doctoral (with Juan de Pablo and Arun Yethiraj), Department of Chemical Engineering and Department of Chemistry, University of Wisconsin-Madison (1995-1997).

Professional Experience

Department of Chemical Engineering, Texas Tech University
Associate Department Chair (02/2018 – present)
Professor (09/2016 – present)
Associate Professor (09/2010 – 08/2016)
Assistant Professor (09/2005 – 08/2010)

Department of Chemical Engineering, University of Wisconsin-Madison
Visiting Senior Scientist (with Juan de Pablo and Michael Graham), (09/2004 – 08/2005)

Physics Department, San Diego State University, San Diego, CA
Adjunct Professor (01/2004 – 08/2004)

Accelrys Inc. (formerly Molecular Simulations Inc.), San Diego, CA
Manager, Materials Science Modeling R&D-San Diego (2002–01/2004)
Manager, Atomistic Polymer R&D (2000–2002)
Product Development Scientist, Polymers (1997-2000)

Department of Chemical Engineering, University of Wisconsin-Madison
Associate Lecturer, concurrent with the post-doc position (1996)

Honors and Awards

George T. and Gladys Abell-Hanger Faculty Award, College of Engineering, Texas Tech University (2013).

Ed and Linda Whitacre Faculty Fellow, College of Engineering, Texas Tech University (2009-2012).

3M Non-tenured Faculty Award (2005, 2006, 2007).

National Talent Search (Science) Scholarship, Government of India (1983-1989).

RESEARCH ACTIVITIES

Publications

h-index: **24** (Google Scholar), **21** (Web of Science)

Refereed Book Chapters

(57) Muthukumar, L.; Khare R.; "Molecular dynamics simulation of free energy of desorption of cellohexaose from a cellulose crystal surface" in *Applications of Molecular Modeling to Challenges in Clean Energy*, ACS Symposium Series (ACS Books), Eds.: G. Fitzgerald and N. Govind, Vol. 1133, pp. 1-17 (2013). **DOI:** 10.1021/bk-2013-1133.ch001.

(56) Eichinger, B. E.; Khare, R.; "Molecular Modeling" in *Encyclopedia of Polymer Science and Technology*, Wiley Interscience (2002), available online at http://www.mrw.interscience.wiley.com/epst/articles/pst205/frame.html.

Refereed Journal Articles

Published:

(55) Fogel, A. L.; Ravichandran, A.; Mani, S.; Upadhyay, B.; Khare, R.; Morgan, S. E.; "Water structure and mobility in acrylamide copolymer glycohydrogels with galactose and siloxane pendant groups", *J. Polym. Sci. B Polym. Phys.*, published online (2019). **DOI:** 10.1002/polb.24815.

(54) Saravi, S. H.; Ravichandran, A.; Khare, R.; Chen, C.-C.; "Bridging two-liquid theory with molecular simulations for electrolytes: An investigation of aqueous NaCl solution", *AIChE J.*, **65**, 1315-1324 (2019).

(53) Ravichandran, A.; Chen, C.-C.; Khare, R.; "Prediction of χ parameter of polymer blends by combining molecular simulations and integral equation theory", *J. Phys. Chem. B.*, **122**, 9022–9031 (2018).

(52) Hossain, N.; Ravichandran, A.; Khare, R.; Chen, C.-C.; "Revisiting electrolyte thermodynamic models: Insight from molecular simulations", *AIChE J.*, **64**, 3728-3734 (2018).

(51) Ravichandran, A.; Khare, R.; Chen, C.-C.; "Predicting NRTL binary interaction parameters from molecular simulations", *AIChE J.*, **64**, 2758-2769 (2018).

(50) Khabaz, F.; Khare, R.; "Molecular simulations of asphalt rheology: Application of time-temperature superposition principle", *J. Rheol.*, **62**, 941-954 (2018).

(49) Khabaz, F.; Zhang, Y.; Xue, L.; Quitevis, E. L.; Maginn, E. J.; Khare, R.; "Temperature dependence of volumetric and dynamic properties of imidazolium-based ionic liquids", *J. Phys. Chem. B.*, **122**, 2414-2424 (2018).

(48) Mani, S.; Khare, R.; "Effect of chain flexibility and interlayer interactions on the dynamics of layered polymer systems", *Macromolecules*, **51**, 576-588 (2018).

