

Brian Joseph Edwards

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Department of Chemical and Biomolecular Engineering
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Technical Interests

Fluid Mechanics
Nonequilibrium Dynamics
Molecular Dynamics Simulations

Graphene Applications
Computational Fluid Mechanics
Polymeric Materials

Education

UNIVERSITY OF DELAWARE, Newark, DE
Ph.D. in Chemical Engineering, August 1991.
Dissertation title: *The Dynamical Continuum Theory of Liquid Crystals*.
Advisor: Professor A.N. Beris.
Minor area of specialization: Mathematics.

UNIVERSITY OF ILLINOIS, Urbana, IL
B.S. in Chemical Engineering with Highest Distinction, May 1986.
Senior thesis title: *Phase Separation in Dilute Polymer Solutions*.
Advisor: Professor A.J. McHugh.

Experience

Position: Associate Head of Department of Chemical Engineering (September 2006 -- present),
University of Tennessee-Knoxville

Position: Professor of Chemical and Biomolecular Engineering (August 2008 -- present),
University of Tennessee-Knoxville

Position: Cofounder (January 2021 -- present), International Graphene LLC, Columbia, SC

Position: Chief Executive Officer and Founder (January 2015 – December 2020), Celtig LLC, Knoxville,
TN

Position: Associate Professor of Chemical Engineering (January 2001 -- August 2008),
Department of Chemical Engineering, University of Tennessee-Knoxville

Position: Oberassistent (June 1996 – December 2000).
Institute for Polymers, Swiss Federal Institute of Technology: ETH-Zurich

Explored fundamental relationships between non-Newtonian fluid dynamics and thermodynamics. Developed new methodology for modelling complex fluids encompassing more traditional approaches. Investigated specific examples of complex fluids, such as multi-phase blends, nonisothermal polymer melts, and polymer/colloid mixtures. Performed molecular dynamics and stochastic simulations of these materials.

Position: Research Associate (January 1996-May 1996).
Department of Chemical Engineering, University of Delaware.

Performed intensive computational fluid dynamics simulation of two-dimensional Newtonian flows with a free surface. A spectral representation of the spatial coordinates was used involving Fourier and Chebyshev discretization and conformal mapping. Several difference and splitting methods were used for the temporal problem.

Position: Research Associate (August 1991-December 1994).
Department of Chemical Engineering, University of Illinois.

Performed experimental investigations to study the structural changes induced in polymeric systems by a flow field, as well as the implications for the rheological characterization of the materials. Investigated the effects of a flow field upon fundamental stress/structural relationships for various polymer solutions and melts. A new modulated polarimetry instrument was developed which measured transient and steady state circular (as well as linear) optical properties of flowing macromolecular solutions.

Position: Research Assistant (September 1986-June 1991).
Department of Chemical Engineering, University of Delaware.

Performed independent research for Ph.D. dissertation. Research involved the development of a novel technique for deriving complex constitutive equations for various hydrodynamic systems. Specifically, a liquid-crystalline system was extensively studied. Intensive large-scale numerical computations were performed on many existing models of polymeric flow behavior.

Position: Research Assistant (June 1985-August 1986).
Department of Chemical Engineering, University of Illinois.

Performed viscometric experiments to quantify the flow-induced phase separation and shear thickening in dilute polymer solutions. Studied fiber and monofilament growth from polymeric solutions and melts using a variety of experimental procedures of industrial importance. Determined the molecular weight fractionation in laboratory-grown polymeric fibers.

Awards

Roy L. McCullough Scholars Award (for most outstanding graduate student), University of Delaware, 1990.
Outstanding Faculty Advisor Award, College of Engineering, University of Tennessee, 2003.
Outstanding Teacher Award, Department of Chemical Engineering, University of Tennessee, 2003.
Engineering Research Fellow Award, University of Tennessee, 2007.
Outstanding Advisor Award, Department of Chemical Engineering, University of Tennessee, 2007.
Tom and Ruth Clark Excellence Award in Teaching, University of Tennessee, 2007.
Outstanding Advisor Award, Department of Chemical and Biomolecular Engineering, University of Tennessee, 2009.
Outstanding Teacher Award, Department of Chemical and Biomolecular Engineering, University of Tennessee, 2009.
Chancellor's Award for Excellence in Advising, University of Tennessee, 2009.

College of Engineering Outstanding Advisor Award, University of Tennessee, 2009.
College of Engineering Research Fellow Award, University of Tennessee, 2009.
Best of EPL 2010 Award for paper "Atomistic simulation of flow-induced crystallization at constant temperature," C. Baig and B.J. Edwards, *Europhys. Lett.*, **89**, 36003 (2010).
Outstanding Advisor Award, Department of Chemical and Biomolecular Engineering, University of Tennessee, 2011.
College of Engineering Leon and Nancy Cole Superior Teaching Award, University of Tennessee, 2011.
Tom and Ruth Clark Excellence Award in Teaching, University of Tennessee, 2012.
Outstanding Teacher Award, Department of Chemical and Biomolecular Engineering, University of Tennessee, 2013.
Honorary Distinguished Professor, Jiangsu University, China, 2013.
Outstanding Advisor Award, Department of Chemical and Biomolecular Engineering, University of Tennessee, 2015.
Distinguished Collaborative Professor, Shenyang University of Technology, China, 2015.
Distinguished Affiliated Professor, Southwest University of Science and Technology, China, 2015; renewed 2017.

Publications

Books

- 1.) *The Thermodynamics of Flowing Systems*, A.N. Beris and B.J. Edwards, Oxford University Press, New York (1994). Volume 36 of the Oxford Engineering Science Series.

Edited Volumes (Book Chapters)

- 1.) Flow-induced structure formation in polymer solutions, A.J. McHugh and B.J. Edwards, in *Rheo-Physics of Multiphase Polymer Solutions*, Technomic Publishing Co., Lancaster, PA, eds. K. Sondergaard and J. Lyngaae-Jorgensen, pp. 185-226 (1995).
- 2.) Flow-induced structuring and conformational rearrangements in flexible and semiflexible polymer solutions, A.J. McHugh, A. Immaneni, and B.J. Edwards, in *Flow-Induced Structure in Polymers*, American Chemical Society, eds. A.I. Nakatani and M.D. Dadmun, pp. 75-90 (1995).
- 3.) Translational and rotational motion of a uniaxial liquid crystal as derived using Hamilton's principle of least action, B.J. Edwards, in *Variational and Extremum Principles in Macroscopic Systems*, Elsevier Press, Oxford, S. Sieniutycz and H. Farkas, eds., pp. 131-156, (2005).

I quit accepting invitations to write book chapters in 2006 because I felt that it was not appropriate that the editors were paid but not the contributors.

Journal Articles

- 1.) Molecular weight fractionation in tubular flow-induced crystallization of polyethylene, A.J. McHugh, E. Vrahopoulou, and B.J. Edwards, *J. Polym. Sci.: Polym. Phys. Ed.*, **25**, 953-956 (1987).
- 2.) Flow-induced orientation in monodomain systems of polymeric liquid crystals, B.J. Edwards and A.N. Beris, *J. Rheol.*, **33**, 537-557 (1989).
- 3.) Order parameter representation of spatial inhomogeneities in polymeric liquid crystals, B.J. Edwards and A.N. Beris, *J. Rheol.*, **33**, 1189-1193 (1989).

- 4.) Poisson bracket formulation of incompressible flow equations in continuum mechanics, A.N. Beris and B.J. Edwards, *J. Rheol.*, **34**, 55-78 (1990).
- 5.) Generalized constitutive equation for polymeric liquid crystals, part 1. model formulation using the Hamiltonian formulation, B.J. Edwards, A.N. Beris, and M. Grmela, *J. Non-Newtonian Fluid Mech.*, **35**, 51-72 (1990).
- 6.) Poisson bracket formulation of viscoelastic flow equations of differential type: a unified approach, A.N. Beris and B.J. Edwards, *J. Rheol.*, **34**, 503-538 (1990).
- 7.) Generalized constitutive equation for polymeric liquid crystals, part 2. non-homogeneous systems, B.J. Edwards, A.N. Beris, M. Grmela, and R.G. Larson *J. Non-Newtonian Fluid Mech.*, **36**, 243-254 (1990).
- 8.) Remarks concerning compressible viscoelastic fluid models, B.J. Edwards and A.N. Beris, *J. Non-Newtonian Fluid Mech.*, **36**, 411-417 (1990).
- 9.) A unified view of transport phenomena based on the generalized bracket formulation, B.J. Edwards and A.N. Beris, *Ind. Eng. Chem. Res.*, **30**, 873-881 (1991).
- 10.) The dynamical behavior of liquid crystals: a continuum description through generalized brackets, B.J. Edwards, A.N. Beris, and M. Grmela, *Mol. Cryst. Liq. Cryst.*, **201**, 51-86 (1991).
- 11.) Noncanonical Poisson bracket for nonlinear elasticity with extensions to viscoelasticity, B.J. Edwards and A.N. Beris, *J. Phys. A: Math. Gen.*, **24**, 2461-2480 (1991).
- 12.) The dynamics of a thermotropic liquid crystal, B.J. Edwards and A.N. Beris, *Eur. J. Mech., B/Fluids*, **11**, 121-142 (1992).
- 13.) Internal variables for relaxation phenomena in heat and mass transfer, N.S. Kalospiros, B.J. Edwards, and A.N. Beris, *Int. J. Heat Mass Trans.*, **36**, 1191-1200 (1993).
- 14.) A rheo-optical study of flow-induced pretransitional ordering in solutions of lyotropic semi-rigid macromolecules, B.J. Edwards and A.J. McHugh, *J. Rheol.*, **37**, 743-774 (1993).
- 15.) On the admissibility criteria for linear viscoelasticity kernels, A.N. Beris and B.J. Edwards, *Rheol. Acta*, **32**, 505-510 (1993).
- 16.) Flow-induced ordering and conformational rearrangement in hydroxypropyl-cellulose solutions, B.J. Edwards, A.J. McHugh, and A. Immaneni, *J. Rheol.*, **39**, 527-544 (1995).
- 17.) Continuum dynamic behavior of homogeneous liquid-crystalline polymers under the imposition of shear and magnetic fields, N.C. Andrews, B.J. Edwards, and A.J. McHugh, *J. Rheol.*, **39**, 1161-1181 (1995).
- 18.) A model with two coupled Maxwell modes, B.J. Edwards, V.G. Mavrantzas, and A.N. Beris, *J. Rheol.*, **40**, 917-942 (1996).
- 19.) Out-of-plane orientational dynamics of polymer liquid crystals under flow, N.C. Andrews, A.J. McHugh, and B.J. Edwards, *J. Rheol.*, **40**, 459-469 (1996).
- 20.) Time/structure invariance criteria for closure approximations, B.J. Edwards and H.C. Öttinger, *Phys. Rev. E*, **56**, 4097-4103 (1997).
- 21.) On the relationships between thermodynamic formalisms for complex fluids, B.J. Edwards, H.C. Öttinger, and R.J.J. Jongschaap, *J. Non-Equilib. Thermodyn.*, **22**, 356-373 (1997).

