Comprehensive Curriculum Vitae
Steven Raymond Lustig, PhD, FRSC

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EDUCATION

Ph.D. Chemical Engineering, Purdue University, December 1989.
M.S. Chemical Engineering, Purdue University, April 1985.
B.S.Ch.E. with Distinction, University of Virginia, May 1983.

CONTINUED EDUCATION

- American Sailing Association (https://asa.com/)certifications ASA 101, 103, 104 (2005), 105 (2006), 118 (2010); New Castle Sailing Club certification (2007); Annapolis School of Sailing marine diesel maintenance and repair (2012)
- Marshal Bridge Welding Workshop, Stan Smokler (http://www.stansmokler.com/), Kennett Square, PA, Summers 2009, 2010, 2012
- Techniques in Microbiology, Pennsylvania State University, State College, PA. Summer 2005
- The Florida School on Applied Molecular Orbital Theory, University of Florida, Gainesville, FL. May 1993
- Los Alamos Workshop Program on Scientific Supercomputing, Los Alamos National Laboratory, NM. Summer 1991.

EMPLOYMENT HISTORY

Associate Professor with Tenure **2016-Present**
Department of Chemical Engineering, Northeastern University, Boston, Massachusetts

Chemical Engineer Joint Faculty Appointment **2019-2021**
Army Research Laboratory, U.S. Army, Aberdeen, Maryland

Adjunct Professor **1992-1996, 2012-2016**
Department of Chemical & Biomolecular Engineering, Department of Materials Science & Engineering
University of Delaware, Newark, Delaware

- Collaborative research in statistical thermodynamics of solutions with Prof. Stanley Sandler results: a new, more accurate revision of COSMO-SAC theory implemented in new, high-performance software that predicts pure liquid and mixture solution thermodynamic properties; successful project funding by a National Science Foundation GOALI grant and a DuPont Ventures research grant; a joint development agreement for commercialization with a world-class vendor of molecular modeling software. Coauthored textbook in progress.

- Collaborative research with Prof. Bruce Chase resulted in the development of a novel rheological characterization method with simultaneous polarized Raman scattering, particularly applied to

industrially-relevant liquid crystalline polymer solutions. Crossed-angle and magic angle polarization methods quantitatively characterize molecular alignment, heterogeneity and rotational dynamics. The method is being adopted in an industrial development and manufacturing facility.

- Collaborative research in massively-parallel computational colloid rheology with Prof. Norman Wagner resulted in: the largest contemporary ensemble nonequilibrium Brownian dynamics simulations of monodisperse and polydisperse colloids in shear; understanding why Brownian dynamics is the more accurate method for comparing colloidal structural and transport properties with experimental data than nonequilibrium molecular dynamics methods; discovery why the discontinuous shear-induced ordering transition is inhibited at a critical polydispersity.

- Courses taught: Graduate: Advanced Polymer Science (CHEG-867), Polymer Physics (MSEG-835), Classical and Statistical Thermodynamics (CHEG-825), Green Engineering (CHEG-625), Undergraduate: Chemical Process Analysis (CHEG-432)

Principal Investigator, Research Associate, Sr Research Engineer, Research Engineer 1990–2016
Central Research & Development, E.I. du Pont de Nemours & Co., Inc., Wilmington, Delaware

- Conceived and developed COSMOdesign© theory and software that directly solves molecular design, inverse-thermodynamic problems in which a required thermodynamic property objective in a chemical process or reaction is specified and new molecular structures or material components are derived from the statistical thermodynamics of molecular solvation surfaces. The methodology also provides an attainable bound to the objective based on the chemical physics of molecular interactions. The design process is detailed in six pending patents and one granted patent. COSMOdesign© was applied to several DuPont research programs, specific results are either published, trade secret or proprietary.

- Collaborative research with Kevlar® business resulted in 2023 commercial debut of Kevlar® EXO™, a novel, ultra-high performance copolymer. My contributions include: (i) optimization of comonomer structure for enabling novel imidazole compositions with greatly improved thermal processability, transverse compression response, and greatly improved anti-ballistic armor performance, (ii) design of process technology that enables effective heat treatment, (iii) innovation of new fundamental improvements in pre-spinning, solution process technology, and (iv) inventorship covered in 7 issued patents. New copolymer compositions with poly(phenylene terephthalamide) were scouted and assessed after developing a novel hydrogen bond network model based on molecular theory of liquid crystalline polymers. Representative hydrogen bond energies were calculated with accurate density functional theory, mobility temperatures were predicted using rigorous statistical thermodynamic alignment probabilities of hydrogen bond acceptors and donors. Benchmarked predictions for several dozen compositions matched quantitatively trends in experimental tenacity with processing treatments. Thousands of new comonomer structures and compositions were evaluated *in silico* to identify the best candidates for new, high strength fibers . This work guided long-term, strategic business decisions on the fiber research and development and has significant commercial impact with a new product launch by DuPont.

- Supported development of novel lithium ion battery electrolyte using molecular spectroscopy and quantum chemical calculations to analyze solid electrolyte interface (SEI) chemistry and structural evolution. Evaluated electrolyte freezing temperature. Used novel chemical solvation theory to predict ionic and ion-pair species concentrations, ionic strength, and ionic mobilities. Designed chemistry exhibited vastly improved recharging lifetime.

- Consulted with Kapton® polyimide polymerization and films development project team on polymerization equilibria and multi-phase equilibria needed for improving trade-secret manufacturing and processing equipment. Project team enabled 2X capacity increase.

- Discovery research resulted in novel enzyme-catalyzed air cathodes for microbial fuel cells as well as other fuel cells based on proton producing anodes. Catalytic conversion of oxygen, electrons and hydronium ions is very efficient with laccase encapsulated on electrically-conductive non-woven membranes. Technology and market analyses indicate substantial business opportunity.

