Rajesh Khare

Department of Chemical Engineering, Texas Tech University
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EDUCATION

B.S., Chemical Engineering**,** Institute of Chemical Technology (formerly UDCT), India (1989).
Ph.D., Chemical Engineering, University of Delaware (1994).
Post-Doctoral, Department of Chemical Engineering and Department of Chemistry, University of Wisconsin-Madison (1995-1997).

PROFESSIONAL EXPERIENCE

Academic

Whitacre College of Engineering, Texas Tech University
Whitacre Department Chair, Department of Chemical Engineering (07/2023 – present, Interim from 07 – 2023 to 08/2024))
Professor (2016 – present)
Associate Dean of Research and Graduate Programs (2022 - 2024)
Assistant Dean of Strategic Initiatives (2019 –2022)
Interim Chair, Department of Chemical Engineering (06/2019 – 07/2019)
Associate Department Chair, Department of Chemical Engineering (2018 –2019)
Associate Professor (2010 –2016)
Assistant Professor (2005 –2010)

Department of Chemical Engineering, University of Wisconsin-Madison
Visiting Senior Scientist (with Juan de Pablo and Michael Graham, 2004 –2005)
Associate Lecturer, concurrent with the post-doc position (1996)

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

Industrial

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)

Honors and Awards

- More than 35 invited lectures at Universities, Industry, and National/International Conferences.
- 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 (2005-2008).
- National Talent Search (Science) Scholarship, Government of India (1983-1989).

PROESSIONAL SERVICE

Committee Memberships in Professional Societies

Member, Nominating Committee, Society of Rheology (2024 – present)
Member, Metzner Award Committee, Society of Rheology (2021 – 2023)
Member, AIChE Awards Committee (2019 – 2021)

Conference/Session Organization

Chair (elected), AIChE Thermodynamics and Transport Properties (Area 1a) Programming Committee (2013 - 2015).
Technical Program Co-Chair, Society of Rheology Annual Meeting, Baltimore, MD (October 2015).
Lecturer, DPOLY (Division of Polymer Physics) Short Course on Glasses, American Physical Society (APS) March Meeting, San Antonio, TX (March 2015).
Discussion Leader for Biomacromolecules, Gordon Research Conference on Polymer Physics (July 2014).
Area Chair, Thermodynamics and Transport Properties (Area 1a) Session Programming, AIChE Annual Meeting, San Francisco, CA (2013).
Member (by election), Thermodynamics and Transport Properties (Area 1a) Programming Committee, AIChE (October 2011 - September 2014).
Conference Co-organizer, Seventh Annual Mini-Symposium of Texas and Southwest Thermal Analysis and Rheology Forum (NATEX), Dallas, TX (2008).
Session Chair, AIChE Annual Meetings (2005 - 2008, 2011, 2012, 2014 - 2019).
Session Chair, Society of Rheology Annual Meetings (2007, 2009, 2010, 2018).

INTERNAL SERVICE AT TEXAS TECH UNIVERSITY

SERVICE TO THE DEPARTMENT OF CHEMICAL ENGINEERING, TEXAS TECH UNIVERSITY

- Member, Faculty Search Committee (2006 – 2009, 2014 – 2016, 2019 - 2020, 2021 - 2022)
- Chair, Department Awards Committee (2019 – 2022)
- Interim Department Chair (06/2019 – 07/2019)
- Associate Department Chair (2018 – 05/2019)
- Graduate Advisor (2010 – 2013, 2016 – 2017) and Director of Graduate Studies (2018 – 2019)
- Member, Graduate Committee (2006 – 2019)
- Member, Chemical Engineering Building Renovation Committee (2018 – 2019)
- Chair, Faculty Search Committee, Computational Soft Matter position (2016)

- Member, Whitacre Chair Search Committee (2010 – 2014)
- Member, Scholarship Committee (2008)
- Member, Graduate Brochure Committee (2006)
- State Employee Charitable Campaign (SECC) Coordinator for the Department (2005 – 2006)

SERVICE TO THE COLLEGE OF ENGINEERING, TEXAS TECH UNIVERSITY

- Chair, College of Engineering Faculty Research Awards Committee (2020 – 2022)
- Member, Koh Scholarship Committee, Graduate Section (2020 – present)
- Member, STEM Outreach & Engagement Program Manager Search Committee (2022)
- Chair, Computational Thinking Lecturer Search Committee (2020)
- External Member, Post-tenure Review Committee, Department of Mechanical Engineering, TTU (2020)
- Member, Tenure & Promotion Committee (2011 – 2013)
- Member, Petroleum Engineering Department Chair Search Committee (2010)
- Member, Donovan Maddox Chair Recruiting Team (2009)
- Member, Committee to Design the MS in Bioengineering Degree Program (2006)
- Member, Associate Dean for Research Search Committee (2006)

SERVICE TO TEXAS TECH UNIVERSITY

- Member, TTU Intellectual Property Review Committee (2024 – present)
- Member, TTU Strategic Enrollment Planning Team (2024 – 2025)
- Member, TTU One Health Curriculum Working Group (2023 – present)
- Member, TTU Internal Committee for Selecting Candidates for Goldwater Scholarship (2016 – 2023)
- Member, 2021 Chancellor's Council Distinguished Research Awards Selection Committee
- External Member, Tenure & Promotion Committee, TTU College of Human Sciences (2018 - 2019)
- Member, Graduate Program Review Committee for Department of Chemistry and Biochemistry, TTU (2015)
- Member, India Task Force (for establishing collaborations) (2014)
- Faculty Advisor to Texas Tech University Society of Plastics Engineers Student Chapter (2006 – 2009)

RESEARCH ACTIVITIES

Publications

Sum of times cited: **3296**, h-index: **31** (Google Scholar)

Refereed Book Chapters

(66) Khabaz, F.; Islam, R.; Khare, R.; "Thermal conductivity of polymer nanocomposites: Applications of molecular dynamics simulations", in *Thermal Behaviour and Application of Carbon-Based Nanomaterials*, Elsevier, pp. 305-324 (2020). **DOI:** 10.1016/B978-0-12-817682-5.00011-8.