- 22.) Efficient pseudospectral flow simulations in moderately complex flow geometries, C.D. Dimitropoulos, B.J. Edwards, K.-S. Chae, and A.N. Beris, *J. Comp. Phys.*, *144*, 517-549 (1998).
- 23.) An analysis of single and double generator thermodynamic formalisms for the macroscopic description of complex fluids, B.J. Edwards, *J. Non-Equilib. Thermodyn.*, *23*, 301-333 (1998).
- 24.) An analysis of single and double generator thermodynamic formalisms for complex fluids. Part II. The microscopic description, B.J. Edwards, A.N. Beris, and H.C. Öttinger, *J. Non-Equilib. Thermodyn.*, *23*, 334-350 (1998).
- 25.) Rotational motion and Poisson bracket structures in rigid particle systems and anisotropic fluid theory, B.J. Edwards and A.N. Beris, *Open Syst. Information Dyn.*, *5*, 333-368 (1998).
- 26.) Generalized Doi-Ohta model for multiphase flow developed via GENERIC, N.J. Wagner, H.C. Öttinger, and B.J. Edwards, *AIChE J.*, *45*, 1169-1181 (1999).
- 27.) Macroscopic thermodynamics of flowing polymeric liquids, M. Dressler, B.J. Edwards, and H.C. Öttinger, *Rheol. Acta*, *38*, 2028-2043 (1999).
- 28.) A reversible problem in non-equilibrium thermodynamics: Hamiltonian evolution equations for non-equilibrium molecular dynamics simulations, B.J. Edwards and M. Dressler, *J. Non-Newtonian Fluid Mech.*, *96*, 163-175 (2001).
- 29.) Evaluation of the thermodynamic consistency of closure approximations in several models proposed for the description of liquid crystalline dynamics, B.J. Edwards, *J. Non-Equilib. Thermodyn.*, *27*, 5-24 (2002).
- 30.) An examination of the shear-thickening behavior of high-molecular-weight polymers dissolved in low-viscosity Newtonian solvents, B.J. Edwards, D.J. Keffer, and C. Reneau, *J. Appl. Polym. Sci.*, *85*, 1714-1735 (2002).
- 31.) Noncanonical Poisson brackets and Hamiltonian evolution equations for nonequilibrium molecular dynamics simulations, M. Dressler and B.J. Edwards, *Int. J. Mod. Phys. C*, *13*, 1273-1283 (2002).
- 32.) Rheological models with microstructural constraints, B.J. Edwards, M. Dressler, M. Grmela, and A. Ait-Kadi, *Rheol. Acta*, *42*, 64-72 (2003).
- 33.) Modeling shear thickening in dilute polymer solutions: temperature, concentration, and molecular weight dependencies, B. Jiang, D.J. Keffer, B.J. Edwards, and J.N. Allred, *J. Appl. Polym. Sci.*, *90*, 2997-3011 (2003).
- 34.) A rheological model with constant approximate volume for immiscible blends of ellipsoidal droplets, B.J. Edwards and M. Dressler, *Rheol. Acta*, *42*, 326-337 (2003).
- 35.) A numerical study of the measurement of elongational viscosity of polymeric fluids in a semihyperbolically converging die, K. Feigl, F.X. Tanner, B.J. Edwards, and J.R. Collier, *J. Non-Newtonian Fluid Mech.*, *115*, 191-215 (2003).
- 36.) A rheological and morphological model for blends of flexible and rigid macromolecules, B.J. Edwards and K.L. Williams, *Polym. Sci. Eng.*, *43*, 1778-1787 (2003).
- 37.) The influence of matrix viscoelasticity on the rheology of polymer blends, M. Dressler and B.J. Edwards, *Rheol. Acta*, *43*, 257-282 (2004).
- 38.) A test case for predicting the rheological properties of polymeric liquids: the multiple coupled Maxwell modes model, B. Jiang, P.A. Kamekar, D.J. Keffer, and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, *120*, 11-32 (2004).

- 39.) Determination of statistically reliable transport diffusivities from molecular dynamics simulation, D.J. Keffer, B.J. Edwards, and P. Adhangale, *J. Non-Newtonian Fluid Mech.*, 120, 41-53 (2004).
- 40.) Rheology of polymer blends with matrix viscoelasticity and narrow droplet size distribution, M. Dressler and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 120, 189-205 (2004).
- 41.) Derivation of a pressureless formulation for spectral direct numerical simulation of incompressible channel flows based on a functional formalism, B.J. Edwards and A.N. Beris, *J. Non-Newtonian Fluid Mech.*, 120, 241-250 (2004).
- 42.) Nonequilibrium thermodynamics and complex fluids, B.J. Edwards and A.N. Beris, *J. Non-Newtonian Fluid Mech.*, 120, 1-2 (2004).
- 43.) Letter to the Editor: Comments on "Thermodynamic admissibility of the reptation model" [J. Rheol. 48, 53 (2004)], B.J. Edwards, *J. Rheol.*, 48, 705-708 (2004).
- 44.) Shear thickening in dilute polymer solutions: transient analysis, P.A. Kamerkar, B.J. Edwards, D.J. Keffer, and C.W. Reneau, *Chem. Eng. Commun.*, 192, 89-107 (2005).
- 45.) A proper approach for nonequilibrium molecular dynamics simulations of planar elongational flow, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *J. Chem. Phys.*, 122, 114103 (2005).
- 46.) A method for calculating rheological and morphological properties of constant-volume polymer blend models in inhomogeneous flow fields, M. Dressler and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 130, 77-95 (2005).
- 47.) Modeling the dynamic propagation of shear bands, B.J. Edwards, K. Feigl, M.L. Morrison, B. Yang, P.K. Liaw, and R.A. Buchanan, *Scripta Mater.*, 53, 881-885 (2005).
- 48.) On the relationship between Fickian diffusivities at the continuum and molecular levels, D.J. Keffer, C.Y. Gao, and B.J. Edwards, *J. Phys. Chem. B*, 109, 5279-5288 (2005).
- 49.) Rheological and structural studies of liquid decane, hexadecane, and tetracosane under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, and H. D. Cochran, *J. Chem. Phys.*, 122, 184906 (2005).
- 50.) An examination of the validity of non-equilibrium molecular dynamics simulation algorithms for arbitrary steady-state flows, B.J. Edwards, C. Baig, and D.J. Keffer, *J. Chem. Phys.*, 123, 114106 (2005).
- 51.) Using multiple-mode models for fitting and predicting the rheological properties of polymeric melts, B. Jiang, P.A. Kamerkar, D.J. Keffer, and B.J. Edwards, *J. Appl. Polym. Sci.*, 99, 405-423 (2006).
- 52.) Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, H.D. Cochran, and V.A. Harmandaris, *J. Chem. Phys.*, 124, 084902 (2006).
- 53.) A comparison of simple rheological models and simulation data of n-hexadecane under shear and elongational flow, C. Baig, B. Jiang, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *J. Rheol.*, 50, 625-640 (2006).
- 54.) Structure formation under steady-state isothermal planar elongational flow of n-eicosane: a comparison between simulation and experiment, T.C. Ionescu, C. Baig, B.J. Edwards, D.J. Keffer, and A. Habenschuss, *Phys. Rev. Lett.*, 96, 037802 (2006).

- 55.) Channel, tube, and Taylor-Couette flow of complex viscoelastic fluid models, M. Dressler and B.J. Edwards, *Rheol. Acta*, **46**, 59-82 (2006).
- 56.) Estimation and analysis of the rheological properties of a perfluoropolyether through molecular dynamics simulation, B. Jiang, D.J. Keffer, and B.J. Edwards, *J. Fluor. Chem.*, **127**, 787-795 (2006).
- 57.) A validation of the p-SLLOD equations of motion for homogeneous steady-state flows, B.J. Edwards, C. Baig, and D.J. Keffer, *J. Chem. Phys.*, **124**, 194104 (2006).
- 58.) A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the isobaric-isothermal ensemble, D.J. Keffer, C. Baig, P. Adhangale, and B.J. Edwards, *Molecul. Simul.*, **32**, 345-356 (2006).
- 59.) Structure formation under steady-state isothermal planar elongational flow of *n*-eicosane: a comparison between simulation and experiment, T.C. Ionescu, C. Baig, B.J. Edwards, D.J. Keffer, and A. Habenschuss, *Virt. J. Biol. Phys. Res.*, **11**, 3 (2006).
- 60.) A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards, and D.J. Keffer, *Rheol. Acta*, **46**, 1171-1186 (2007).
- 61.) An experimental study of slip flow in capillaries and semi-hyperbolically converging dies, P.A. Kamerkar and B.J. Edwards, *Polym. Eng. Sci.*, **47**, 159-167 (2007).
- 62.) A molecular dynamics study of a nafion polyelectrolyte membrane and the aqueous phase structure for proton transport, S. Cui, J. Liu, M. Esai Selvan, D.J. Keffer, B.J. Edwards, and W.V. Steele, *J. Phys. Chem. B*, **111**, 2208-2218 (2007).
- 63.) Using multiple-mode models for fitting and predicting the rheological properties of polymeric melts. Part II. Single and double step-strain flows, B. Jiang, P.A. Kamerkar, D.J. Keffer, and B.J. Edwards, *J. Appl. Polym. Sci.*, **105**, 2884-2892 (2007).
- 64.) Comparison of rheological properties of perfluoropolyethers through simulation and experiment, B. Jiang, N.J. Crawford, D.J. Keffer, B.J. Edwards, and J.J. Adcock, *Mol. Sim.*, **33**, 881-888 (2007).
- 65.) Energetic and entropic elasticity of nonisothermal flowing polymers: experiment, theory, and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer, and V.G. Mavrantzas, *J. Rheol.*, **52**, 105-140 (2008).
- 66.) A multiscale modeling demonstration based on the pair correlation function, C.Y. Gao, D.M. Nicholson, D.J. Keffer, and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, **152**, 140-147 (2008).
- 67.) An examination of droplet deformation and break-up between concentrically rotating cylinders, M. Dressler and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, **152**, 86-100 (2008).
- 68.) A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the canonical ensemble, D.J. Keffer, C. Baig, P. Adhangale, B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, **152**, 129-130 (2008).
- 69.) Rheological and entanglement characteristics of linear chain polyethylene liquids in planar Couette and planar elongational flows, J.M. Kim, D.J. Keffer, M. Kröger, and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, **152**, 168-183 (2008).
- 70.) Visualization of conformational changes of linear short-chain polyethylenes under shear and elongational flows, J.M. Kim, B.J. Edwards, and D.J. Keffer, *J. Mol. Graph. Model.*, **26**, 1046-1056 (2008).

- 71.) Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes, T.C. Ionescu, V.G. Mavrantzas, D.J. Keffer, and B.J. Edwards, *J. Rheol.*, *52*, 567-589 (2008).
- 72.) Molecular dynamics study of structure and transport of water and hydronium ions at the membrane/vapor interface of nafion, M. Esai Selvan, J. Liu, D.J. Keffer, S. Cui, B.J. Edwards, and W.V. Steele, *J. Phys. Chem. C*, *112*, 1975-1984 (2008).
- 73.) Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J., Keffer, and W.V. Steele, *J. Phys. Chem. C*, *112*, 1984-1993 (2008).
- 74.) A quantum mechanical study of the decomposition of CF_3OCF_3 and $\text{CF}_3\text{CF}_2\text{OCF}_2\text{CF}_3$ in the presence of AlF_3 , B. Jiang, D.J. Keffer, and B.J. Edwards, *J. Phys. Chem. A*, *112*, 2604-2609 (2008).
- 75.) Temperature increases caused by shear banding in as-cast and relaxed Zr-based bulk-metallic glasses in compression, W.H. Jiang, F.X. Liu, H.H. Liao, H. Choo, P.K. Liaw, B.J. Edwards, and B. Khomami, *J. Mat. Res.*, *23*, 2967-2974 (2008).
- 76.) Comparison of perfluoropolyethers and n-alkanes under shear via nonequilibrium molecular dynamics simulation, B. Jiang, J.M. Kim, D.J. Keffer, and B.J. Edwards, *Mol. Sim.*, *34*, 231-242 (2008).
- 77.) Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes, T.C. Ionescu, V.G. Mavrantzas, D.J. Keffer, and B.J. Edwards, *Virt. J. Biol. Phys. Res.*, *15*, 6 (2008).
- 78.) Comparison of the hydration and diffusion of protons of perfluorosulfonic acid membranes with molecular dynamics simulations, S. Cui, J. Liu, M. Esai Selvan, S.J. Paddison, D.J. Keffer, and B.J. Edwards, *J. Phys. Chem. B*, *112*, 13273-13284 (2008).
- 79.) A reactive molecular dynamics study of the thermal decomposition of perfluorodimethyl ether, B. Jiang, M. Esai Selvan, D.J. Keffer, and B.J. Edwards, *J. Phys. Chem. B*, *113*, 13670-13677 (2009).
- 80.) Single-chain dynamics of linear polyethylene liquids under shear flow, J.M. Kim, B.J. Edwards, D.J. Keffer, and B. Khomami, *Phys. Lett. A*, *373*, 769-772 (2009).
- 81.) Dynamics of individual molecules of linear polyethylene liquids under shear: atomistic simulation and comparison with a free-draining bead-rod chain, J.M. Kim, B.J. Edwards, D.J. Keffer, and B. Khomami, *J. Rheol.*, *54*, 283-310 (2010).
- 82.) Atomistic simulation of flow-induced crystallization at constant temperature, C. Baig and B.J. Edwards, *Europhys. Lett.*, *89*, 36003 (2010).
- 83.) Atomistic simulation of crystallization of a polyethylene melt in steady uniaxial extension, C. Baig and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, *165*, 992-1004 (2010).
- 84.) Analysis of the configurational temperature of polymeric liquids under shear and elongational flows using nonequilibrium molecular dynamics and Monte Carlo simulations, C. Baig and B.J. Edwards, *J. Chem. Phys.*, *132*, 184906 (2010).
- 85.) Elucidating the formation of block copolymer nanostructures on patterned surfaces: a self-consistent field theory study, X. Ye, B.J. Edwards, and B. Khomami, *Macromolecules*, *43*, 9594-9597 (2010).
- 86.) A mean-field anisotropic diffusion model for unentangled polymeric liquids and semi-dilute solutions: model development and comparison with experimental and simulation data, J.M. Kim, P.S. Stephanou, B.J. Edwards, and B. Khomami, *J. Non-Newtonian Fluid Mech.*, *166*, 593-606 (2011).