- Collaboration with DuPont Inkjet business resulted in the development and commercialization of Artistri™ P5910W™ white inkjet ink producing multiple million dollar profits and my invention of trade secret: thermally-cleavable dispersants and surfactants; microwave curing hardware for aqueous, high print speed textile inks; and nanoparticle Nucrel® fusants for ultra-durable aqueous inks. P5910W™ ink is the leading, state-of-the-art heat-curable aqueous white ink. My significant technology improvement in P5910W™ ink is the highly-enhanced colloidal stability of titania pigment within the aqueous vehicle. Titania pigment is over four times denser than the aqueous vehicle, has the 120 nm particle size with narrow distribution for optimum optical scattering and yet remains stable for months without appreciable settling. Although the ink was specifically developed for the Artistri™ printer, the product displaced most competitive offerings for all other digital textile printers. Developed heat-fusible quantum dot solutions that worked as pigmented inkjet inks.

- Invented polytransesterification catalysts that provide high polymerization rates, environmental and biological compatibility, and colorless polymers. These catalysts are currently applied in the manufacturing of DuPont Sorona® as well as newer condensation polymers based on biologically-sourced trimethylene glycol. Prior to the commercial adoption of these catalysts, polyester fibers, films and resins were manufactured using antimony catalysts that present environmental and biological liabilities when either landfilled or recycled. Prior titanate catalysts were known to be environmentally-safe and effective, but created strong chromophores that rendered the polymer opaque and unmarketable. My identifying the titanate chromophores provided a fundamental understanding of how even minute quantities of aldol condensation by-products lead to polymer color thus enabling my invention of environmentally-safe zirconate co-catalyst chemistries that annihilate the titanate chromophores. A dramatic example of this technology was demonstrated by adding these zirconate compounds to remove the existing color and impart transparency to highly colored polymer manufactured with only titanates. Several countries including the United States granted patents to this technology by allowing claims both to the co-catalyst combinations as well as composition of matter of polyesters containing titanates with improved optical properties.

- Discovery research explored the manipulation of carbon single wall nanotubes (SWNTs) with biological molecules that resulted in: invention of the first process to cut SWNTs to narrow length distribution while chemically functionalizing only the tube ends; discovery of polypeptides that selectively bind and disperse SWNTs in water; structural and electrostatic characterization of SWNT/DNA hybrids; discovery of polypeptides that selectively bind to SWNT/DNA hybrids; development of chemistries to guide the self-assembly placement of SWNTs on silicon wafers with various surface compositions; my theory that describes quantitatively SWNT/DNA hybrid separation based on SWNT chirality; invention of the potentiostat-HPLC method to separate SWNT/DNA hybrids based on SWNT chirality with complete yield.

- Discovery research and engineering of room temperature ionic liquids and ionic compounds resulted in my invention of proprietary compositions that greatly improve: aqueous absorption cooling refrigeration by increasing thermodynamic efficiency and decreasing lifetime process cost; carbon

dioxide capture from coal-burning power plant flue gas by decreasing parasitic energy and lifetime process cost; and thermodynamic separation of nitrogen from natural gas by selective adsorption. Although absorption cooling is a very mature technology, COSMOdesign discovered a novel absorbent that increased the coefficient of performance 10% and decreased the lifetime process cost 7% (equivalent to millions of dollars for typical office buildings) relative to the state-of-the-art processes. Carbon capture technology was advanced with the development of novel, low molecular weight, vicinal diamine based ionic liquids that absorb(desorb) carbon dioxide at 30°C(70°C) with over 90% theoretical capacity involving very low latent heats of adsorption. Since absorption and stripping operations are cooled/heated entirely by the available excess energy provided from intercooler transfer fluid from the multiple-stage compression required for sequestration distribution, the parasitic loss to the power plant is restricted only to that required to compress the separated carbon dioxide. This technology was awarded by the Pittsburgh Coal Conference and has attracted the interest of the Alberta Innovates, Canadian government, for further development funding.

- Research on M5, poly(hydroquinone-diimidazopyridine), high performance fiber resulted in a mechanistic, quantum-chemical prediction for the loss in tensile modulus in the presence of trace absorbed water that agrees quantitatively with experimental measurements. A single water molecule was found to form a stable hydrogen bonds between the hydroquinone hydroxyl and imidazole nitrogen, thus breaking the direct inter-monomer hydrogen bond. This chemistry diminishes the modulus along the chain backbone and can only be reversed by drying at substantially high temperatures. This fundamental understanding provided the DuPont Protection Technologies business with sufficient confidence to cease all development of M5.

- Exploratory research on hydrogen storage materials resulted in a patented nano-porous, ultra-high surface area carbon that met the U.S. D.o.E. Stage I gravimetric and volumetric capacity metrics. High molecular weight polysaccharides were reduced at high temperature in pure hydrogen atmosphere to produce a novel, reduced form of carbon in which capillary condensation of hydrogen occurs at high pressure but ambient temperatures.

- Engineering research resulted in new patent estates of new polyester manufacturing technologies: high yield syntheses and ring-opening polymerizations of cyclic oligomers, suspension condensation polymerization, and clay-based coatings for high barrier applications. Nonequilibrium size distributions of cyclic oligomers can be produced that melt at low eutectic temperatures, thus fast ring opening polymerizations can occur at temperatures low enough to avoid substantial thermal degradation obviating diffusion-limited condensation polymerization. The novel suspension polymerization method also obviates diffusion-limited condensation and enhances polymerization rates 10-100X over bulk melt polymerizations by dispersing melted monomer in high surface area droplets and boiling off the condensation by-product through the continuous suspending phase. New chemistries were developed to produce ionic functionality on polyester surfaces so exfoliated clays coatings are stable.

- Investigation of DuPont PETRETEC (polyester regeneration technology) plant revealed the source of a strong exciplex chromophore formed from recycled Mylar® X-ray films. Purifications of specific feedstocks enabled the manufacturing plant to double its capacity of recycled products with comparable physical and chemical properties to virgin materials.

- Exploratory research on lithium ion battery electrolytes for hybrid electric vehicles resulted in: new correlation between electrolyte solvent's electronic structure and redox stability; new speciation method for COSMO theory that accurately predicts temperature-dependent solubility of $LiPF_6$ and ionic conductivity; combined spectroscopic and quantum chemical calculation method that infers the

structure and composition of the solid-electrolyte interface that provided diagnostic information for improved electrolyte design.