(47) Dehghani, N. L.; Khare, R.; Christopher, G. F.; "2D Stokesian approach to modeling flow induced deformation of particle laden interfaces", *Langmuir*, **34**, 904-916 (2018).

(46) Godbole, R.; Khabaz, F.; Khare, R.; Hedden, R. C.; "Swelling of random copolymer networks in pure and mixed solvents: Multi-component Flory-Rehner theory", *J. Phys. Chem. B*, **121**, 7963−7977 (2017).

(45) Khare, R.; Devarajan, D. S.; "Molecular simulations of nanocolloids", *Current Opinion in Chemical Engineering*, **16**, 86-91 (2017).

(44) Habib, T.; Devarajan, D. S.; Khabaz, F.; Parviz, D.; Achee, T. C.; Khare, R.; Green, M. J.; "Co-solvents as liquid surfactants for boron nitride nanosheet (BNNS) dispersions", *Langmuir*, **32**, 11591−11599 (2016).

(43) Khabaz, F.; Mani, S.; Khare, R.; "Molecular origins of dynamic coupling between water and hydrated polyacrylate gels", *Macromolecules*, **49**, 7551-7562 (2016).

(42) Sirk, T. W.; Karim, M.; Lenhart, J. L.; Andzelm, J. W.; Khare, R.; "Bi-modal polymer networks: Viscoelasticity and mechanics from molecular dynamics simulation", *Polymer*, **90**, 178–186 (2016).

(41) Karim, M..; Indei, T.; Schieber, J. D.; Khare, R.; "Determination of linear viscoelastic properties of an entangled polymer melt by probe rheology simulations", *Phys. Rev. E.*, **93**, 012501 (2016).

(40) Mani, S.; Khabaz, F.; Godbole, R. V.; Hedden, R. C.; Khare, R.; "Structure and hydrogen bonding of water in polyacrylate gels: Effects of polymer hydrophilicity and water concentration", *J. Phys. Chem. B.*, **119**, 15381-15393 (2015).

(39) Zhang, Y.; Xue, L.; Khabaz, F.; Doerfler, R.; Quitevis, E. L.; Khare, R.; Maginn, E. J.; "Molecular topology and local dynamics govern the viscosity of imidazolium-based ionic liquids", *J. Phys. Chem. B.*, **119**, 14934-14944 (2015).

(38) Khabaz, F.; Khare, R.; "Glass transition and molecular mobility in styrene-butadiene rubber modified asphalt", *J. Phys. Chem. B.*, **119**, 14261-14269 (2015).

(37) Bari, R.; Parviz, D.; Khabaz, F.; Klaassen, C. D.; Metzler, S. D.; Hansen, M. J.; Khare, R.; Green, M. J.; "Liquid phase exfoliation and crumpling of inorganic nanosheets", *Physical Chemistry Chemical Physics*, **17**, 9383-9393 (2015).

(36) Sirk, T. W.; Karim, M.; Khare, K. S.; Lenhart, J. L.; Andzelm, J. W.; Khare, R.; "Bi-modal polymer networks: Composition-dependent trends in thermal, volumetric and structural properties from molecular dynamics simulation", *Polymer*, **58**, 199–208 (2015).

(35) Khabaz, F.; Khare, R.; “Effect of chain architecture on the size, shape, and intrinsic viscosity of chains in polymer solutions: A molecular simulation study”, *J. Chem. Phys.*, **141**, 214904 (2014).

(34) Khare, K. S.; Khabaz, F.; Khare, R.; “Effect of carbon nanotube functionalization on mechanical and thermal properties of cross-linked epoxy–carbon nanotube nanocomposites: Role of strengthening the interfacial interactions”, *ACS Applied Materials & Interfaces*., **6**, 6098-6110 (2014).

(33) Sirk, T. W.; Khare, K. S.; Karim, M.; Lenhart, J. L.; Andzelm, J. W.; McKenna, G. B.; Khare, R.; “High strain rate mechanical properties of a cross-linked epoxy across the glass transition”, *Polymer*, **54**, 7048-7057 (2013).