- 87.) Morphology tailoring of thin film block copolymers on patterned substrates, X. Ye, B.J. Edwards, and B. Khomami, *Macromol. Rapid Comm.*, **33**, 392-395 (2012).
- 88.) A macroscopic model of proton transport through the membrane-ionomer interface of a polymer electrolyte membrane fuel cell, M. Kumar, B.J. Edwards, and S.J. Paddison, *J. Chem. Phys.*, **138**, 064903 (2013).
- 89.) A self-consistent field study of diblock copolymer/charged particle system morphologies for nanofiltration membranes, B. Zhang, X. Ye, and B.J. Edwards, *J. Chem. Phys.*, **139**, 244909 (2013).
- 90.) Block copolymer morphology formation on topographically complex surfaces: A self-consistent field theoretic study, X. Ye, B.J. Edwards, and B. Khomami, *Macromol. Rapid Comm.*, **35**, 702-707 (2014).
- 91.) Characterization of the Flory-Huggins interaction parameter of polymer thermodynamics, T.H. Russell, B.J. Edwards, and B. Khomami, *EPL*, **108**, 66003 (2014).
- 92.) Individual chain dynamics of a polyethylene melt undergoing steady shear flow, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *J. Rheol.*, **59**, 119-153 (2015). (Cover and featured article.)
- 93.) The effect of particle size on the morphology and thermodynamics of diblock copolymer/tethered-particle membranes, B. Zhang and B.J. Edwards, *J. Chem. Phys.*, **142**, 214907 (2015).
- 94.) Proton conductivity in perfluorosulfonate acid membranes via continuum percolation theory, B. Zhang and B.J. Edwards, *J. Electrochem. Soc.*, **162**, F1088-F1095 (2015).
- 95.) Modeling of proton conductivity through perfluorosulfonate acid electrolyte membranes, B. Zhang and B.J. Edwards, *ECS Trans.*, **66**, 163-177 (2015).
- 96.) Steady shearing flow of a moderately entangled polyethylene liquid, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *J. Rheol.*, **60**, 1227-1244 (2016).
- 97.) Modeling controlled release from hollow porous nanospheres, A.L. Wang and B.J. Edwards, *Int. J. Heat Mass Trans.*, **103**, 997-1007 (2016).
- 98.) Evaluation of reptation-based modeling of entangled polymeric fluids including chain rotation via nonequilibrium molecular dynamics simulation, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Phys. Rev. Fluids*, **2**, 083301 (2017).
- 99.) Improvement of the tribological properties of a lithium-based grease by addition of graphene, J. Zhang, J. Li, A. Wang, B.J. Edwards, Z. Li, Y. Ding, and H. Yin, *J. Nanosci. Nanotechnol.*, **18**, 7163-7169 (2018).
- 100.) In-plane and out-of-plane rotational motion of individual chain molecules in steady shear flow of polymer melts and solutions, C.N. Edwards, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *J. Mol. Graph. Model.*, **81**, 184-196 (2018).
- 101.) Communication: A coil-stretch transition in planar elongational flow of an entangled polymeric melt, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *J. Chem. Phys.*, **148**, 141103 (2018). [Chosen as Editor's Pick.]
- 102.) Editorial: Introducing Engineered Science, H. Gu, D. Cao, J. Kong, J. Gu, Q. Jiang, Y. Li, B. Wang, X. Yan, Y. Chen, J.E. Ryu, M. Hu, Y. Yan, Z. Guo, B.J. Edwards, and D.P. Young, *Eng. Sci.*, **1**, 1-3 (2018).
- 103.) Ion transport through single-walled carbon nanotubes: effects of electric field and fixed surface charge, M. Aranha and B.J. Edwards, *Chem. Phys. Lett.*, **712**, 95-101 (2018).

- 104.) Accuracy of the single-mode model of controlled release from hollow porous nanospheres, B.J. Edwards, A. Wang, C.N. Edwards, and H. Yin, *Eng. Sci.*, **3**, 41-47 (2018).
- 105.) Configurational microphase separation in elongational flow of an entangled polymer liquid, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Phys. Rev. Lett.*, **121**, 247802 (2018).
- 106.) Individual molecular dynamics of an entangled polyethylene melt undergoing steady shear flow: steady-state and transient dynamics, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Polymers*, **11**, 476-501 (2019).
- 107.) Elucidating the molecular rheology of entangled polymeric fluids via comparison of atomistic simulations and model predictions, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Macromolecules*, **52**, 8124-8143 (2019).
- 108.) High-fidelity scaling relationships for determining dissipative particle dynamics parameters from atomistic molecular dynamics simulations of polymeric liquids, M.H. Nafar Sefiddashti, M. Boudaghi-Khajehnohar, B.J. Edwards, and B. Khomami, *Scient. Rep.*, **10**, 4458 (2020).
- 109.) Flow-induced crystallization of a polyethylene liquid above the melting temperature and its nonequilibrium phase diagram, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Phys. Rev. Res.*, **2**, 013035 (2020).
- 110.) Flow-induced phase separation and crystallization in entangled polyethylene solutions under elongational flow, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Macromolecules*, **53**, 6432-6451 (2020) [cover article].
- 111.) Effects of chain length and polydispersity on shear banding in simple shear flow of polymeric melts, M. Boudaghi-Khajehnohar, B.J. Edwards, and B. Khomami, *Soft Matter*, **16**, 6468-6483 (2020) [cover article].
- 112.) A simple thermodynamic method for quantifying phase transitions in polymeric liquids, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Macromolecules*, **53**, 10487-10502 (2020).
- 113.) A theory for the coexistence of coiled and stretched configurational phases in the extensional flow of entangled polymer melts, M.H. Nafar Sefiddashti, B.J. Edwards, B. Khomami, and E.S.G. Shaqfeh, *J. Chem. Phys.*, **154**, 204907 (2021).

Conference Proceedings

- 1.) Calculations of steady-state flows of polymeric liquid crystals, B.J. Edwards, S. Piliitsis, and A.N. Beris, *Proceedings of the Xth International Congress on Rheology, Sydney, Australia*, **1**, 312-314 (1988).
- 2.) Thermodynamics of flowing systems: What have we learned?, A.N. Beris and B.J. Edwards, in *Proceedings of the XIIth International Congress on Rheology*, eds. A. Ait-Kadi, J.M. Dealy, D.F. James, and M.C. Williams, Quebec City (Canada), August 18-23, pp. 327-328 (1996).
- 3.) Predicting rheological behavior of polymer melts using a coupled relaxation mode model, B. Jiang, P.A. Kamerkar, D.J. Keffer, and B.J. Edwards, *Proceedings of the 2003 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 16-21 (2003).
- 4.) Polymer elongational rheology: comparison of hyperbolically convergent flow and simple extension techniques, J.R. Collier, B.J. Edwards, S. Petrovan, and K. Feigl, *Proceedings of the 2003 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 16-21 (2003).

- 5.) A proper approach for nonequilibrium molecular dynamics simulations of planar elongational flow, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *Proceedings of the 2004 AIChE Annual Meeting*, [CD-ROM], Austin, TX, Nov. 7-12 (2004).
- 6.) Simulating and measuring elongational flow properties in special geometries, B.J. Edwards, S. Petrovan, J.R. Collier, K. Feigl, and F.X. Tanner, *7th World Congress of Chemical Engineering*, [CD-ROM], Glasgow, Scotland, July 10-14 (2005).
- 7.) Non-equilibrium thermodynamics based modeling of viscoelastic emulsion flow processing and comparison with experiments, M. Dressler, B.J. Edwards, and E.J. Windhab, *7th World Congress of Chemical Engineering*, [CD-ROM], Glasgow, Scotland, July 10-14 (2005).
- 8.) The performance of multiple-mode models in single and double step-strain flows, B. Jiang, P. Kamekar, D.J. Keffer, and B.J. Edwards, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 9.) Experimental study of slip flow in the semi-hyperbolically converging dies, P.A. Kamekar and B.J. Edwards, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 10.) A Hamiltonian-based algorithm for rigorous molecular dynamics simulation in the NVE, NVT, NpT, and NpH ensembles, D.J. Keffer, C. Baig, B.J. Edwards, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 11.) Crystalline structure formations under steady-state isothermal planar elongational stretching of n-alkanes: a molecular dynamics study, T. C. Ionescu, C. Baig, B.J. Edwards, D.J. Keffer, and A. Habenschuss, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 12.) Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 13.) Evaluation of energetic and entropic contributions to the free energy of oriented polymer melts, T.C. Ionescu, B.J. Edwards, D.J. Keffer, and V. Mavrantzas, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 14.) Test of viscoelastic models for predicting the rheological properties of short-chain alkanes under shear and elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B. Jiang, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 15.) Rheological and structural studies of liquid decane, hexadecane, and tetracosane under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *Proceedings of the 2005 AIChE Annual Meeting*, [CD-ROM], Cincinnati, OH, Oct. 30-Nov. 5-12 (2005).
- 16.) A generalized Hamiltonian-based algorithm for rigorous nonequilibrium molecular dynamics simulation in the NVT ensemble, J.G. Rajkumar, D.J. Keffer, B.J. Edwards, and C. Baig, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).
- 17.) A comparison of rheological and structural properties of linear polyethylene melts under shear and elongational flow using nonequilibrium molecular dynamics simulations, J.M. Kim, C. Baig, D.J. Keffer, and B.J. Edwards, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).

- 18.) A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards, and D.J. Keffer, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).
- 19.) Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer, and V. Mavrantzas, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).
- 20.) A molecular dynamics study of nafion polyelectrolyte membrane and the aqueous phase structure for proton transport, S.T. Cui, J. Liu, M. Esai-Selvan, D.J. Keffer, B.J. Edwards, and W.V. Steele, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).
- 21.) Estimation and analysis of the rheological properties of perfluoropolyethers, B. Jiang, D.J. Keffer, and B.J. Edwards, *Proceedings of the 2006 AIChE Annual Meeting*, [CD-ROM], San Francisco, CA, Nov. 12-17 (2006).
- 22.) Correlation-based coarse-graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer, and B.J., Edwards, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 23.) Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer, and W.V. Steele, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 24.) Rheological and entanglement characteristics of polyethylene liquids and visualization of conformational changes in shear and elongational flows, J.M. Kim, D.J. Keffer, M. Kröger, and B.J. Edwards, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 25.) Reactive molecular dynamics of the thermal decomposition of CF_3OCF_3 , B. Jiang, B.J. Edwards, and D.J. Keffer, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 26.) Quantum mechanics study of decomposition of CF_3OCF_3 and $(\text{CF}_3\text{CF}_2)_2\text{O}$ catalyzed by AlF_3 , B. Jiang, B.J. Edwards, and D.J. Keffer, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 27.) Understanding the relationship between molecular architecture and thermophysical and rheological properties of perfluoropolyethers, B. Jiang, J.L. Adcock, N.J. Crawford, J.T. Fern, A.F. Pangloli, B.J. Edwards, W.V. Steele, and D.J. Keffer, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 28.) Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai, Selvan, J. Liu, D.J. Keffer, B.J. Edwards, S. Cui, and W.V. Steele, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 29.) Correlation-based coarse graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer, B.J. Edwards, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Salt Lake City, UT, November 4-9, 2007.
- 30.) Single-chain dynamics of linear polyethylene liquids under shear, J.M. Kim, B.J. Edwards, B. Khomami, and D.J. Keffer, *Proceedings of the XVth International Congress on Rheology*, Monterey, CA, August 3-8, 2008.
- 31.) Rheology of short-chain branched polyethylene melts under shear: results from NEMD simulations and comparison with linear and H-shaped analogues, J.M. Kim, C. Baig, and B.J. Edwards, *Proceedings of the XVth International Congress on Rheology*, Monterey, CA, August 3-8, 2008.