- Exploratory research for the DuPont FluoroProducts business resulted in the identification of next generation refrigerants for automotive air conditioning that feature low global warming potential, low ozone depletion, low biological toxicity potential and low fire hazard potential. Theoretical COSMO methods were used to predict pure-component and mixture properties. COSMOdesign© was extended to predict molecules with requisite azeotropy.

- Scientific research in polymer-polymer inter-diffusion resulted in: the invention of the ATR-FTIR method and an established analysis method to infer the diffusion coefficient; validation of the method via successful agreement with prior SIMS and RBS literature data; the first measurements of polymer diffusion in semi-crystalline polymers and discovery of the associated non-Fickian kinetics; a novel model of diffusion in random, disordered media that reproduces the non-Fickian kinetics in semi-crystalline systems; a practical and quantitative diagnostic tool to help develop polymer welding and fusion-bonding resins.

- Mathematical modeling of the contemporary DuPont research & development project history in a product development pipeline was done to: examine common modes of project failure and success; balance the overall R&D portfolio with short- and long-term growth objectives; predict dynamic cyclicality in the portfolio; benchmark and test improving the overall rate of business growth against management processes and strategies; set appropriate expectations for growth with R&D budgetary resources. These results were communicated to the succession of Senior Vice President, Chief Science & Technology Officers as well as Directors in Central Research & Development. New work compares the relative merits of funding in-house discovery *versus* purchasing external intellectual property.

Visiting Scientist **Summer 1985**
Faculté de Pharmacie, Université de Paris-Sűd XI, France

- As a graduate student of Prof. N.A. Peppas in collaboration with Prof. A. Puisieux I synthesized hydrophilic, swelling-controlled release systems for several peptides and proteins, characterized polymer deformation and measured solute release kinetics.

Physical Scientist Aide **Summers 1980- 1983**
Chemistry Department, Naval Research Laboratory, Washington, D.C.

- I initiated and completed a fire-scaling and modeling project by starting theoretical analysis, designing and fabricating instrumentation; interfaced laser Doppler anemometer hardware to a minicomputer and wrote operating software in assembly and Fortran languages; arranged gas mixing and data-logging instrumentation; wrote software to reduce and analyze the data.

Undergraduate Research **1982-1983**
Chemistry Department, University of Virginia, Charlottesville, VA

- I designed and assembled a tunable, high-power pulse-NMR probe for measuring quadrupolar relaxations of deuterated proteins in phospholipid bilayers.

Visiting Scientist **1979**
Biochemistry Department, National Bureau of Standards, Gaithursburg, MD

- I performed and analyzed kinetic measurements of glycol fission by periodate oxidation using stopped-flow photometric spectrometry to elucidate the molecular mechanisms. This work was recognized in the top 300 finalists in the National Westinghouse Science Talent Search.

SYNERGISTIC ACTIVITIES

- Collaborative research with Dr. Ken Strawhecker, Army Research Laboratory, Aberdeen, MD focuses on the mesoscale structure of high performance, anti-ballistic fibers and the mechanism of fiber failure under tension. We jointly developed a novel *iso-locus* atomic force microscopy characterization method for monitoring changes in the mesoscale structure of fibers during dynamic extension. This method shows Kevlar® fibers deform very non-uniformly, with minute sections yielding with large deformations at characteristic defects while the fiber majority remains static. This provides clues how to increase fiber strength with improved manufacturing. Additional research is currently active.

- I was a principal investigator in a multidisciplinary, multi-institutional Cooperative Research And Development Agreement (CRADA) program to develop the high-performance, parallel-scalable software LAMMPS, Large-scale Atomic/Molecular Massively Parallel Simulator. This collaboration developed and implemented novel computational molecular dynamics methodologies to simulate large, complex chemical systems with realistic forcefields. The project was sponsored by the Department of Energy. The CRADA institutions included Sandia National Lab, Lawrence-Livermore National Lab, Cray Research, Bristol Myers Squibb and DuPont. The project is summarized and freely distributed at http://lammps.sandia.gov where the first version was released in 1999.

- I was a principal investigator in a multidisciplinary, multi-institutional CRADA program to develop the high-performance, parallel-scalable software MCCCS TOWHEE, Monte Carlo for Complex Chemical Systems, for modeling the thermodynamic properties of complex chemical systems. The project was sponsored by the Department of Energy. The CRADA institutions included Sandia National Lab, Ford, Air Products and DuPont. The project is summarized and freely distributed at http://towhee.sourceforge.net

- I was a principal investigator in a National Science Foundation Nanoscale Interdisciplinary Research Team grant “Solution-Based Dispersion, Sorting and Placement of Carbon Nanotubes”. The research provided new theoretical understanding and experimental techniques resolving the structure of single-stranded DNA wrapped around SWNTs and the manipulation of these hybrid materials to separate SWNTs according to chirality. The program in 2006-2008 involved investigators from DuPont, Lehigh University and Massachusetts Institute of Technology.

- As Somerset Lake Civic Association President (1995-1996) and Somerset Lake Service Corporation Director (1996-1997), I managed organizational operations, legal and transition issues of my 427-home neighborhood as the builder finished construction and homeowners took possession of common property and operation of the clubhouse and pool facilities. I initiated the neighborhood website www.somersetlake.org and the web-based functional software.

- In the New Garden Elementary School Parent-Teacher Organization I participated as an active Board Member (2001-2006) and served as President (2005-2006) managing organizational operations, fund-raising events, school benefit projects and multicultural, multidisciplinary supplementary educational programs for the elementary school students. I instituted and continued to organize the school's first science fair program for grades 1-5. This non-competitive program comprises a student or student team writing a proposal based on a scientific method outline, receiving individual review, giving a classroom oral project presentation and presenting the poster display during Open House. Since the 2000/2001 school year, the science fair is still held annually. Fundraising efforts achieved over $20,000 per year from within community resources.