(65) 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.

(64) 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:

(63) Sundaravadivelu Devarajan, D.; Khare, R.; "Linear viscoelasticity of nanocolloidal suspensions from probe rheology molecular simulations", *J. Rheol.*, **66**, 837-852 (2022).

(62) Ethier, J.; Nourian, P.; Islam, R.; Khare, R.; Schieber, J. D., "Microrheology analysis in molecular dynamics simulations: Finite box size correction", *Journal of Rheology*, **65**, 1255-1267 (2021).

(61) Balogun, A.; Lazarenko, D.; Khabaz, F.; Khare, R.; "Extending timescale of molecular simulations by using time-temperature superposition: Rheology of ionic liquids", *Soft Matter*, **17**, 7210-7220 (2021).

(60) Nourian, P.; Islam, R.; Khare, R.; "Implementation of active probe rheology simulation technique for determining the viscoelastic moduli of soft matter", *Journal of Rheology***, 65**, 617-632 (2021).

(59) Sami, S. N.; Islam, R.; Khare, R.; Joshi, R. P.; "Simulations of hydrogen outgassing from a carbon fiber electrode", *Journal of Applied Physics***, 129**, 213303 (2021).

(58) Islam, R.; Mani, S.; Khare, R.; "Chain and solvent dynamics in polymer membrane films supported on a polymeric substrate", *ACS Applied Polymer Materials***, 3**, 3164-3174 (2021).

(57) Ravichandran, A.; Tun, H.; Khare, R.; Chen, C.-C.; "Prediction of thermodynamic properties of organic mixtures: Combining molecular simulations with classical thermodynamics", *Fluid Phase Equilibria*, **523**, 112759 (2020).

(56) Sundaravadivelu Devarajan, D.; Nourian, P.; McKenna, G. B.; Khare, R.; "Molecular simulation of nanocolloid rheology: Viscosity, viscoelasticity, and time-concentration superposition", *Journal of Rheology*, **64**, 529-543 (2020).

(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).

(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 timetemperature 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.; "Cosolvents 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**, 72037209 (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**, 262265 (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

(39) "From Molecules to Rheology: A Journey Across Length and Time Scales", Department of Chemical, Biological and Materials Engineering, University of South Florida (April 2025).

(38) "From Molecules to Rheology: A Journey Across Length and Time Scales", Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute (April 2025).

(37) "What Can Molecules Tell Us About Rheology?", School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma (November 2024).

(36) "Rheological deductions from simulations: Time-temperature superposition and probe rheology", JD Lindsay Seminar Series, Department of Chemical Engineering, Texas A&M University (April 2022).

(35) "Interfacial dynamics in layered polymeric systems", AIChE Virtual Annual Meeting (November 2020).

(34) "Predicting Properties of Complex Fluids from Molecular Simulations", Oil & Gas Chemistry + Polymers 2019 Workshop, Houston, TX (November 2019).

(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 > 100. Selected recent presentations are:

- “Viscoelasticity of nanocolloidal suspensions from probe rheology: Direct and indirect interactions”, Society of Rheology Annual Meeting, Chicago, IL (October 2022).
- “Active probe rheology simulations: General formalism and applications”, Society of Rheology Annual Meeting, Bangor, ME (October 2021).
- “Linear viscoelasticity of nanocolloidal suspensions from probe rheology molecular simulations”, AIChE Virtual Annual Meeting (November 2020).
- “Rheological characterization of polymer networks and heavily entangled polymer melts using particle rheology simulations”, AIChE Annual Meeting, Orlando, FL (November 2019).
- "Probe rheology molecular simulations of nanocolloidal suspensions", AIChE Annual Meeting, Orlando, FL (presented by D. Sundaravadivelu Devarajan, November 2019).

TEACHING/STUDENT MENTORING

Ph.D. Students Currently Supervised

(18) Prabesh K. C., 2025 – present

(17) Mohammad Khosravikia, 2023 – present.

(16) Masoumeh Pourasgharoshtebin (co-advised with C. Chen), 2022 – present.

(15) Kolawole Sonibare, 2020 – present.

Ph. D. Students Graduated

(14) Adegbola Balogun, “Long Time Dynamics and Viscoelasticity of Soft Matter Systems from Molecular Simulation”, 2024.

(13) Rafikul Islam, “Viscoelastic Properties and Dynamics of Cross-linked Polymer Network Systems”, 2021.

(12) Dinesh Sundaravadivelu Devarajan, “Molecular Investigations of Nanocolloid Rheology”, 2020.

(11) Pouria Nourian, “Application of Probe Rheology Simulation Technique in Rheological Characterization of Soft Matter”, 2020.

(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 Crosslinked 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 Graduated

(3) Thong Le, 2020.

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

(1) 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.