- 32.) Single-chain dynamics and nonisothermal rheology of linear polyethylene liquids under shear, J.M. Kim, B.J. Edwards, B. Khomami, and D.J. Keffer, *Proceedings of the North American Thermal Analysis Society 36th Annual Conference*, [CD-ROM], Atlanta, GA, August 18-20, 2008.
- 33.) A coarse-grained reactive molecular dynamics algorithm for proton transport in hydrogen fuel cells, M. Esai-Selvan, D.J. Keffer, S. Cui, and B.J. Edwards, *Proceedings of the 2007 AIChE Annual Meeting*, [CD-ROM], Philadelphia, PA, November 16-22, 2008.

I stopped keeping track of these in 2008 because I believe this category of publications provides a meaningless indicator of productivity.

Presentations since July, 2000 (Approximately 30 prior to this date)

Invited Lectures

- 1.) Nonequilibrium thermodynamics in microstructural dynamical theory, Oak Ridge National Laboratory, Oak Ridge, TN, October 25, 2000.
- 2.) The influence of coupled relaxation modes on viscoelastic fluid dynamics, Michigan Technological University, Houghton, MI, November 3, 2000.
- 3.) Shear thickening in dilute polymer solutions, The University of Tennessee, Knoxville, TN, August 27, 2001.
- 4.) Shear thickening in dilute polymer solutions, University of Alabama, Tuscaloosa, AL, February 21, 2002
- 5.) Shear thickening in dilute polymer solutions, Ecole Polytechnique de Montreal, Montreal, Canada, April 9, 2002.
- 6.) Rheology of blends of thermoplastic and liquid-crystalline polymers, ETH-Zurich, Zurich, Switzerland, January 6, 2003.
- 7.) Transient analysis of shear thickening, ETH-Zurich, Zurich, Switzerland, January 7, 2003.
- 8.) Multi-mode relaxation models for polymer melts, ETH-Zurich, Zurich, Switzerland, January 8, 2003.
- 9.) Applying recent developments in nonequilibrium thermodynamics to multi-scale simulations, Knoxville Area Theoretical Chemists (KATC), The University of Tennessee, May 16, 2003.
- 10.) Shear thickening in dilute polymer solutions: transient analysis, Michigan Technological University, Houghton, MI, Jun 8, 2003.
- 11.) Predicting rheological behavior of polymer melts using a coupled relaxation modes model, Tennessee Tech University, Cookeville, TN, Feb. 19, 2004.
- 12.) Predicting rheological behavior of polymer melts using models with multiple relaxation modes, Washington University, St. Louis, MO, April 12, 2004.
- 13.) Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, University of Alabama-Huntsville, Huntsville, AL, Sept. 22, 2006.
- 14.) Current research activities in microstructured materials of potential interest to Eastman Chemical, with D.J. Keffer and B. Khomami, Kingsport, TN, Jan. 30, 2007.

- 15.) Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, University of Patras, Patras, Greece, June 21, 2007.
- 16.) Applying nonequilibrium thermodynamics principles to NEMD simulations, Department of Materials Science, ETH-Zurich, June 13, 2008.
- 17.) Thermodynamics of nonisothermal polymer flows: experiment, theory and simulation, University of Kentucky, Lexington, KY, February 18, 2009.
- 18.) Direct atomistic simulation of flow-induced crystallization of a short-chain polyethylene liquid at constant temperature, Lehigh University, Bethlehem, PA, November 4, 2009.
- 19.) Anisotropic tube model for semi-concentrated polymer solutions, ETH-Zurich, Zurich, Switzerland, January 6, 2011.
- 20.) High shear tumbling of chain molecules, University of Patras, Patras, Greece, January 12, 2011.
- 21.) Flow-induced crystallization in short chain polyethylene melts, Jiangsu University, Zhenjiang, China, October 21, 2013.
- 22.) Direct atomistic simulation of flow-induced crystallization of a short-chain polyethylene liquid at constant temperature, Oklahoma State University, Stillwater, OK, May 20, 2015.
- 23.) Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, Jiangsu University, Zhenjiang, China, July 9, 2015.
- 24.) Direct atomistic simulation of flow-induced crystallization of a short-chain polyethylene liquid at constant temperature, Shenyang University of Technology, Shenyang, China, July 17, 2015.
- 25.) Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, Southwest University of Science and Technology, Mianyang, China, July 15, 2015.
- 26.) Direct atomistic simulation of flow-induced crystallization of a short-chain polyethylene liquid at constant temperature, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China, July 23, 2015.
- 27.) Flow-induced crystallization of polyethylene via atomistic simulations, Zhengzhou University, Zhengzhou, China, July 16, 2016.
- 28.) Thermodynamics of non-isothermal liquids, Sichuan University, Chengdu, China, July 18, 2016.
- 29.) Steady shearing flow of an entangled polymeric liquid, University of Delaware, Newark, DE, April 7, 2017.
- 30.) Individual molecular motion in the flow of entangled polymeric liquids, Southwest University of Science and Technology, Mianyang, China, July 6, 2017.
- 31.) Molecular individuality of polymeric liquids, Jiangsu University, Zhenjiang, China, July 21, 2017.
- 32.) Progress in chemical and Biomolecular Engineering, Jiangsu University, Zhenjiang, China, November 5, 2017.
- 33.) Individual molecular motion in viscoelastic fluid flow, Hainan University, Haikou, China, November 13, 2017.

- 34.) Individual molecular motion in viscoelastic fluid flow, Zhongbei University, Taiyuan, China, November 15, 2017.
- 35.) Coil-stretch transition and configurational microphase separation in elongational flow of entangled polymeric liquids, ETH, Zürich, Switzerland, November 7, 2018.
- 36.) The nonequilibrium phase diagram of an entangled polymeric liquid under elongational flow, University of Nebraska, Lincoln, Nebraska, October 25, 2019.
- 37.) Flow-induced crystallization of a polyethylene melt under elongational flow, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, Retirement Celebration of Dr. Anthony J. McHugh, Lehigh University, February 5, 2021.

Conference Presentations (since 2000)

Plenary Lectures

- 1.) Successes of non-equilibrium thermodynamics, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.
- 2.) Applying nonequilibrium thermodynamics principles to NEMD simulations, European Community Marie Curie Lectures: Nanostructured Materials and Modelling and Simulation, Patras, Greece, June 18-27, 2008.

Invited Presentations

- 1.) Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer and V.G. Mavrantzas, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
- 2.) Modeling the propagation of shear bands in bulk metallic glasses, B.J. Edwards, B. Khomami, and P.K. Liaw, *TMS 2007 Annual Meeting*, Orlando, FL, February 25-March 1, 2007.
- 3.) A computational investigation of proton transport through the electrode/electrolyte interface of proton exchange membrane fuel cell systems, D.J. Keffer, M. Esai Selvan, J. Liu, S. Cui, B.J. Edwards, and W.V. Steele, Southeast Regional Meeting of the American Chemical Society (SERMACS), Greenville, SC, October 24-27, 2007.
- 4.) Effect of relaxation on plastic flows and temperature rises of a Zr-based bulk-metallic glass, P.K. Liaw, W.H. Jiang, F.X. Liu, H. Choo, B.J. Edwards, and B. Khomami, 2007 MRS Fall Meeting, Boston, MA, November 26-30, 2007.
- 5.) Single-chain dynamics and nonisothermal rheology of linear polyethylene liquids under shear, J.M. Kim, B.J. Edwards, and D.J. Keffer, North American Thermal Analysis Society 36th Annual Conference, Atlanta, GA, August 18-20, 2008.
- 6.) Combining atomistic and mesoscopic simulations to understand high shear dynamics of chain molecules, B.J. Edwards, AIChE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.
- 7.) Molecular rheology of entangled polymeric fluids: Understanding bulk flow behavior based on single molecule dynamics, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, Annual European Rheology Conference, Sorrento, Italy, April 17-20, 2018.

- 8.) Nonequilibrium thermodynamics of polymeric liquids via atomistic simulation, B.J. Edwards, M.H. Nafar Sefiddashti, and B. Khomami, Joint European Thermodynamic Conference, Prague, Czech Republic, June 14-18, 2021.

Regular Contributions

- 1.) Evaluation of the thermodynamic consistency of closure approximations in several models proposed for the description of liquid crystalline dynamics, B. J. Edwards, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.
- 2.) Reversible contributions to non-equilibrium thermodynamics, B.J. Edwards, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.
- 3.) Shear thickening in dilute polymer solutions, B.J. Edwards, D.J. Keffer, and C.W. Reneau, *AIChE* Annual Meeting, Reno, NV, November 4-9, 2001.
- 4.) Thermodynamics and numerical studies concerning the structure-rheology-process relationship in microstructural fluids and its possible relevance for food process engineering, M. Dressler, B.J. Edwards, M. Grmela, and A. Ait-Kadi, European Colloquium on Food Science and Engineering, Grindelwald, Switzerland, March 18-21, 2002.
- 5.) Applications of nonequilibrium thermodynamics to NEMD simulations, M. Dressler and B.J. Edwards, Symposium: Stochastic processes applied to complex systems: Computational endeavors versus conceptual frontiers, University of Technology and Agriculture, Bydgoszcz, Poland, May 21-23, 2002.
- 6.) A constant volume model for immiscible polymer blends, M. Dressler and B.J. Edwards, Society of Rheology Annual Meeting, Minneapolis, MN, October 13-17, 2002.
- 7.) Thermodynamic description of polymer blends, M. Dressler and B.J. Edwards, Rheologentagung 2003, Meeting of the German Rheological Society and the German Society of Process Engineering and Chemical Engineering, Berlin, Germany, May 5-6, 2003.
- 8.) How nonequilibrium thermodynamics leads to models for viscoelastic fluid properties that actually work, B.J. Edwards, B. Jiang, D.J. Keffer, and P. A. Kamekar, 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton, NJ, August 14-17, 2003.
- 9.) Thermodynamic modeling of polymer blends with droplet morphology and matrix phase viscoelasticity, M. Dressler and B.J. Edwards, 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton, NJ, August 14-17, 2003.
- 10.) Thermodynamic modeling of polymer blends with matrix phase viscoelasticity, B.J. Edwards and M. Dressler, The Society of Rheology 75th Annual Meeting, Pittsburgh, PA, Oct. 12-16, 2003.
- 11.) Predicting rheological behavior of polymer melts using a coupled relaxation mode model, B. Jiang, P.A. Kamekar, D.J. Keffer, and B.J. Edwards, The Society of Rheology 75th Annual Meeting, Pittsburgh, PA, Oct. 12-16, 2003.
- 12.) Investigation of semihyperbolically converging dies for the measurement of elongational viscosity of polymeric fluids, K. Feigl, F.X. Tanner, B.J. Edwards, and J.R. Collier, The Society of Rheology 75th Annual Meeting, Pittsburgh, PA, Oct. 12-16, 2003.
- 13.) Predicting rheological behavior of polymer melts using a coupled relaxation mode model, B. Jiang, P.A. Kamekar, D.J. Keffer, and B.J. Edwards, *AIChE* Annual Meeting, San Francisco, CA, Nov. 16-21, 2003.