- DuPont TechCon is an annual, week-long conference of typically 900-1,100 employees representing all global businesses and sites for the purposes of: innovating with customers, sharing advances in science and technology, networking and learning new initiatives from corporate leadership. I was the conference chairperson in 1996 and participated as a core organizer between 1994 and 2015. My responsibilities included: training the annual chairperson, conference financing, assisting program development, developing original web-based software to handle: dissemination of conference information, abstract submission, technical abstract reviews, registration, cost recovery as a credit card merchant, proceedings documentation and archiving technical information in the program.

- I was a Delaware certified Medical First Responder and participated in the Experimental Station Emergency Medical Team between 1995-2016.

HONORS AND AWARDS

- Fellow of the Royal Society of Chemistry (2023)
- Finalist Cahn Prize (2019)
- AIChE Industrial Research & Development Institute Award (2013)
- DuPont Central Research Accomplishment Awards (1997, 1998, 1999, 2000, 2001, 2002, 2013, 2014, 2015)
- DuPont TechCon Award (2011)
- DuPont Information Security Organization Accomplishment Award (2011)
- Pittsburgh Coal Conference Top Three Conference Innovations (2011)
- DuPont Crop Protection DevStars Award (2011, 2014)
- DuPont Polyester Leapfrog Technology Award (1992)
- DuPont Materials Science and Engineering Accomplishment Award (1993, 1995, 2005)
- Phi Lambda Upsilon (1986)
- Award in the Sigma Xi University-wide Student Research Competition (1985)
- Sigma Xi (1984)
- Plastics Institute of America National Fellowship (1984)
- Purdue University Fellowship (1983)
- Dean's List, University of Virginia (1979-1983), Purdue University (1984-1989)
- Special Achievement Award, Naval Research Laboratory (1981 ,1983)
- Certificate of Honors, University of Virginia (1981)
- Westinghouse Science Talent Search (Top 300 in nation in 1979)

PUBLICATIONS as of January 22, 2023
Google Scholar h-index: 31
Google Scholar i10 index: 48
Google Scholar Citations: 7,560

Names of students and trainees are underlined

Peer-Reviewed Journal Publications

1. A.M. Rahimi, **S.R. Lustig**, J.P. Bardhan, S. Jamali, "Drag reduction and the Vogel exponent of a flexible beam intransient shear flows" *Phys. Fluids*, 34, 104111 (2022) https://doi.org/10.1063/5.0106700
2. D. Rana, K. Lachmayr, **S.R. Lustig**, "A Review of Covetics– Current Understanding and Future Perspectives" *Nanoscale Advances*, **5**, 11-26 (2023) DOI: https://doi.org/10.1039/D2NA00500J
3. A.M. Rahimi, S. Jamali, J.P. Bardhan, **S.R. Lustig**, "Solvation Thermodynamics of Solutes in Water and Ionic Liquids Using the Multiscale Solvation-Layer Interface Condition Continuum Model", *J. Chem. Theory & Comput.*, **18**(9),5539-5558 (2022) DOI: https://doi.org/10.1021/acs.jctc.2c00248
4. **S.R. Lustig**, S.R., Allen, J.D. Londono, J. Lowery "Mechanistic Impact of Water on Polypyridobisimidazole (M5) Structure and Properties", *Polymer Int.*, 2021, 70(6), 795-802, DOI: https://doi.org/10.1002/pi.6194
5. **S.R. Lustig**, J.W. Andzelm, E.D. Wetzel "Highly Thermostable Dynamic Structures of Polyaramid Two-Dimensional Polymers" *Macromolecules*, **54**, 1291-1303 (2021) DOI: https://doi.org/10.1021/acs.macromol.0c01931
6. J.J.S. Biswakarma, D.A. Cruz, E.D. Bain, J.M. Dennis, J.W. Andzelm, **S.R. Lustig**, 2021, "Modeling Brittle Fractures in Epoxy Nanocomposites Using Extended Finite Element and Cohesive Zone Surface Methods" *Polymers*, 2021, 13(19), 3387. DOI: https://doi.org/10.3390/POLYM13193387
7. J. Xu, A.M. Scurto, M.B. Shiflett, **S.R. Lustig**, F.R. Hung, F.R. "Power Generation from Waste Heat: Ionic Liquid-Based Absorption Cycle versus Rankine Cycle" *AIChE J.*, **67**, e17038 (2020), DOI: https://doi.org/10.1002/aic.17038
8. **S.R. Lustig**, "Speciation in Electrolytes Using the COSMO-RS Solution Model" *Fluid Phase Equilibria*, **521**, 112717 (2020) DOI: https://doi.org/10.1016/j.fluid.2020.112717
9. **S.R. Lustig**, J.J.S. Biswakarma, D. Rana, S.H. Tilford, W. Hu, M. Su, M.S. Rosenblatt, "Effectiveness of Common Fabrics to Block Aqueous Aerosols of Virus-like Nanoparticles" *ACS Nano*, **14**(6), 7651–7658 (2020), DOI: https://doi.org/10.1021/acs.nanolett.0c04230
10. T.A. Stockdale, D.P. Cole, J.M. Staniszewski, M.R. Roenbeck, D. Papkov, **S.R. Lustig**, Y.A. Dzenis, K.E. Strawhecker "Hierarchical Mechanisms of Lateral Interactions in High- Performance Fibers" *ACS Appl. Mater. Interfaces*, **12**, 22256−22267 (2020), DOI: https://doi.org/10.1021/acsami.9b23459
11. M. Gao, R. Chang, D. Wang, Y. Li, L. Sun, **S.R. Lustig**, T.J. Webster, "Fructose- Enhanced Antibacterial Activity of Self-Assembled Nano-Peptide Amphiphiles for Treating Antibiotic-Resistant Bacteria" *Int. J. Nanomedicine*, **15**, 513-519 (2020), DOI: https://doi.org/10.2147/IJN.S200505
12. M.R. Roenbeck, J. Cline, V. Wu, M. Afshari, S. Kellner, P. Martin, J.D. Londono, L.E. Clinger, D. Reichert, **S.R. Lustig**, K.E. Strawhecker "Structure–property relationships of aramid fibers via X-ray scattering and atomic force microscopy" *J. Mater. Sci.*, **54**, 6668–6683 (2019) http://doi.org/10.1007/S10853-018-03282-X (April Finalist for the 2019 Cahn Prize)
13. M. Jennings, I. Kendrick, C. Green, **S. Lustig** "PEDOT:PSS-DVS Crosslinking Reaction Monitored via ATR-FTIR for Air Cathode Application in Microbial Fuel Cells", *Embark*, **2**, 4-8 (2018)
14. M.R. Roenbeck, E.J. Sandoz-Rosado, J. Cline, V. Wu, P. Moy, M. Afshari, D. Reichert, **S.R. Lustig**, K.E. Strawhecker, "Probing the internal structures of Kevlar® fibers and their impacts on mechanical performance", *Polymer*, **128**, 200-210 (2017).
15. M.B. Shiflett, B.A. Elliott, **S.R. Lustig**, S. Sabesan, M.S. Kelkar, A. Yokozeki, "Phase Behavior of CO2 in Room-Temperature Ionic Liquid 1-Ethyl-3-Ethylimidazolium Acetate" *Chem. Phys. Chem.*, **13**, 1806-1817 (2012).