(32) Khare, K.; Khare, R.; “Effect of carbon nanotube dispersion on glass transition in cross-linked epoxy – carbon nanotube nanocomposites: Role of interfacial interactions”, *J. Phys. Chem. B*, **117**, 7444-7454 (2013).

(31) Karim, M..; Kohale, S. C.; Indei, T.; Schieber, J. D.; Khare, R.; “Determination of viscoelastic properties by analysis of probe particle motion in molecular simulations”, *Phys. Rev. E.*, **86**, 051501 (2012).

(30) Peri, S.; Karim, Muthukumar, L.; Karim, M. N.; Khare R.; “Dynamics of cello-oligosaccharides on a cellulose crystal surface”, *Cellulose*, **19**, 1791-1806 (2012).

(29) Khare, K.; Khare, R.; "Directed diffusion approach for preparing atomistic models of cross-linked epoxy for use in molecular simulations", *Macromolecular Theory and Simulations*, **21**, 322-327 (2012).

(28) Soni, N.; Lin, P.-H.; Khare R.; “Effect of cross-linker length on the thermal and volumetric properties of cross-linked epoxy networks: A molecular simulation study”, *Polymer*, **53**, 1015-1019 (2012).

(27) Hegde, G.; Chang, J.-F.; Chen, Y.-L.; Khare, R.; “Conformation and diffusion behavior of ring polymers in solution: A comparison between molecular dynamics, multiparticle collision dynamics and lattice Boltzmann simulations”, *J. Chem. Phys.*, **135**, 184901 (2011).

(26) Lin, P.-H.; Kohale S. C.; Khare, R.; "Effect of nanoconfinement on kinetics of cross-linking reactions: A molecular simulation study", *J. Phys. Chem. B*, **115**, 12348–12355 (2011).

(25) Peri, S.; Karim, M. N.; Khare R.; “Potential of mean force for separation of the repeating units in cellulose and hemicellulose”, *Carbohydrate Research*, **346**, 867-871 (2011).

(24) Lin, P.-H.; Khare, R.; "Glass transition and structural properties of glycidyloxypropyl-heptaphenyl polyhedral oligomeric silsesquioxane-epoxy nanocomposites: A molecular simulation study", *Journal of Thermal Analysis and Calorimetry*, **102**, 461-467 (2010).

(23) Lin, P.-H.; Khare, R.; "Local chain dynamics and dynamic heterogeneity in cross-linked epoxy in the vicinity of glass transition", *Macromolecules*, **43**, 6505-6510 (2010).

(22) Kohale S. C.; Khare R.; "Molecular dynamics simulation study of friction force and torque on a rough spherical particle", *J. Chem. Phys.*, **132**, 234706 (2010).

(21) Lin, P.-H.; Khare, R.; "Molecular simulation of crosslinked epoxy and epoxy-POSS nanocomposite", *Macromolecules*, **42**, 4319-4327 (2009).

(20) Kohale, S.; Khare, R.; "Cross-stream chain migration in nanofluidic channels: Effects of chain length, channel height and chain concentration", *J. Chem. Phys.*, **130**, 104904 (2009). *Also selected for Virtual Journal of Biological Physics Research (March 15, 2009 issue).*

(19) Kohale, S.; Khare, R.; "Molecular simulation of cooperative hydrodynamic effects in motion of a periodic array of spheres between parallel walls", *J. Chem. Phys.*, **129**, 164706 (2008).

(18) Alexiadis, O.; Mavrantzas, V.; Khare, R.; Beckers, J.; Baljon, A.; "End-bridging Monte Carlo simulation of bulk and grafted amorphous polyethylene above and below the glass transition", *Macromolecules*, **41**, 987-996 (2008).

(17) Lin, P.-H.; Khare, R.; Weeks, B. L.; Gee, R. H.; "Molecular modeling of diffusion on a crystalline pentaerythritol tetranitrate surface", *Appl. Phys. Lett.*, **91**, 104107 (2007).

(16) Kohale, S.; Molina, S. M.; Weeks, B. L.; Khare, R.; Hope-Weeks, L. J.; "Monitoring the formation of self-assembled monolayers of alkanedithiols using a micromechanical cantilever sensor", *Langmuir*, **23**, 1258-1263 (2007).