- 14.) Polymer elongational rheology: comparison of hyperbolically convergent flow and simple extension techniques, J.R. Collier, B.J. Edwards, S. Petrovan, and K. Feigl, *AICHE Annual Meeting*, San Francisco, CA, Nov. 16-21, 2003.
- 15.) Modeling the propagation of shear bands in bulk metallic glasses, B.J. Edwards, K. Feigl, and P.K. Liaw, *TMS Annual Meeting*, Charlotte, NC, Mar. 14-18, 2004.
- 16.) A proper approach for nonequilibrium molecular dynamics simulations of planar elongational flow, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *AICHE Annual Meeting*, Austin, TX, Nov. 7-12, 2004.
- 17.) Modeling shear band propagation in bulk metallic glasses, B.J. Edwards, K. Feigl, P.K. Liaw, M. Morrison, B. Yang, and R.A. Buchanan, *TMS Annual Meeting*, San Francisco, CA, Feb. 13-17, 2005.
- 18.) Modeling the propagation of shear bands in bulk metallic glasses, B.J. Edwards, K. Feigl, M.L. Morrison, B. Yang, P. K. Liaw, and R.A. Buchanan, *The Fourth International Bulk Metallic Glasses Conference*, Gatlinburg, Tennessee, May 1-5, 2005.
- 19.) Non-equilibrium thermodynamics based modeling of viscoelastic emulsion flow processing and comparison with experiments, M. Dressler, B.J. Edwards, and E.J. Windhab, *7th World Congress of Chemical Engineering*, Glasgow, Scotland, July 10-14, 2005.
- 20.) Simulating and measuring elongational flow properties in special geometries, B.J. Edwards, S. Petrovan, J.R. Collier, and K. Feigl, *7th World Congress of Chemical Engineering*, Glasgow, Scotland, July 10-14, 2005.
- 21.) The performance of multiple-mode models in single and double step-strain flows, B. Jiang, P. Kamerkar, D.J. Keffer, and B.J. Edwards, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 22.) Experimental study of slip flow in the semi-hyperbolically converging dies, P.A. Kamerkar and B.J. Edwards, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 23.) A Hamiltonian-based algorithm for rigorous molecular dynamics simulation in the NVE, NVT, NpT, and NpH ensembles, D.J. Keffer, C. Baig, B.J. Edwards, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 24.) Crystalline structure formations under steady-state isothermal planar elongational stretching of n-alkanes: a molecular dynamics study, T. C. Ionescu, C. Baig, B.J. Edwards, D.J. Keffer, and A. Habenschuss, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 25.) Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 26.) Evaluation of energetic and entropic contributions to the free energy of oriented polymer melts, T.C. Ionescu, B.J. Edwards, D.J. Keffer, and V. Mavrantzas, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 27.) Test of viscoelastic models for predicting the rheological properties of short-chain alkanes under shear and elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B. Jiang, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.
- 28.) Rheological and structural studies of liquid decane, hexadecane, and tetracosane under planar elongational flow using nonequilibrium molecular dynamics simulations, C. Baig, B.J. Edwards, D.J. Keffer, and H.D. Cochran, *AICHE Annual Meeting*, Cincinnati, OH, Oct. 30-Nov. 5, 2005.

- 29.) The molecular structure of hydrated nafion membrane interfaces: developing a model for proton transport, by D.J. Keffer, S. Cui, B.J. Edwards, and W.V. Steele, Annual Meeting of The Electrochemical Society, Denver, CO, May 7-12, 2006.
- 30.) Correlation based coarse graining approach to coupling length scales: atomistic to continuum, D.M. Nicholson, P. Nukala, Y. Osetskiy, R. Stoller, C. Gao, D.J. Keffer, and B.J. Edwards, NanoFocUL 2006 Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, August 24-25, 2006.
- 31.) A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards, and D.J. Keffer, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
- 32.) A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the NVT, NpT, and MuVT ensembles, J. Santiago, D.J. Keffer, B.J. Edwards, and C. Baig, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
- 33.) Flow of polymer blends between concentric cylinders, M. Dressler, B.J. Edwards and E.J. Windhab, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.
- 34.) A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards, D.J. Keffer, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
- 35.) Thermodynamics of non-isothermal polymer flows: experiment, theory, and simulation, T. Ionescu, B.J. Edwards, D.J. Keffer, and V. Mavrantzas, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
- 36.) Comparison of short and long chain polyethylene atomistic dynamics under shear and planar elongational flows, J.M. Kim, C. Baig, B.J. Edwards, and D.J. Keffer, The Society of Rheology 78th Annual Meeting, Portland, ME, Oct. 8-12, 2006.
- 37.) A generalized Hamiltonian-based algorithm for rigorous nonequilibrium molecular dynamics simulation in the NVT ensemble, J.G. Rajkumar, D.J. Keffer, B.J. Edwards, and C. Baig, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
- 38.) A comparison of rheological and structural properties of linear polyethylene melts under shear and elongational flow using nonequilibrium molecular dynamics simulations, J.M. Kim, C. Baig, D.J. Keffer, and B.J. Edwards, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
- 39.) A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards, and D.J. Keffer, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
- 40.) Thermodynamics of non-isothermal polymer flows: experiment, theory and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer, and V. Mavrantzas, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
- 41.) A molecular dynamics study of nafion polyelectrolyte membrane and the aqueous phase structure for proton transport, S.T. Cui, J. Liu, M. Esai-Selvan, D.J. Keffer, B.J. Edwards, and W.V. Steele, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.
- 42.) Estimation and analysis of the rheological properties of perfluoropolyethers, B. Jiang, D.J. Keffer, and B.J. Edwards, *AIChE* Annual Meeting, San Francisco, CA, Nov. 12-17, 2006.

- 43.) Understanding fuel cell operation through neutron imaging, D. Aaron, S. Yiacoumi, C. Tsouris, S.T. Cui, J. Liu, M. Esai Selvan, D.J. Keffer, B.J. Edwards, and W.V. Steele, Imaging and Neutrons 2006 Workshop, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN, October, 2006.
- 44.) A molecular-level reaction algorithm for proton transport consistent with quantum mechanical transition state theory and macroscopic conductivity, by D.J. Keffer, M. Esai Selvan, J. Liu, S. Cui, B.J. Edwards, and W.V. Steele, Electrochemical Society Annual Meeting, Chicago, IL, May 6-10, 2007.
- 45.) Rheological and entanglement characteristics of linear chain polyethylene liquids in planar Couette and planar elongational flows, J.M. Kim, D.J. Keffer, M. Kröger, and B.J. Edwards, XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007), Rhodes, Greece, June 6-10, 2007.
- 46.) Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer, and W.V. Steele, 15th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tennessee, October 21-25, 2007.
- 47.) Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, J. Liu, D.J. Keffer, B.J. Edwards, S. Cui, and W.V. Steele, 15th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tennessee, October 21-25, 2007.
- 48.) Correlation-based coarse-graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer, and B.J., Edwards, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 49.) Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer, and W.V. Steele, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 50.) Rheological and entanglement characteristics of polyethylene liquids and visualization of conformational changes in shear and elongational flows, J.M. Kim, D.J. Keffer, M. Kröger, and B.J. Edwards, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 51.) Reactive molecular dynamics of the thermal decomposition of CF_3OCF_3 , B. Jiang, B.J. Edwards, and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 52.) Quantum mechanics study of decomposition of CF_3OCF_3 and $(\text{CF}_3\text{CF}_2)_2\text{O}$ catalyzed by AlF_3 , B. Jiang, B.J. Edwards, and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 53.) Understanding the relationship between molecular architecture and thermophysical and rheological properties of perfluoropolyethers, B. Jiang, J.L. Adcock, N.J. Crawford, J.T. Fern, A.F. Pangloli, B.J. Edwards, W.V. Steele, and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 54.) Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, J. Liu, D.J. Keffer, B.J. Edwards, S. Cui, and W.V. Steele, AIChE Annual Meeting, Salt Lake City, UT, November 4-9, 2007.
- 55.) Correlation-based coarse graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer, B.J. Edwards, AIChE Annual Meeting, [Salt Lake City, UT, November 4-9, 2007.
- 56.) Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, D.J. Keffer, B.J. Edwards, S. Cui, J. Liu, and W.V. Steele, The Electrochemical Society Annual Meeting, Phoenix, AZ, May 18-23, 2008.

- 57.) Molecular-Level modeling of the structure and wetting of electrode/electrolyte interfaces, J. Liu, S. Cui, D.J. Keffer, B.J. Edwards, and M. Esai Selvan, The Electrochemical Society Annual Meeting, Phoenix, AZ, May 18-23, 2008.
- 58.) A comparison of the aqueous phase structures of hydrated Nafion and short side-chain polymer electrolyte membranes through molecular dynamics simulation, J. Liu, S. Cui, D.J. Keffer, B.J. Edwards, S. Paddison, and M. Esai Selvan, The Electrochemical Society Annual Meeting, Phoenix, AZ, May 18-23, 2008.
- 59.) Single-chain dynamics of linear polyethylene liquids under shear, J.M. Kim, B.J. Edwards, B. Khomami, and D.J. Keffer, The XVth International Congress on Rheology, Monterey, CA, August 3-8, 2008.
- 60.) Rheology of short-chain branched polyethylene melts under shear: results from NEMD simulations and comparison with linear and H-shaped analogues, C. Baig, J.M. Kim, V.G. Mavrantzas, and B.J. Edwards, The XVth International Congress on Rheology, Monterey, CA, August 3-8, 2008.
- 61.) A coarse-grained reactive molecular dynamics algorithm for proton transport in hydrogen fuel cells, M. Esai-Selvan, D.J. Keffer, S. Cui, and B.J. Edwards, AIChE 2008 Annual Meeting, Philadelphia, PA, November 16-22, 2008.
- 62.) Flow-induced temperature change and anisotropic heat capacity of a linear short-chain polyethylene liquid, C. Baig and B.J. Edwards, AIChE 2008 Annual Meeting, Philadelphia, PA, November 16-22, 2008.
- 63.) Dynamics of individual chains in linear polyethylene liquids under shear, J.M. Kim, D.J. Keffer, B. Khomami, and B.J. Edwards, AIChE 2008 Annual Meeting, Philadelphia, PA, November 16-22, 2008.
- 64.) Dynamics of entangled polyethylenes under shear via single-chain in mean-field simulations, K.Ch. Daoulas, B.J. Edwards, B. Khomami, M. Kröger, and M. Müller, AIChE 2008 Annual Meeting, Philadelphia, PA, November 16-22, 2008.
- 65.) Mechanistic dynamics of single chains in dense liquids under shear flow, J.M. Kim and B.J. Edwards, AIChE 2009 Annual Meeting, Nashville, TN, November 8-13, 2009.
- 66.) Nonequilibrium Monte Carlo simulation of flow-induced crystallization of a short-chain polyethylene liquid in uniaxial elongational flow, C. Baig and B.J. Edwards, AIChE 2009 Annual Meeting, Nashville, TN, November 8-13, 2009.
- 67.) Comparison of individual chain dynamics of a short-chain polyethylene dense liquid with equivalent free-draining dilute solution using an atomistic and mesoscopic level approach, J.M. Kim, B.J. Edwards, B. Khomami, and D.J. Keffer, AIChE 2009 Annual Meeting, Nashville, TN, November 8-13, 2009.
- 68.) Direct nonequilibrium Monte Carlo simulation of flow-induced crystallization of a linear short-chain polyethylene liquid in uniaxial elongational flow, C. Baig and B.J. Edwards, The Society of Rheology 81st Annual Meeting, Madison, WI, October 18-22, 2009.
- 69.) An experimental study of slip flow in capillaries and semi-hyperbolically converging dies, P.A. Kamerkar and B.J. Edwards, The Society of Rheology 81st Annual Meeting, Madison, WI, October 18-22, 2009.
- 70.) Single droplet dynamics in the framework of non-equilibrium thermodynamics, M. Dressler and B.J. Edwards, 5th International Workshop on Nonequilibrium Thermodynamics IWNET 2009, Cuernavaca, Mexico, August 24-30, 2009.
- 71.) Nonequilibrium Monte Carlo simulation of flow-induced crystallization of a short-chain polyethylene liquid in uniaxial elongational flow, C. Baig and B.J. Edwards, 5th International Workshop on Nonequilibrium Thermodynamics IWNET 2009, Cuernavaca, Mexico, August 24-30, 2009.