16. L.M. Grieco, G.A. Halliday, C.P. Junk, **S.R. Lustig**, W.J. Marshall, V.A. Petrov, "Reactions of 1,1,2,2-tetrafluoroethyl-N,N-dimethylamine with linear and cyclic 1,3-diketones." *J. Fluorine Chem.*, **132**, 1198-1206 (2011).
17. R.H. French, V.A. Parsegian, R. Podgornik, R.F. Rajter, A. Jagota, J. Luo, D. Asthagiri, M.K. Chaudhury, Y.M. Chiang, S. Granick, S. Kalinin, M. Kardar, R. Kjellander, D.C. Langreth, J. Lewis, **S. Lustig**, D. Wesolowski, J.S. Wettlaufer, W.Y. Ching, M. Finnis, F. Houlihan, O.A. von Lilienfeld, C.J. van Oss, T. Zemb, "Long range interactions in nanoscale science" *Rev. Mod. Phys*., **82**, 0034-6861/2010/82 2 /1887 58 1887 (2010)
18. J.S. Meth, **S.R. Lustig**, "Polymer interphase structure near nanoscale inclusions: Comparison between random walk theory and experiment" *Polymer*, **51**, 4259-4266 (2010)
19. C. Gu, **S. Lustig**, C. Jackson, B.L. Trout, "Design of Surface-Active Soluble Peptide Molecules at the Air/Water Interface" *J. Phys. Chem. B*, **112**, 2970-2980 (2008).
20. V.A. Petrov, **S. Lustig**, W. Marshall, "Reactivity of fluorinated sulfur-containing heterocycles towards nucleophilic and oxidizing reagents" *J. Fluorine Chem.*, **128**, 1227-1234 (2007).
21. C. Gu, **S. Lustig**, B.L. Trout, "Solvation Model Based on Order Parameters and a Fast Sampling Method for the Calculation of the Solvation Free Energies of Peptides." *J. Phys. Chem. B*, **110**, 1476-1484 (2006)
22. G. Grigoryan, F. Zhou, **S.R. Lustig**, G. Ceder, D. Morgan, A.E. Keating, "Ultra-fast evaluation of protein energies directly from sequence." PLoS Computational Biology, **2**, 551-563 (2006)
23. F. Zhou, G. Grigoryan, **S.R. Lustig**, A.E. Keating, G. Ceder, D. Morgan, "Coarse-Graining Protein Energetics in Sequence Variables." *Phys. Rev. Lett*., **95**, 148103/1-148103/4 (2005)
24. **S.R. Lustig**, A. Jagota, C. Khripin, M. Zheng, "Theory of structure-based carbon nanotube separations by ion-exchange chromatography of DNA/CNT hybrids." *J. Phys. Chem. B*, **109**, 2559-2566. (2005)
25. R.A. Segalman, A. Jacobson, E.J. Kramer, **S.R. Lustig**, "Polymer diffusion in semicrystalline polymers using secondary ion mass spectroscopy." *Macromolecules*, **37**, 2613-2617 (2004).
26. M. Zheng, A. Jagota, E.D. Semke, B.A. Diner, R.S. McLean, **S.R. Lustig**, R.E. Richardson, N.G. Tassi, "DNA-assisted dispersion and separation of carbon nanotubes." *Nature Materials*, **2**, 338-342 (2003).
27. **S.R. Lustig**, E.D. Boyes, R.H. French, T.D. Gierke, M.A. Harmer, P.B. Hietpas, A. Jagota, R.S. McLean, G.P. Mitchell, G.B. Onoa, "Lithographically Cut Single-Walled Carbon Nanotubes: Controlling Length Distribution and Introducing End-Group Functionality." *Nano Letters,* **3**, 1007-1012 (2003).
28. S. Wang, E.S. Humphreys, S.Y. Chung, D.F. Delduco, **S.R. Lustig,** H. Wang, K.N. Parker, N.W. Rizzo, S. Subramoney, Y.M. Chiang, "Peptides with selective affinity for carbon nanotubes." *Nature Materials*, **2**, 196-200 (2003)
29. **S.R. Lustig,** G.J. Everlof and G.D. Jaycox, "Stimuli-Responsive Polymers. 5. Azobenzene modified polyaramides containing chiral binaphthyl linkages: tuning chiroptical behavior with light and heat." *Macromolecules,* **34**, 2364-2372 (2001).
30. R.R. Burch, **S.R. Lustig** and M. Spinu, "Synthesis of Cyclic Oligoesters and Their Rapid Polymerization to High Molecular Weight." *Macromolecules*, **33**, 5053-5064 (2000).
31. **S.R. Lustig,** "Peak-referenced integral method for size exclusion chromatography and its application to aromatic polyesters." *J. Chromatogr. A*., **839**, 1-14 (1999).
32. V.J. Rao, S.R. Uppili, D.R. Corbin, S. Schwarz, **S.R. Lustig** and V. Ramamurthy, "Facial Selective Photoreduction of Steroids: Role of Zeolites." *J. Am. Chem. Soc.*, **120**, 2480-2481 (1998).
33. S.R. Rastogi, N.J. Wagner and **S.R. Lustig**, "Rheology, self-diffusion and microstructure of charged colloids under simple shear by massively parallel nonequilibrium Brownian dynamics." *J. Chem. Phys.,* **104**, 9234-9248 (1996).
34. S.R. Rastogi, N.J. Wagner and **S.R. Lustig,** "Microstructure and rheology of polydisperse, charged suspensions," *J. Chem. Phys.,* **104**, 9249-9258 (1996).