(15) Khare, R.; Keblinski, P.; Yethiraj, A.; "Molecular dynamics simulations of heat and momentum transfer at a solid-fluid interface: Relationship between thermal and velocity slip", *International Journal of Heat and Mass Transfer*, **49**, 3401-3407 (2006).

(14) Khare, R.; Graham, M. D.; de Pablo, J. J.; "Cross-stream migration of flexible molecules in a nanochannel", *Phys. Rev. Lett.*, **96**, 224505 (2006).

(13) Baljon, A. R. C.; Van Weert, M. H. M.; DeGraff, R. B.; Khare, R.; "Glass transition behavior of polymer films of nanoscopic dimensions", *Macromolecules*, **38**, 2391-2399 (2005).

(12) Baljon, A. R. C.; Billen, J.; Khare, R.; "Percolation of immobile domains in supercooled thin polymeric films", *Phys. Rev. Lett.*, **93**, 255701 (2004).

(11) Khare, R.; Sum, A. K.; Nath, S. K.; de Pablo, J. J.; "Simulation of vapor-liquid phase equilibria of primary alcohols and alcohol-alkane mixtures", *J. Phys. Chem. B*, **108**, 10071-10076 (2004).

(10) Nath, S. K.; Khare, R.; "New forcefield parameters for branched hydrocarbons", *J. Chem. Phys.*, **115**, 10837-10844 (2001).

(9) Khare, R.; de Pablo, J. J.; Yethiraj, A.; "Molecular simulation and continuum mechanics investigation of viscoelastic properties of fluids confined to molecularly thin films", *J. Chem. Phys.*, **114**, 7593-7601 (2001).

(8) Garde, S.; Khare, R.; Hummer, G.; "Microscopic density fluctuations and solvation in polymeric fluids", *J. Chem. Phys.*, **112**, 1574-1578 (2000).

(7) Khare, R.; de Pablo, J. J.; Yethiraj, A.; "Rheological, thermodynamic and structural studies of linear and branched alkanes under shear", *J. Chem. Phys.*, **107**, 6956-6964 (1997).

(6) Khare, R.; de Pablo, J. J.; Yethiraj, A.; "Molecular simulation and continuum mechanics study of non-isothermal planar Couette flows", *J. Chem. Phys.*, **107**, 2589-2596 (1997).

(5) Xu, Z.; Khare, R.; de Pablo, J. J.; Kim, S.; "On the calculation of transport properties of polymer melts from nonequilibrium molecular dynamics", *J. Chem. Phys.*, **106**, 8285-8286 (1997).

(4) Khare, R.; de Pablo, J. J.; Yethiraj, A.; "Rheology of confined polymer melts", *Macromolecules*, **29**, 7910-7918 (1996).

(3) Khare, R.; Paulaitis, M. E.; "A study of cooperative phenyl ring flip motions in glassy polystyrene by molecular simulations", *Macromolecules*, **28**, 4495-4504 (1995).

(2) Khare, R.; Paulaitis, M. E.; "Molecular simulations of cooperative ring flip motions in single chains of polystyrene", *Chem. Eng. Sci.*, **49**, 2867-2879 (1994).

(1) Khare, R.; Paulaitis, M. E.; Lustig, S. R.; "Generation of glass structures for molecular simulations of polymers containing large monomer units: Application to polystyrene", *Macromolecules*, **26**, 7203-7209 (1993).

Conference Proceedings and Other Articles

(8) Fardin Khabaz, Ketan S. Khare and Rajesh Khare, "Temperature dependence of creep compliance of highly cross-linked epoxy: A molecular simulation study", *AIP Conference Proceedings*, **1599**, 262-265 (2014).

(7) Swapnil C. Kohale and Rajesh Khare, "Molecular Hydrodynamics in Nanoparticle Suspensions", *Proceedings of The XVth International Congress on Rheology and The Society of Rheology 80th Annual Meeting*, CP 1027, American Institute of Physics, 644-646 (2008).

(6) Swapnil C. Kohale and Rajesh Khare, "Shear Induced Chain Migration in Flowing Polymeric Solutions: A Molecular Dynamics Study", *Proceedings of The XVth International Congress on Rheology and The Society of Rheology 80th Annual Meeting*, CP 1027, American Institute of Physics, 558-560 (2008).