- 72.) Non-equilibrium thermodynamics modeling of concentrated polymer blends, M. Dressler and B.J. Edwards, 5th International Workshop on Nonequilibrium Thermodynamics IWNET 2009, Cuernavaca, Mexico, August 24-30, 2009.
- 73.) Multiscale simulations of chain dynamics in polymeric liquids undergoing shear, J.M. Kim, B.J. Edwards, and B. Khomami, American Physical Society Annual Meeting, Portland, OR, March 15-20, 2010.
- 74.) Fabrication of complex three-dimensional nanostructures from self-assembling block copolymer materials on two striped patterned templates with mismatched symmetry, X. Ye, B.J. Edwards, and B. Khomami, American Physical Society Annual Meeting, Portland, OR, March 15-20, 2010.
- 75.) A mean-field anisotropic diffusion model for unentangled polymeric liquids and semi-dilute solutions, J.M. Kim, P.S. Stephanou, B.J. Edwards, and B. Khomami, XVIth International Workshop on Numerical Methods for Non-Newtonian Flows, Northampton, MA, June 13-16, 2010.
- 76.) A mean-field anisotropic diffusion model for unentangled polymeric liquids and semi-dilute solutions, J.M. Kim, P.S. Stephanou, B.J. Edwards, and B. Khomami, The Society of Rheology 82st Annual Meeting, Santa Fe, NM, October 24-28, 2010.
- 77.) Elucidating the formation of block copolymer nanostructures on patterned surfaces: a self-consistent field theory study, X. Ye, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Salt Lake City, UT, November 7-12, 2010.
- 78.) Rational design of block copolymer morphologies via control of the film thickness and substrate patterning: A self consistent field study, X. Ye, B.J. Edwards, and B. Khomami, American Physical Society Annual Meeting, Dallas, TX, March 21-25, 2011.
- 79.) Macroscopic model of proton transport through the membrane-ionomer interface, M. Kumar, B.J. Edwards, and S.J. Paddison, AIChE Annual Meeting, Minneapolis, MN, October 16-21, 2011.
- 80.) Tailoring block copolymer morphology via control of topographical surface: A self consistent field theoretic study, X. Ye, B. J. Edwards, and B. Khomami, APS Annual Meeting, Boston, MA, February 27-March 2, 2012.
- 81.) A self-consistent field study of diblock copolymer/charged particle system morphologies for nanofiltration membranes, B. Zhang and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
- 82.) First-principles modeling of proton conductivity in perfluorosulfonate fuel cell membranes, B. Zhang and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
- 83.) Atomistic simulation of dynamics of individual molecules in entangled polymers undergoing homogenous shear flow, M. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
- 84.) Composition dependency of the Flory-Huggins χ parameter in isotopic polymer blends, T. Russell, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 3-8, 2013.
- 85.) Atomistic simulation of dynamics of individual molecules in entangled polymers undergoing homogenous shear flow, M. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, Society of Rheology Annual Meeting, Montreal, Canada, October 13-17, 2013.
- 86.) Composition dependency of the Flory-Huggins χ parameter in isotopic polymer blends, T.H. Russell, B.J. Edwards, and B. Khomami, APS Annual Meeting, Denver, CO, March 3-7, 2013.

- 87.) Modeling proton conductivity in perfluorosulfonate acid fuel cell membranes, B. Zhang and B.J. Edwards, TN-SCORE Annual Conference, Nashville, TN, June 26-27, 2014.
- 88.) A self-consistent field study of diblock copolymer/charged particle system morphologies for nanofiltration membranes, B. Zhang and B.J. Edwards, TN-SCORE Annual Conference, Nashville, TN, June 26-27, 2014.
- 89.) Dynamics of individual molecules in entangled polymeric melts under homogenous shear flow: an atomistic simulation study, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 86th Annual Meeting, Philadelphia, PA, October 5-9, 2014.
- 90.) Single chain dynamics of entangled linear polyethylene liquids under shear flow: an atomistic simulation study, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Atlanta, GA, November 16-21, 2014.
- 91.) Modeling of proton conductivity through perfluorosulfonate acid electrolyte membranes, B. Zhang and B.J. Edwards, 227th Meeting of the Electrochemical Society, Chicago, IL, May 24-28, 2015.
- 92.) Single chain dynamics of entangled linear polyethylene liquids under homogenous shear and planer elongational flows using nonequilibrium molecular dynamics simulations, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 87th Annual Meeting, Baltimore, MD, October 11-15, 2015.
- 93.) Atomistic simulation of dynamics of individual molecules in entangled polymers undergoing homogenous shear and planer elongational flows, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015.
- 94.) Selective ion transport through carbon nanotubes, M. Aranha and B.J. Edwards, AIChE Annual Meeting, Salt Lake City, UT, November 8-13, 2015.
- 95.) Influence of charge on the transport of water and ions through carbon nanotubes: a molecular dynamics study, M. Aranha and B.J. Edwards, 14th International Conference on Inorganic Membranes, Atlanta, GA, July 10-13, 2016.
- 96.) Graphene and carbon nanotubes: absorption, separations, and transport processes, M. Aranha and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
- 97.) Modeling controlled release from hollow porous nanospheres, A.L. Wang and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
- 98.) Molecular dynamics simulation of water and ion transport through carbon nanotubes, M. Aranha and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
- 99.) A molecular dynamics study of the influence of charge on the transport of water and ions through carbon nanotubes, M. Aranha and B.J. Edwards, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
- 100.) Atomistic and molecular modeling and simulation of polymers, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.
- 101.) Atomistic simulation of dynamics of individual molecules in entangled polymers undergoing homogenous shear flow, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 13-18, 2016.

- 102.) Nonequilibrium molecular dynamics simulations of entangled polymer melts and solutions undergoing planar elongational flows, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 88th Annual Meeting, Tampa, FL, February 12-16, 2017.
- 103.) Nonequilibrium molecular dynamics simulations of entangled polymer solutions undergoing planar elongational flows, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 89th Annual Meeting, Denver, CO, October 8-12, 2017.
- 104.) Evaluation of reptation-based modelling of entangled polymeric fluids including chain rotation via NEMD simulation, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 89th Annual Meeting, Denver, CO, October 8-12, 2017.
- 105.) Out-of-plane rotational motion in shear flow of polymer melts and solutions, M.H. Nafar Sefiddashti, C.N. Edwards, B.J. Edwards, and B. Khomami, The Society of Rheology 89th Annual Meeting, Denver, CO, October 8-12, 2017.
- 106.) Ion transport through carbon nanotubes: a molecule dynamics study, M. Aranha and B.J. Edwards, AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.
- 107.) Magnetic polymer nanocomposites for giant magnetoresistance and electromagnetic shielding, J. Guo, A. Galaska, B.J. Edwards, B. Khomami, and Z. Guo, AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.
- 108.) Tunable magnetoresistance of conductive polymer nanocomposites, J. Guo, A. Galaska, S. Wei, B.J. Edwards, B. Khomami, and Z. Guo, AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.
- 109.) Magnetic polymer nanocomposites for electromagnetic interference shielding, J. Guo, A. Galaska, S. Wei, B.J. Edwards, B. Khomami, and Z. Guo, AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.
- 110.) Nonequilibrium molecular dynamics simulations of entangled polymer solutions undergoing planar elongational flow, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Minneapolis, MN, October 29-November 3, 2017.
- 111.) A coil-stretch transition in planar elongational flow of an entangled polymeric melt, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 90th Annual Meeting, Houston, TX, October 14-18, 2018.
- 112.) Configurational microphase separation in elongational flow of an entangled polymer liquid, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 90th Annual Meeting, Houston, TX, October 14-18, 2018.
- 113.) Microphase separation in entangled polymeric solutions, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 91st Annual Meeting, Raleigh, NC, October 20-24, 2019.
- 114.) Elucidating the molecular rheology of entangled polymeric fluids via direct comparison of NEMD simulations and model predictions, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, The Society of Rheology 91st Annual Meeting, Raleigh, NC, October 20-24, 2019.
- 115.) Microphase separation in entangled polymeric solutions, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
- 116.) Elucidating the molecular rheology of entangled polymeric fluids via direct comparison of NEMD simulations and model predictions, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.

- 117.) Microphase separation in entangled polymeric solutions in extensional flows, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, American Physical Society March Meeting, Denver, CO, March 2-6, 2020.
- 118.) Flow-induced phenomena in planar extensional flows of entangled polyethylene liquids, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, 18th International Congress on Rheology, Rio de Janeiro, Brazil, August 2-7, 2020.
- 119.) Flow-induced crystallization of a polyethylene liquid above the melting temperature and its nonequilibrium phase diagram, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 15-20, 2020.
- 120.) Effects of chain length and polydispersity on shear banding in simple shear flow of polymeric melts, M. Boudaghi-Khajehnohar, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, San Francisco, CA, November 15-20, 2020.
- 121.) A thermodynamically inspired method for quantifying phase transitions in polymeric liquids with application to flow-induced crystallization of a polyethylene melt, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, APS Annual Meeting, held virtually, March 15-19, 2020.
- 122.) Flow-induced crystallization of a polyethylene liquid above the melting temperature and its nonequilibrium phase diagram, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, Society of Rheology 92nd Annual Meeting, Bangor, ME, October 10-14, 2021.
- 123.) Microphase separation and flow-induced crystallization in entangled polymeric solutions in extensional flows, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, Society of Rheology 92nd Annual Meeting, Bangor, ME, October 10-14, 2021.
- 124.) A thermodynamically inspired method for quantifying phase transitions in polymeric liquids with application to flow-induced crystallization of a polyethylene melt, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, *Society of Rheology 92nd Annual Meeting, Bangor, ME, October 10-14, 2021.*
- 125.) Calculating the entropy of an entangled linear polyethylene melt under shear and elongational flows via atomistic simulation, B.J. Edwards, M.H. Nafar Sefiddashti, and B. Khomami, AIChE Annual Meeting, Boston, MA, November 7-11, 2021.
- 126.) Flow-induced crystallization of a polyethylene liquid above the melting temperature and its nonequilibrium phase diagram, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Boston, MA, November 7-11, 2021.
- 127.) A thermodynamically inspired method for quantifying phase transitions in polymeric liquids with application to flow-induced crystallization of a polyethylene melt, M.H. Nafar Sefiddashti, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Boston, MA, November 7-11, 2021.
- 128.) Effects of chain length and polydispersity on shear banding in simple shear flow of entangled polymeric melts, M. Boudaghi-Khajehnohar, B.J. Edwards, and B. Khomami, AIChE Annual Meeting, Boston, MA, November 7-11, 2021.

Visiting Professor

Department of Applied Mathematics, Michigan Technological University, Summer 2003.
Department of Chemical Engineering, University of Patras, Greece, Summer 2007 and Summer 2008.
School of Chemical Sciences and Chemical Engineering, Jiangsu University, Fall 2013, Summer 2015, and Summer 2017.

Editorial Board Member

Journal of Thermodynamics, Associate Editor, 2010-2017.
Polymers, Editorial Board Member, 2018-present.
Engineered Science, Associate Editor, 2018-present.

Technical Conference Participation

Member of the organizing committee, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.

Session chair: Recent theoretical advances in non-equilibrium thermodynamics, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.

Co-Chairman: 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton, NJ, August 14-17, 2003.

Session chair: Statistical mechanics and nonequilibrium thermodynamics, 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton, NJ, August 14-17, 2003.

Guest editor, Journal of Non-Newtonian Fluid Mechanics, dedicated issue to the 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton, NJ, August 14-17, 2003.

Session chair: Nonequilibrium thermodynamics, *AIChE* Annual Meeting, Austin, TX, November 7-12, 2004.

Member of the organizing committee, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.

Session chair: Coarse-graining and mesoscopic dynamics—some mathematical aspects, 4th International Congress on Non-Equilibrium Thermodynamics, Rhodes, Greece, September 3-7, 2006.