35. **S.R. Lustig,** R.M. Shay and J.M. Caruthers, "Thermodynamic Constitutive Equations with Memory using a Material Time Scale," *J. Rheology*, **40**, 69-106 (1996).
36. **S.R. Lustig**, S.R. Rastogi and N.J. Wagner, "Telescoping the Fast Multipole Method using Chebyshev Economization," *J. Comput. Phys.*, **122**, 317-322 (1995).
37. J.G. Van Alsten, **S.R. Lustig** and B.S. Hsiao, "Polymer Diffusion in Semicrystalline Polymers. 2. Atactic Polystyrene-d Transport into Atactic and Isotactic Polystyrene," *Macromolecules*, **28**, 3672-3680 (1995).
38. R. Khare, M.E. Paulaitis and **S.R. Lustig,** "Generation of Glass Structures for Molecular Simulations of Polymers Containing Large Monomer Units: Application to Polystyrene," *Macromolecules,* **26**, 7203-7209 (1993)
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Disclosures

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CONFERENCE PROCEEDINGS
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Podiums

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26. **S.R. Lustig***, *Digital Presentation Tools* (Invited), TEXPO, Northeastern University, April 25, 2017.
27. **S.R. Lustig***, *Thermochemical Design* (Invited), Department of Chemical Engineering, University of Kansas, February 21, 2017.
28. **S.R. Lustig*,** A*dvancing the Understanding of Rigid Rod Polymers with Statistical Mechanics and Analytical Chemistry* (Invited), PittCon 2016, March 10, 2016
29. **S.R. Lustig*,** *Thermochemical Design for Chemical & Materials Engineering* (Invited), 2016 Annual AIChE Meeting, November 13, 2016.
30. **S.R. Lustig*,** A*dvancing the Understanding of Rigid Rod Polymers with Statistical Mechanics and Analytical Chemistry* (Invited), Army Research Laboratory, Aberdeen, MD, May 12, 2016
31. **S.R. Lustig*,** A*dvancing the Understanding of Rigid Rod Polymers with Statistical Mechanics and Analytical Chemistry* (Invited), U.S. Army Natick Soldier Systems Center, Natick, MA, October 26, 2016.

Posters

1. A. Murphy*, K.K. Lachmayr, D.C. McLeod, R.H. Lambeth, **S.R. Lustig**, *Synthesis of hexagonally pored, imine-linked two-dimensional covalent organic frameworks with amine functionalities for selective bioremediation applications*, ChE Research Showcase, Northeastern University, 2022
2. I. C. Taylor*, D. Rana, **S.R. Lustig**, *Engineering a Porous Conductive PEDOT:PSS Polymeric Scaffold for Bioelectric Fuel Cell Cathodes*, Paper 2524, Research Innovation Scholarship Entrepreneurship (RISE), Northeastern University, 2019
3. M. Galietti*, F. Gritti, M. Fogwill, **S.R. Lustig**, H*igh Throughput, Ultra-Fast, Turbulent SFC in Open Tubular Columns"* HPLC 2019, Milan, Italy, June 18, 2019
4. A.M. Rahimi*, **S.R. Lustig**, *Continuum Electrostatics of Bio-Membranes: Multiscale Modeling of Boundary Condition Using a Solvation-Layer Interface Condition (SLIC)*, Molecular Biophysics in the Northeast 2019, 9 November 2019
5. M. Jennings*, **S.R. Lustig**, *PEDOT:PSS-DVS Crosslinking Reaction Monitored via ATR-FTIR for Air Cathode Application in Microbial Fuel Cells*, Research Innovation Scholarship Entrepreneurship (RISE), Northeastern University, April 5, 2018

6. M. Gao*, T.J. Webster, **S.R. Lustig**, *Fructose-Enhanced Antibacterial Activity of Self-Assembled Nano Peptide Amphiphiles: A Combination of Computational Modeling and Experiments for Treating Antibiotic Resistant Orthopedic Implant Infection*, Research Innovation Scholarship Entrepreneurship (RISE), Northeastern University, April 5, 2018

GRANTS and RESEARCH SUPPORT

External Current Research Support

1. 2022 Army Research Laboratory, *Processing and Characterization of 2D Polymers for Extreme Environments.* PI $275,000 (100%)
2. 2022 Fount Bio. Sponsored Research Agreement. PI $700 (100%)
3. 2022 DuPont. *Expediting Next Generation Aramid Development & Advanced Antiballistic Performance with Collaborative Research & Development - Fee for Service*. PI $30,000 (100%)
4. 2022 KRI at Northeastern University, LLC. *Expeditionary Maneuver Support*. PI $50,000 (100%)
5. 2021 Genentech. *Analysis of the impact of mucus on drug precipitation*. Co-PI with Rebecca Carrier $100,000 (50%)

External Pending Research Support
None

Completed Research Support (incomplete draft still under construction)
1. 2021 DuPont. *Expediting Next Generation Aramid Development & Advanced Antiballistic Performance with Collaborative Research & Development - Fee for Service*. PI $98,000 (100%)
2. 2021 Oak Ridge National Lab, *Inelastic Neutron Scattering of Aluminum Graphide*, Beam time on L-16B VISION facility (100%)
3. 2020 Akastek. *Evaluation of Novel Mask Design for COVID PPE – Fee for Service.* PI $1,400 (100%)
4. 2020 DetraPel. *Evaluation of Novel Mask Design for COVID PPE – Fee for Service.* PI $3,030 (100%)
5. 2020 FXI. *Evaluation of Novel Mask Design for COVID PPE – Fee for Service.* PI $3,745 (100%)
6. 2020 Hygienics. *Evaluation of Novel Mask Design for COVID PPE – Fee for Service.* PI $550 (100%)
7. 2020 Provost Office Northeastern University. *Emergency COVID Program*, PI $20,000
8. 2017 NSF CBET Award 1604369. *Hybrid mixed-resolution solvation models,* Co-PI $179,998 (100%) https://www.nsf.gov/awardsearch/showAward?AWD_ID=1604369
9. 2019 DuPont. *Expediting Next Generation Aramid Development & Advanced Antiballistic Performance with Collaborative Research & Development - Fee for Service*. PI $90,000 (100%)
10. 2019 Army Research Laboratory, *Processing and Characterization of 2D Polymers for High Strength Applications,* PI $150,000 (100%)
11. 2019 Army Research Laboratory, *Multiscale Modeling of Epoxy Nanocomposites,* PI $60,000 (100%)