(5) Khare, R.; "Microscopic mechanisms of cross-stream migration of chain molecules in nanochannels", *Polymeric Materials Science and Engineering Preprints*, **231**, 507 (2006).

(4) Garde, S.; Hummer, G.; Khare, R.; "Effect of chain length on microscopic density fluctuations and solvation in polymeric fluids", *Polymeric Materials Science and Engineering Preprints*, **85**, 449 (2001).

(3) Khare, R.; de Pablo, J. J.; Yethiraj, A.; "Dynamics of polymers confined to molecularly thin films", *Polymeric Materials Science and Engineering Preprints*, **77**, 642 (1997).

(2) Khare, R.; Paulaitis, M. E.; "Molecular simulations of phenyl ring flip motion in glassy polystyrene", *Polymer Preprints*, **36**, 655 (April 1995).

(1) Khare, R; Lazaridis, T.; Paulaitis, M. E.; "An internal coordinate approach to reaction path determinations for conformational transitions in polymers", *Chemical Design Automation News*, **8**, 1 (August 1993).

Invited Lectures

(33) "Deducing flow properties and phase behavior from molecular characteristics", Oil & Gas Chemistry Workshop, Houston, TX (November 2018).

(32) "Comparing simulation predictions of viscosity with experiments: Successes and challenges", AIChE Annual Meeting, Minneapolis, MN (October 2017).

(31) "Glass transition in layered polymeric systems: Role of the interphase", 8th International Discussion Meeting on Relaxations in Complex Systems (8 IDMRCS), Wisla, Poland (July 2017).

(30) "Dynamics of solvent molecules in polyacrylate gels supported on a polymeric substrate", ACS National Meeting, San Francisco, CA (April 2017).

(29) "Interaction of flow and chemistry: Insights from molecular simulations", SMART FLOW 2017 Workshop on Flow Problems in Oil & Gas Industry, Houston, TX (February 2017).

(28) "Properties of cross-linked polymers: Insights from molecular simulations", School of Polymers and High Performance Materials, The University of Southern Mississippi, Hattiesburg, MS (January 2017).

(27) "Molecular simulations of dynamics in glassy soft matter systems", ACS Southwest Regional Meeting (SWRM), Galveston, TX (October 2016).

(26) "Design of polymeric pervaporation membranes for energy efficient separation of alcohol-water mixtures", Polymer Composites and High Performance Materials Workshop, ACS Division of Polymer Chemistry, Santa Rosa, CA (July 2016).

(25) "Guidance for the design of pervaporation membranes from molecular simulations and experiments", ACS National Meeting, San Diego, CA (March 2016).

(24) "Mechanical and thermal properties of polymers: Insights from atomistic simulations", School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ (January 2015).

(23) “Mechanical and thermal properties of polymer nanocomposites: Insights from atomistic simulations”, National Institute of Standards and Technology (NIST), Gaithersburg, MD (January 2015).

(22) “Importance of Matrix –Filler Interactions in Cross-linked Epoxy-Carbon Nanotube Composites: A Molecular Simulation Investigation”, Polymer Composites and High Performance Materials Meeting, ACS Division of Polymer Chemistry, Santa Rosa, CA (July 2013).

(21) “Molecular Simulation Techniques for Characterizing the Structure and Rheology of Polymer Solutions and Melts”, Corporate Strategic Research Laboratory, ExxonMobil Research and Engineering Company, NJ (August 2012).

(20) “Particle Nanorheology Simulations: A New Technique for Determining Nanoscale Viscoelastic Properties of Complex Fluids”, Department of Biomedical and Chemical Engineering, Syracuse University (April 2012).

(19) “Molecular simulations of thermophysical properties of cross-linked epoxy and its nanocomposites”, Air Force Research Laboratory, Dayton, OH (December 2011).

(18) “Local viscoelastic properties of polymeric materials from particle nanorheology simulations”, Army Research Laboratory, Aberdeen Proving Ground, MD (September 2011).

(17) “Investigation of glass transition phenomenon in polymers: Molecular simulations vs. experiments”, ACS Joint Southeastern Regional Meeting (SERM) and Southwestern Regional Meeting (SWRM), New Orleans, LA (December 2010).

(16) “Local viscoelastic properties of complex fluids from active nanorheology simulations”, Department of Chemical and Biomolecular Engineering, Tulane University (October 2010).