Member, Organizing and Scientific Committees, 5th International Workshop on Nonequilibrium Thermodynamics, Cuernavaca, Mexico, August 24-28, 2009.

Session chair: Complex Fluids, 5th International Workshop on Nonequilibrium Thermodynamics, Cuernavaca, Mexico, August 24-28, 2009.

Member, Scientific Committees, 6th International Workshop on Nonequilibrium Thermodynamics, Roros, Norway, August 19-24, 2012.

Session co-chair: Where are the limits of thermodynamics in nonequilibrium situations?, Joint European Thermodynamic Conference, Prague, Czech Republic, June 14-18, 2021.

Funding History

A constant volume model for polymer blends and foodstuffs, B.J. Edwards, Professional Development Award, University of Tennessee, October 2002, \$1,500.

A multi-scale approach to advanced materials simulations, B.J. Edwards, Center for Information Technology Research, University of Tennessee, November 2002, \$7,084.

Energetic and entropic elasticity in nonisothermal flows of polymeric materials, B.J. Edwards (PI), Petroleum Research Fund Type-AC Grant, September 1, 2004 through August 31, 2006, \$80,000, Grant No. 41000-AC7.

Joint experimental and simulation project for precise determination of physical properties of interest to D.O.E., D.J. Keffer (PI), B.J. Edwards (co-PI), and W.V. Steele (co-PI), Department of Energy, Fossil Energy Program, March 1, 2004 through February 28, 2005, \$150,000.

Joint experimental and simulation project for precise determination of physical properties of interest to D.O.E. (Renewal), D.J. Keffer (PI), B.J. Edwards (co-PI), and W.V. Steele (co-PI), Department of Energy, Fossil Energy Program, March 1, 2005 through February 28, 2006, \$150,000.

Computational and experimental study of high-performance lubricants in extreme environments, D.J. Keffer (PI), B.J. Edwards (co-PI), and J.L. Adcock (co-PI), Air Force Office of Scientific Research, May 1, 2005 through April 30, 2008, \$525,000, Grant No. AF FA9550-05-1-0342.

Simulating the impossible: non-equilibrium molecular dynamics simulations of uniaxial and biaxial elongational flow, B.J. Edwards (PI) and D.J. Keffer (co-PI), University of Tennessee Computational Sciences Initiative, August 1, 2005 through July 31, 2006, \$52,000.

A unified computational, theoretical and experimental investigation of proton transport through the electrode/electrolyte interface of proton exchange membrane fuel cell systems, D.J. Keffer (PI), B.J. Edwards (co-PI), W.V. Steele (co-PI), and S. Cui (co-PI), Department of Energy, Hydrogen Fuel Initiative, August 1, 2005 through July 31, 2008, \$825,000, Grant No. DE-FG02-05ER15723.

Simulation of long-chain molecules in elongational flows, Professional Development Award, University of Tennessee, November 2005, \$5,000.

Multi-scale modeling: application to hydrogen and helium in steels, D.J. Keffer (PI), B.J. Edwards (co-PI), and D. Nicholson (co-PI), University of Tennessee Science Alliance, Joint Directed Research and Development Program, January 1, 2006 through December 31, 2006, \$51,200, Grant No. D06-101.

Joint experimental and simulation project for precise determination of physical properties of interest to D.O.E. (Renewal), D.J. Keffer (PI), B.J. Edwards (co-PI), and W.V. Steele (co-PI), Department of Energy, Fossil Energy Program, March 1, 2006 through February 28, 2007, \$100,000.

Multi-scale modeling: application to hydrogen and helium in steels (Renewal), D.J. Keffer (PI), B.J. Edwards (co-PI), and D. Nicholson (co-PI), University of Tennessee Science Alliance, Joint Directed Research and Development Program, January 1, 2007 through December 31, 2007, \$52,200, Grant No. D06-101.

EXP-LA: Collaborative Research: Exploiting geometry and chemistry at the nanoscale to selectively preconcentrate explosive molecules, D.J. Keffer (PI) and B.J. Edwards (co-PI), National Science Foundation, CMMI, October 1, 2007 through September 30, 2009, \$265,819, Grant No. CMMI-0730207.

Scholarships for Engineering Students from Underrepresented Groups in the East Tennessee Region, B.J. Edwards (PI), D. Jackson (co-PI), J. Wu (co-PI), D.J. Keffer (co-PI), and W. Odom (co-PI), National Science Foundation, DUE, August 15, 2007 through July 31, 2011, \$600,000, Grant No. DUE-0726564.

From nanoscale simulation to process engineering: Building a network for understanding polymer dynamics, B.J. Edwards (PI), B. Khomami (co-PI), D.J. Keffer (co-PI), J.D. Schieber (co-PI), and E. Shaqfeh (co-PI), National Science Foundation, CBET, November 15, 2007 through October 31, 2009, \$189,959, Grant No. CBET 0742679.

Multiscale simulation of flow-induced structuring in entangled polymeric fluids, B.J. Edwards (PI), National Center for Supercomputing Applications, DAC-NCSA, 30,000 service units, October 15, 2007 until spent, Grant No. TG-CTS080002N.

Metal-porphyrin frameworks: A novel class of metal-organic frameworks, D.J. Keffer (PI), B.J. Edwards (co-PI), S. Agnihotri (co-PI), and C.Rawn (co-PI), Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, August 1, 2007 through December 31, 2007, \$25,000.

Convective and mass transfer models of the dynamics of reactive systems in C-tray polyester finishing reactors, D.J. Keffer (PI), B.J. Edwards (co-PI), B. Khomami (co-PI), and S. Petrovan (co-PI), Eastman Chemical Co., January 1, 2008 through December 31, 2010, \$120,000.

Self-consistent field and single chain in mean-field simulations of diblock and triblock copolymer systems, B.J. Edwards (PI), Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, January 1, 2009 through December 31, 2009, \$37,751.

A unified computational, theoretical, and experimental investigation of proton transport through the electrode/electrolyte interface of fuel cell membranes, D.J. Keffer (PI), S.J. Paddison (co-PI), and B.J. Edwards (co-PI), Department of Energy, National Energy Technology Initiative, \$210,000.

Nonisothermal flows of viscoelastic polymers, Professional Development Award, University of Tennessee, October 2008, \$5,000.

IGERT: STAIR: Sustainable technology through advanced interdisciplinary research, D.J. Keffer, B. Khomami, P.D. Frymier, C.J. Rawn, and B.D. Bruce, National Science Foundation, 08/01/2008 – 07/31/13, \$2,941,396. Edwards' portion: \$282,720.

Development of an experimentally validated master simulation module for PEM fuel cells, S.J. Paddison (PI) and B.J. Edwards (co-PI), Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, August 1, 2009 through July 31, 2010, \$64,926.

Self-consistent field and single chain in mean-field simulations of diblock and triblock copolymer systems (Extension), B.J. Edwards (PI), Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, January 1, 2010 through June 30, 2010, \$20,650.

Morphology development in multi-component polymeric systems with application to photovoltaic materials, B.J. Edwards, Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, February 1, 2011 through May 31, 2011, \$28,628.

Morphology control of conductivity using systems of diblock copolymers doped with metal ions: application to advanced battery technology, Sustainable Energy Education and Research Center, University of Tennessee-Knoxville August 1, 2011 through May 31, 2012, \$31,406.

Electrolytic removal of heavy metals from frack water, EnergySolutions Inc., January 1, 2013 through June 30, 2013, \$50,000.

EPSCoR: Tennessee Solar Conversion and Storage Using Outreach, Research and Education, T. Zawodzinski (PI), National Science Foundation, August 1, 2010 through July 31, 2015, \$20,000,000. Edwards' portion: \$172,500.

Scholarships for Engineering Students in the East Tennessee Demographic Region, B.J. Edwards (PI), J. Wu (co-PI), C.J. Rawn (co-PI), P.M. Dalhaimer (co-PI), T.T. Griffin, National Science Foundation, June 1, 2013 through May 31, 2018, \$606,800, Grant No. DUE-1258417.

Intra-cellular and inter-cellular transport in drug delivery systems, Professional Development Award, University of Tennessee, May through August, 2015, \$4,000.

Description of the structural, transport and electrochemical features of electrolytes in carbon nanotubes using molecular dynamics simulations, National Center for Supercomputing Applications, DAC-NCSA, 50,000 service units, June 1, 2016 until spent, Grant No. TG-CTS160032.

Nanocomposites manufacturing innovation hub, B.J. Edwards (PI), M. Dadmun (co-PI), B. Khomami (co-PI), R. Kalyanaraman (co-PI), G. Bhat (co-PI), and D. Mukherjee (co-PI), Transdisciplinary Academy Program, University of Tennessee, July 1, 2016 through June 30, 2017, \$90,300.

Flow-induced disentanglement in shear and elongational flows of entangled polymers: a hi-fidelity molecular simulation study, B.J. Edwards (PI) and B. Khomami (co-PI), National Science Foundation, Sept. 1, 2016 through August 31, 2019, \$299,999, Grant No. CBET-1602890.

An assessment of the barriers to ion transport through sub-3 nm diameter carbon nanotubes, National Center for Supercomputing Applications, XSEDE XRAC, 988,000 service units (\$66,855 value), October 1, 2016 through September 30, 2017, Grant No. CTS160038.

Nanoscale ion transport through carbon nanotubes, Oak Ridge Leadership Computing Facility, 2M Titan core hours, 2,500 Rhea node hours, April 25, 2017 through April 24, 2018, Project ID NTI107.

Dilute and semi-dilute polymer solutions: configurational and rheological analysis of flexible and semi-flexible linear and brush polymers and their blends, XSEDE Bridges, 1500 GPU hours (\$25,894), November 10, 2020 through November 9, 2021, Grant No. CHM200004.

Courses Taught at the University of Tennessee

Chemical Engineering 230, Chemical Engineering Thermodynamics I, Summer 2001-2005.

Chemical Engineering 250, Chemical Engineering Thermodynamics II, Spring 2002-2008; Summer 2015.

Chemical Engineering 411, Undergraduate Research Experience, Spring 2007.

Chemical Engineering 501, Chemical Engineering Seminar, every semester from Fall 2001-Spring 2007; Fall 2013.

Chemical Engineering 531, Advanced Chemical Engineering Thermodynamics, Fall 2001-2009.

Chemical Engineering 631, Advanced Topics in Statistical Thermodynamics and Molecular Dynamics, Fall 2005.

Chemical Engineering 691, Nonequilibrium Thermodynamics, Fall 2002, Fall 2006.

Chemical Engineering 691, Fortran Programming for Windows-Based Applications in Chemical Engineering, Fall 2003.

Chemical Engineering 691, Molecular-Scale Chemical Engineering Simulations, Spring 2005, 2012.

Chemical and Biomolecular Engineering 691, Equilibrium Theory of Inhomogeneous Polymers, Spring 2009.

Chemical and Biomolecular Engineering 380, Chemical Engineering Seminar, Spring 2010, 2011.

Chemical and Biomolecular Engineering 407, Chemical Engineering Honors Seminar, Fall of 2006-Spring 2014, Fall 2016-present.

Chemical and Biomolecular Engineering 691, Chemical Engineering Topical Projects, Spring 2010, 2013.

Chemical and Biomolecular Engineering 580, Technical Review and Assessment, Fall and Spring 2009-2011; Fall 2013; Spring 2018.

Chemical and Biomolecular Engineering 394, Chemical and Biomolecular Engineering Co-op, Fall, Spring, and Summer, 2007-present.

Chemical and Biomolecular Engineering 506, Advanced Mathematics for Chemical Engineers, Fall 2010-2012.

Chemical and Biomolecular Engineering 240, Fluid Flow and Heat Transfer, Spring 2012, 2013.

Chemical and Biomolecular Engineering 691, Transport Phenomena in Thin Films and Membranes, Spring 2013.

Chemical and Biomolecular Engineering 447/547, Advanced Transport Phenomena, Spring 2014-2017, Spring 2020.

Chemical and Biomolecular Engineering 590, Special Topics in Chemical Engineering, Fall 2015.