Research Support Not Funded

1. 2022 NIH. RFA-RM-22-020: *Advancing In Vivo Genome Engineering.* Co-I (Auguste, Hung, Auclair) $6,435,163 (10%)
2. 2022 Tier One. College of Engineering, Northeastern University, *Interpretable AI for mRNA Lipid Nanoparticle (LNP) Formulation and Delivery Process Mechanism Learning and Optimization*. Co-I (Wei, Amiji) $50,000

3. 2021 DOD. *Extreme Environment Measurement Platform of Crystallographic, RF, and Dielectric Properties for Research on the Advanced Manufacturing of Ceramics, Metallics, and Covetics* (Erb) $1,330,927
4. 2021 Welcome LEAP, *Intelligent Digital Twin for RNA-based Manufacturing*, (Wei) $7,009,690
5. 2020 Army Research Laboratory, *Ionic Liquid Compositions for Gas Phase Electromagnetic Interference Shielding*, $1,936,000
6. 2020 Army Research Laboratory, *High Strength 2D-Structured Metal-Carbon Covetic Materials*, $430,000
7. 2017, NSF MRI, *Acquisition of Anasys AFM-IR-MS System*, PI, $966,525
8. 2017, NSF CBET, *Collaborative Research: Advanced Absorption Cycle for Power Generation*, Co-PI (Hung, Shiflett, Scurto), $215,444
9. 2016, NSF CBET, *Collaborative Research: Developing Optimal Working Fluid Mixtures for Absorption Refrigeration Systems,* Co-PI (Hung, Shiflett, Scurto), $374,922

TEACHING and ADVISING

New Course Development

1. CHME 5699 *Special Topics in Chemical Engineering: Polymer Physics* (established 2022)
   Polymer Physics offers a graduate-level introduction to the quantitative principles relating macromolecular structure and properties. Statistical mechanics are applied using analytical theory and computational molecular modeling. Homework based on reading covers: single chain conformations, thermodynamics of mixing, polymer solutions, networks and gels, dynamics, thermoviscoelasticity, transport in polymer systems. The project enables students to specialize the course material to their interests.

2. CHME 7330 *Chemical Engineering Thermodynamics* (significantly revised 2021)
   CHME 7330 offers a graduate-level introduction to the fundamental principles relating molecular structure and bulk material properties. The class begins with classical thermodynamics laws that govern macroscopic conservation, equilibrium stability, and irreversible processes, including open processes, multicomponent phase equilibrium, and reaction equilibrium. The class introduces relationships between microscopic states and macroscopic properties, applied to understand systems such as non ideal fluids, crystalline solids, polymers, and electrolytes. Statistical thermodynamics concepts may also be applied using analytical theory and computational molecular modeling.

3. CHME 7260 *Introduction To Statistical Thermodynamics* (established 2017)
   This elective covers the introductory concepts used to predict molecular, bulk and mixture properties from molecular structure. Topics include: non-ideal solutions, high pressure systems, complex reaction equilibria, phase equilibria and molecular modeling. Student projects are self selected to focus on specific applications of individual interest. The material is appropriate for graduate and advanced undergraduate students who have taken classical thermodynamics in either an undergraduate chemical engineering course or similar content in a physical chemistry course.

4. CHME 5101 *Fundamentals of Chemical Engineering Analysis* (established 2017 with Goluch, Hung, West)
   Offers graduate students from undergraduate studies outside of traditional chemical engineering an opportunity to obtain a practical understanding of the core principles behind the chemical engineering discipline. Topics include vector and tensor calculus, continuum mechanics and thermodynamics, macroscopic and microscopic analyses of mass, momentum, and energy conservation; the fundamental principles of processes in which mass, energy, and momentum are transported; consequences of the Second Law of Thermodynamics, the principles governing phase and chemical

reaction equilibrium; the fundamental theories of chemical reaction kinetics and reactor design; and the mathematical formulation and solution of the underlying equations involved in all these topics.