(15) “Local chain dynamics and dynamic heterogeneity in crosslinked polymers near the glass transition: A molecular perspective”, Department of Materials Science and Engineering, University of North Texas (April 2010).

(14) “Hydrodynamic effects in confined nanoparticle suspensions”, MESOSOFT: Workshop on Mesoscale Simulations of Soft Matter Out of Equilibrium, Forschungszentrum Julich, Julich, Germany (March 2009).

(13) “Molecular hydrodynamics at the nanoscale”, National Chemical Laboratory, Pune, India (December 2008).

(12) “Molecular hydrodynamics at the nanoscale”, Golden Jubilee Visiting Fellowship lecture, Institute of Chemical Technology (formerly UDCT), Mumbai, India (December 2008).

(11) “Molecular hydrodynamics near a solid surface”, Science and Engineering Faculty Day, 3M, St. Paul, MN (June 2007).

(10) “Molecular hydrodynamics near a solid-fluid interface”, NATEX Sixth Annual Mini-Symposium, Dallas, TX (April 2007).

(9) “Molecular hydrodynamics near a solid fluid interface”, Mohs Lectures by Placon, Rheology Research Center Seminar Series, University of Wisconsin-Madison (December 2006).

(8) “Microscopic mechanisms of cross-stream migration of chain molecules in nanochannels”, ACS National Meeting, Atlanta (March 2006).

(7) “Chain migration in polymer solutions flowing in nanochannels”, Department of Chemical Engineering Seminar Series, Virginia Tech (October 2005).

(6) “Shear flow induced chain migration in nanochannels”, Rheology Research Center Seminar Series, University of Wisconsin-Madison (March 2005).

(5) “Viscoelastic properties and glass transition behavior of nanoscopic films”, Polymer Group Seminar Series, Rensselaer Polytechnic Institute (March 2004).

(4) “Molecular modeling for nanotechnology applications”, Department of Chemical Engineering, Washington University in St. Louis (March 2004).

(3) “Atomistic and mesoscopic modeling of polymers”, Rheology Research Center Seminar Series, University of Wisconsin-Madison (May 2003).

(2) “Molecular simulations and continuum mechanics investigation of shear flow of confined fluids”, Computational Science Seminar Series, San Diego State University, San Diego (December 2001).

(1) “Rheology of confined polymer melts”, Rheology Research Center Seminar Series, University of Wisconsin-Madison (February 1997).

Contributed Conference Presentations (Oral)

Total contributed presentations > 90. Contributed presentations in last two years are listed here:

(14) "Combining molecular simulations and theory for predicting the binary interaction parameters of the NRTL model", AIChE Annual Meeting, Pittsburgh, PA (presented by A. Ravichandran, November 2018).

(13) "Oscillatory active nanorheology simulations of colloidal suspensions: Effect of probe size", AIChE Annual Meeting, Pittsburgh, PA (presented by D. Sundaravadivelu Devarajan, October 2018).

(12) “Viscoelastic properties of polymer networks from probe rheology simulations: Effect of network mesh size”, AIChE Annual Meeting, Pittsburgh, PA (presented by R. Islam, October 2018).

(11) "Linear viscoelasticity of colloidal suspensions from probe rheology simulations: Application to nanoscopic systems", Society of Rheology Annual Meeting, Houston, TX (presented by D. Sundaravadivelu Devarajan, October 2018).

(10) “Probe rheology simulation of heavily entangled polymer melts”, Society of Rheology Annual Meeting, Houston, TX (presented by P. Nourian, October 2018).

(9) “Determination of viscoelastic properties of polymer networks using probe rheology simulations”, Society of Rheology Annual Meeting, Houston, TX (presented by R. Islam, October 2018).

(8) "Using molecular simulations for predicting the binary interaction parameters of the Non-Random Two-Liquid (NRTL) model", Twentieth Symposium on Thermophysical Properties, Boulder, CO (presented by A. Ravichandran, June 2018).

(7) “Effect of polymer-polymer interface on polymer chain dynamics”**,** APS March Meeting, Los Angeles, CA (March 2018).

(6) “Determination of Polymer Gel Viscoelasticity using Probe Rheology Simulations”, APS March Meeting, Los Angeles, CA (presented by R. Islam, March 2018).