Chemical and Biomolecular Engineering 494, Special Problems in Chemical Engineering, Spring 2015, Fall 2015, Fall 2017, Summer 2020, Fall 2020.
Chemical and Biomolecular Engineering 498, Honors Thesis, Spring 2015, Fall 2015.
Chemical and Biomolecular Engineering 691, Advanced Engineering Thermodynamics, Spring 2016.
Chemical and Biomolecular Engineering 360, Process Dynamics and Control, Spring 2019 – present.

Students and Postdoctoral Associates Supervised since January, 2001

Direct supervision

Christopher W. Reneau, undergraduate research assistant, spring 2001; fall 2001.
Jonathan N. Allred, undergraduate research assistant, fall 2001; spring 2002.
Prajakta Kamerkar, Ph.D. student, fall 2002-summer 2005.
Bangwu Jiang, Ph.D. student, fall 2002-summer 2005.
Chunggi Baig, Ph.D. student, fall 2003-summer 2005.
Tudor Ionescu, Ph.D. student, fall 2004-summer 2006.
Kenny Tucker, Ronald McNair Post Baccalaureate Achievement Program scholar, summer 2002.
Karen Williams, NSF REU Program fellow (Grant No. EEC-9820489), summer 2002.
Kevin Smith, undergraduate research assistant, fall 2002.
Christopher Otuonye, undergraduate research assistant, summer 2005-fall 2005.
Joseph Rajkumar, M.S. student, fall 2005-summer 2007.
Jun Mo Kim, M.S. student, fall 2005-summer 2008.
Jun Mo Kim, Ph.D. student, fall 2008-summer 2010.
Junwu Liu, Ph.D. student, fall 2005-summer 2009.
Myvizhi Esai Selvan, Ph.D. student, spring 2006-fall 2010.
Johanna Santiago, M.S. student, fall 2004-summer 2006.
Bangwu Jiang, Postdoctoral researcher, fall 2005-spring 2008.
Chunggi Baig, Postdoctoral researcher, fall 2005-spring 2006.
Carrie Gao, Postdoctoral researcher, spring 2006-spring 2007.
Tudor Ionescu, Postdoctoral researcher, fall 2004-fall 2006.
Anne Wells, undergraduate research assistant, spring 2007.
Hannah Bailey, undergraduate research assistant, spring 2007.
Mathew Milazzo, undergraduate research assistant, spring 2007.
Opeoluwa Kolawole, M.S. student, spring 2008-spring 2011.
Travis Russell, M.S. student, fall 2009-fall 2011.
Travis Russell, Ph.D. student, fall 2011-summer 2014.
Abigail Hipp, undergraduate research assistant fall 2009-fall 2011.
Xiangui Ye, Postdoctoral researcher, spring 2009-spring 2012.
Milan Kumar, Ph.D. student, spring 2009-fall 2011.
Mohammad Nafar Sefiddashti, M.S. student, spring 2011-spring 2013.
Mohammad Nafar Sefiddashti, Ph.D. student, spring 2013-summer 2018.
Kaara Anderson, M.S. student, fall 2009-summer 2012.
Bo Zhang, M.S., student, fall 2011-summer 2013.
Bo Zhang, Ph.D. student, fall 2013-summer 2015.
Aaron Oswald, undergraduate research assistant, spring 2013.
Michelle Aranha, M.S. student, fall 2012-spring 2015.
Michelle Aranha, Ph.D. student, summer 2015-summer 2017.
Nicholas Ciparro, B.S. student, fall 2014-spring 2017.
Xuewei Guan, International Exchange B.S. student, fall 2014-spring 2015.
Michael Lin, B.S. student, summer, fall 2015-spring 2016.
Carl Edwards, B.S. student, fall 2016-fall 2017.
Oluwafemi Oyedeji, M.S. student, fall 2017-spring 2018.
Justin Le, B.S. student, fall 2020-present.

Ph.D and M.S. Committee Participation

Parag Patil, Ph.D., J. Collier (chairman), graduation 2002.
Jan van Meervald, Ph.D., H.C. Öttinger (chairman), graduation 2002.
José Luis Rivera-Rojas, Ph.D., P.T. Cummings (chairman), graduation 2002.
Mithun R. Kamat, M.S., D.J. Keffer (chairman), graduation 2002.
Parag Adhangale, Ph.D., D.J. Keffer (chairman), graduation 2003.
Austin Newman, M.S., D.J. Keffer (chairman), graduation 2004.
Chao Li, M.S., D.J. Keffer (chairman), graduation 2006.
Charles W. Alvord, Ph.D., A.E. Ruggles (chairman), graduation 2008.
Jared T. Fern, Ph.D., D.J. Keffer and W.V. Steele (co-chairmen), graduation 2007.
Mohamad Kassaei, M.S., D.J. Keffer (chairman), graduation 2007.
Pavlos Stephanou, University of Patras, Greece, Prof. V.G. Mavrantzas (chairman), graduation 2011.
Lujian Peng, Ph.D., J. Morris (chairman), graduation 2011.
Arash Abedijaberi, Ph.D., B. Khomami (chairman), graduation 2011.
Jeffrey Clark, M.S., S.J. Paddison (chairman), graduation 2012.
Jeffrey Clark, Ph.D., S.J. Paddison (chairman), graduation 2014.
Mahdy Malekzadeh Moghani, M.S., B. Khomami (chairman), graduation 2012.
Mahdy Malekzadeh Moghani, Ph.D., B. Khomami (chairman), graduation 2014.
Mouge Mohagheghi, M.S., B. Khomami (chairman), graduation 2013.
Mohammad Ghanbari, M.S., B. Khomami (chairman), graduation 2013.
Sagar Yadavali, Ph.D., R. Kalyanaraman (chairman), graduation 2014.
Timothy Diedesch, Ph.D., M. Jessup (chairman), graduation 2016.
Nada Mehio, Ph.D., S. Dai (chairman), graduation 2016.
Sina Mirzaeifard, M.S., S. Abel (chairman), graduation 2016.
Robert Golsby, M.S., P. Frymier (chairman), graduation 2016.
Amir Saadat, Ph.D., B. Khomami (chairman), graduation 2016.
Xingru Yan, Ph.D., Z. Guo (chairman), graduation 2016.
Jiang Guo, Ph.D., B. Khomami (chairman), graduation 2018.
Yuanjun Song, Ph.D., S. Laursen (chairman), graduation 2020.
Nobahar Shahidi, M.S., E. Doxastakis (chairman), graduation 2020.
Xubo Luo, Ph.D., S. Paddison (chairman), graduation 2020.
Nobahar Shahidi, Ph.D., E. Doxastakis (chairman), graduation 2021.

University and Community Service

Co-Organizer, 2nd International Congress on Non-Equilibrium Thermodynamics, Oxford University, Oxford, UK, August 14-18, 2000.
Member, Graduate Curriculum Committee, Department of Chemical Engineering, University of Tennessee, 2001-2008.
Organizer, Departmental Seminar Series, Fall, 2001-2014.
Ronald McNair Post Baccalaureate Achievement Program mentor, summer, 2002.
NSF Research Experience for Undergraduates Program mentor (Grant No. EEC-9820489), summer, 2002.
Co-chairman, 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton University, Princeton, NJ, August 14-17, 2003.
Guest co-editor of the special issue of *Journal of Non-Newtonian Fluid Mechanics* devoted to papers from the 3rd International Congress on Non-Equilibrium Thermodynamics, Princeton University, Princeton, NJ, August 14-17, 2003.
National Science Foundation Panelist, divisions and dates omitted for confidentiality (about 40 times, since 2003).
Chairman, Session 1a, Nonequilibrium Thermodynamics, AIChE Annual Meeting, Austin, TX, November 7-12, 2004.
Faculty senator, The University of Tennessee, 2004-2006: member, Faculty Affairs Committee and Student Affairs Committee.

Member, Department Head Search Committee for Chemical Engineering, 2005-06.
Member, Governor's Chair Position Search Committee, 2005-2006.
Member, Organizing Committee, 4th International Congress on Nonequilibrium Thermodynamics, Patras, Greece, September 3-7, 2006.
Chairman, Graduate Curriculum Committee, Department of Chemical Engineering, University of Tennessee, 2006-present.
Associate Head, Department of Chemical and Biomolecular Engineering, September 2006-present.
Member, Department of Chemical Engineering Faculty Search Committee, 2006-2007.
Chairman, Undergraduate Curriculum and Affairs Committee, Dept. of Chemical and Biomolecular Engineering, UTK, 2006-present.
Member, Facilities and Infrastructure Committee, Dept. of Chemical Engineering, UTK, 2006-present.
Representative, College of Engineering ABET Committee, UTK, 2006-2015.
Member, University Coeus Steering Committee, 2006-2008.
Member, College of Engineering Business Manager Search Committee, 2007.
Member, College of Engineering Scholarship Committee, 2008-2012.
Member, Chemical and Biomolecular Engineering Faculty Search Committee, UTK, 2007-2008.
Member, Department of Materials Science and Engineering Academic Program Review team, April 14-16, 2008.
Member, Editorial Board, Journal of Thermodynamics, 2008-2018.
Tenure and Promotion Committee, College of Engineering, UTK, 2009-2015.
Member, Organizing and Scientific Committees, 5th International Workshop on Nonequilibrium Thermodynamics, Cuernavaca, Mexico, August 24-28, 2009.
Member, Chemical and Biomolecular Engineering Faculty Search Committee, UTK, 2009-2010.
Member, College of Engineering Research Fellow Award Committee, UTK, spring 2010 and 2011.
Director and Chairman of the Board of Advisors, PolyHub Engineering Virtual Organization, fall 2007-present.
Director, NSF-funded S-STEM Scholarship Program for Students from Underrepresented Groups, UTK, fall 2006-2018.
Member, College of Engineering Promotion and Tenure Committee, 2009-2014.
Member, College of Engineering ABET Committee, UTK, spring 2010-present.
Member, Chemical and Biomolecular Engineering Faculty Search Committee, UTK, 2010-2011.
Chairman, Chemical and Biomolecular Engineering Strategic Planning Committee, UTK, 2012.
Member, Chemical and Biomolecular Engineering Human Subject Research Committee, UTK, 2012.
Chairman, Chemical and Biomolecular Engineering Faculty Search Committee, UTK, 2013-2014.
Member, College of Engineering Curriculum Committee, UTK, fall 2016-present.

Patents

Manufacture of graphene and graphene composition of matter, B.J. Edwards and N. Ciparro, Provisional Patent Application No. 62/145355, 4/9/2015. Regular utility application No.: 15095729, 4/11/2016.

Engineering Consulting

Nike IHM, Inc., St. Charles, MO 63304.
Kongsberg Automotive, Milan, TN.
The Popham Law Firm, Kansas City, MO.

Reviewer for:

Journals: *Journal of Non-Newtonian Fluid Mechanics; Macromolecular Theory and Simulation; Journal of Chemical Physics; Journal of Non-Equilibrium Thermodynamics; Journal of Rheology; Journal of Applied Polymer Science; Polymer Engineering and Science; Rheologica Acta; Journal of Nonlinear Science; Chemical Engineering Science; Physics of Fluids; Proceedings of the Royal Society A; Physical Review Letters, Physical Review E; Mathematical Physics, Analysis and Geometry; Polymer; Journal of*

Thermodynamics; Journal of Physical Chemistry B; Journal of Physical Chemistry C; Industrial & Engineering Chemistry Research; Microfluidics and Nanofluidics, Macromolecules; Chemical Engineering Communications; Continuum Mechanics and Thermodynamics; Journal of Polymer Science: Polymer Physics; J. Elasticity; ChemPhysChem; Chemical Physics Letters; Reviews in Chemical Engineering; Molecular Simulation; Entropy; AIChE Journal; Molecular Pharmaceutics; Proceedings of the Royal Society A; Polymers; Engineered Science; Processes; Entropy; Journal of Applied Physics; Soft Matter; ACS Macro Letters; Journal of Computational Chemistry; Physical Review Fluids; Physica A; Physical Review Materials.

Funding organizations: *National Science Foundation; Schweizerischer Nationalfonds zur Förderung der Wissenschaftlichen Forschung (Swiss NSF); Petroleum Research Fund.*

Book publishers: *John Wiley and Sons; Cambridge University Press; Elsevier Ltd., McGraw-Hill.*