(5) “Can molecular simulations predict the binary interaction parameters of the activity coefficient models?”, AIChE Annual Meeting, Minneapolis, MN (presented by A. Ravichandran, November 2017).

(4) “Probe rheology simulation technique for determination of viscoelastic properties of complex fluids”, AIChE Annual Meeting, Minneapolis, MN (presented by P. Nourian, October 2017).

(3) “Probe rheology simulations for determining linear viscoelasticity of colloidal suspensions”, Society of Rheology Annual Meeting, Denver, CO (presented by D. Sundaravadivelu Devarajan, October 2017).

(2) “Probe rheology simulation technique: Polymer melts vs. polymer solutions”, Society of Rheology Annual Meeting, Denver, CO (presented by P. Nourian, October 2017).

(1) “Structure and dynamics of thin polyacrylate gel films supported on a polymeric substrate”, APS March Meeting, New Orleans, LA (presented by S. Mani, March 2017).

TEACHING/STUDENT MENTORING

Ph.D. Students Currently Supervised

(13) Rafikul Islam, 2015 – present.

(12) Dinesh Sundaravadivelu Devarajan, 2015 – present.

(11) Pouria Nourian, 2014 – present.

Ph. D. Students Graduated

(10) Ashwin Ravichandran (co-advised with C. Chen), "Predicting Interaction Parameters of Thermodynamic Models from Simulations: Bridging Classical and Molecular Thermodynamics", 2018.

(9) Sriramvignesh Mani, "Structural and Dynamics Properties of Penetrant Molecules in Unsupported and Supported Hydrated Gels", 2017.

(8) Fardin Khabaz, "Structural, Dynamic, and Viscoelastic Properties of Complex Materials Using Molecular Dynamics Simulations", 2016.

(7) Mir Karim, "Local Linear and Nonlinear Viscoelasticity of Polymeric Systems by Particle Tracking Rheology Simulations", 2015.

(6) Lakshmi Muthukumar, "Computational Study of Cello-Oligosaccharide Adsorption/Desorption from the Cellulose Crystal Surface during Enzymatic Hydrolysis", 2014.

(5) Ketan Khare, "Thermo-Mechanical Properties of Cross-linked Epoxy Based Systems: A Molecular Simulation Study", 2013.

(4) Govind Hegde, "Mesoscale Simulations of the Hydrodynamics of Complex Fluids", 2012.

(3) Po-Han Lin, "Molecular Simulation of Structural, Volumetric and Dynamic Properties of Cross-linked Epoxy and Epoxy Nanocomposites", 2011.

(2) Suma Peri, "Computational Studies of Cellulose Degradation for the Production of Biofuels", 2011.

(1) Swapnil Kohale, "Molecular Hydrodynamics in Complex Fluids", 2010.

MS. Students Currently Supervised

Michael Wurmstein, 2018 – present.

MS Students Graduated

Xiao Zhao, 2017 (co-advised with N. Nuraje).

Amol Bhusari, 2007.

Post-docs Supervised

Nipun Soni, 2010.

Awards Won by Students Supervised

(6) Sriramvignesh Mani and Fardin Khabaz, **Raider Red Award for Outstanding Peer-Reviewed Journal Paper**, Society of Plastics Engineers Student Chapter and Department of Chemical Engineering, Texas Tech University, September 2016.

(5) Michael Wurmstein, **Second Place** (Topical Area: Computing and Process Control), AIChE Annual Meeting Undergraduate Student Poster Competition, Salt Lake City, UT, November 2015.

(4) Michael Wurmstein, **Winner** (Topical Area: Computing and Process Control), AIChE Annual Meeting Undergraduate Student Poster Competition, Atlanta, GA, November 2014.

(3) Ketan Khare, **First Prize,** Poster Contest at the Polymer Composites and High Performance Materials Workshop, Division of Polymer Chemistry, American Chemical Society (ACS), Santa Rosa, CA, July 2013.

(2) Po-Han Lin, **First Prize,** Student Poster Contest at the International Polyolefins Conference, Houston, TX, February 2009.

(1) Swapnil Kohale, **Best Student Poster award,** Student Poster Competition at The XVth International Congress on Rheology and The Society of Rheology 80th Annual Meeting, Monterey, CA, August 2008.