Courses Taught

Semester	Number	Title	[w]Report/ Enroll	[x]Intellectually Challenging	[y]Instructor Effectiveness	[z]Student Learning
2022 Fall	CHEM 4991	Chemistry Undergraduate Research	0*/1	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)
2022 Fall	CHME 5699	Polymer Physics	0*/1	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)
2022 Fall	CHME 7330	Chemical Engineering Thermodynamics	32/32	4.6 (4.5,4.2)	3.6 (4.3,4.4)	3.8 (4.3,4.3)
2022 Spring	CHME 4991	ChE Undergraduate Research	0*/1	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a (n.a.,n.a.).
2022 Spring	CHME 7350	Transport Phenomena	37/39	4.7 (4.5,4.3)	4.0 (4.4,4.5)	4.0 (4.3,4.3)
2021 Fall	CHME 4991	ChE Undergraduate Research	0*/1	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)
2021 Fall	CHME 7330	Chemical Engineering Thermodynamics	33/34	4.7 (4.5,4.2)	3.9 (4.2,4.4)	4.0 (4.2,4.3)
2021 Spring	CHME 7330	Chemical Engineering Thermodynamics	12/20	4.6 (4.5,4.3)	3.5 (4.5,4.5)	3.8 (4.5,4.4)
2020 Fall	CHME 7330	Chemical Engineering Thermodynamics	20/22	4.8 (4.5,4.2)	4.4 (4.5,4.4)	4.4 (4.5,4.3)
2020 Spring	CHME 4703	Process Design	1/3	4.0 (4.4,4.3)	5.0 (4.6,4.5)	4.0 (4.2,4.1)
2019 Fall	CHME 7330	Chemical Engineering Thermodynamics	29/34	4.6 (4.2,4.1)	4.4 (4.4,4.4)	4.4 (4.3,4.3)
2019 Fall	CHME 5101	Fundamentals of Chemical Engineering Analysis	10/19	4.2 (4.2,4.1)	4.5 (4.4,4.4)	4.2 (4.3,4.3)
2019 Spring	CHME 7235	Introduction to Statistical Thermodynamics	9/10	4.6 (4.1,4.1)	4.3 (4.3,4.4)	4.3 (4.3,4.3)
2019 Spring	CHME 7350	Transport Phenomena	35/37	4.4 (4.1,4.1)	4.1 (4.3,4.4)	4.1 (4.3,4.3)
2018 Fall	CHME 7330	Chemical Engineering Thermodynamics	17/33	4.3 (4.2,4.1)	4.5 (4.3,4.4)	4.3 (4.3,4.3)
2018 Fall	CHME 5101	Fundamentals of Chemical Engineering Analysis	13/20	4.1 (4.2,4.1)	4.7 (4.3,4.4)	4.6 (4.3,4.3)
2018 Spring	CHME 7260	Introduction to Statistical Thermodynamics	7/7	4.3 (4.0,4.1)	4.6 (4.0,4.4)	4.4 (4.1,4.3)
2018 Spring	CHME 7350	Transport Phenomena	75/78	4.6 (4.0,4.1)	4.1 (4.0,4.4)	4.1 (4.1,4.3)
2017 Fall	CHME 5101	Fundamentals of Chemical Engineering Analysis	0*/17	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)
2017 Fall	CHME 7330	Chemical Engineering Thermodynamics	15/17	4.7 (4.1,4.1)	3.0 (4.1,4.1)	3.5 (4.3,4.2)
2017 Spring	CHME 7260	Introduction to Statistical Thermodynamics	0*/4	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)	n.a. (n.a.,n.a.)
2017 Spring	CHME 7350	Transport Phenomena	58/58	4.4 (4.1,4.1)	3.6 (4.2,4.4)	3.9 (4.2,4.2)
2016 Fall	CHME 2311-1	Lab for CHME 2310	10/19	4.3 (4.1,4.1)	4.1 (4.3,4.3)	4.1 (4.2,4.2)
2016 Fall	CHME 2311-2	Lab for CHME 2310	10/18	3.8 (4.1,4.1)	3.5 (4.3,4.3)	4.2 (4.2,4.2)

[w] Number of reponses to teaching evaluation survey, and total number enrolled in the class
[x] "I found this course intellectually challenging." Strongly agree = 5, Agree = 4, Neutral = 3, Disagree = 2, Strongly disagree = 1
[y] "What is your overall rating of this instructor's teaching effectiveness?" Almost always effective = 5, Usually Effective = 4, Sometimes Effective = 3, Rarely Effective = 2, Never Effective = 1
[z] "I learned a lot in this course." Strongly agree = 5, Agree = 4, Neutral = 3, Disagree = 2, Strongly disagree = 1
Numbers in parentheses show ChE department and university mean scores for that semester
n.a. indicates data not collected by NU Office of the Registrar
0* indicates data not collected by NU Office of the Registrar

Postdoctoral Supervision
(Period, Name, Status, Institution, *Project title*, Current position)

2021-2022 Kätchen Lachmayr — Senior Research Associate, Northeastern University
Novel Hexavalent Monomers and their Two-Dimensional Polymers
Current position: Chemours

2020-2021 Ali Mehdizadeh Rahimi — Post-doctoral Fellow , Northeastern University
Solvation Thermodynamics of Two-Dimensional Polymers
Current position: 6 River Systems

Graduate Supervision
(Period, Name, Status, Institution, *Project title*, Current position, Coadvisor where applicable)

2022- Emma Egli — Doctoral Student, Northeastern University
Macromolecular Orientation and Dynamics of Rigid-Rod Liquid Crystal Polymers

2022- Victus Korduwu — Doctoral Student, Northeastern University
Thermodynamics of Bioactive Molecules in Intestinal Mucus
Co-advised with Rebecca Carrier, ChE

2019- John Biswakarma — Doctoral Student, Northeastern University
Polymerization and Processing Two-Dimensional Polymer Films

2018- Devyesh Rana — Industrial Doctoral Candidate, Northeastern University
Understanding Aluminum Graphide: From Theory to Synthesis
Current position: DELO Industrial Adhesives

2017- Michael Ploch — Doctoral Candidate, Northeastern University
Microstructural Deformation of Aramid Fibers in Response to Ballistic Impact

2017- Artem Isakov — Industrial Doctoral Student, Northeastern University
Molecular Orientation and Continuum Dynamics in a Periodic Extensional Flow Reactor
Current position: Gentuity

2016-2020 Ali Mehdizadeh Rahimi — Ph.D. Northeastern University

SLIC (Solvation-Layer Interface Condition) - Multiscale Modeling of Boundary Condition in Biomolecular Electrostatics

Co-advised with Safa Jamali, MIE
Current position: 6 River Systems

2017-2021 Ming Gao Ph.D. Northeastern University
Three Strategies to Treat Antibiotic Resistant Bacterial Infections: Self-assembled Nano-peptide Amphiphiles, Selenium Nanorods, and Cold Atmospheric Plasma
Co-advised with Thomas Webster, ChE
Current position: Metagenomi

2019-2021 Michael Galietti M.S. Northeastern University
Turbulent Supercritical Fluid Chromatography in Open Tubular Columns
Current position: Day Zero Diagnostics

Graduate Thesis Committee Memberships (2022)
(Period, Name, Status, Institution, *Project title*, Advisor)

2020- Yujia Wang Doctoral Candidate, Northeastern University
Investigation of Crystal Growth from Liquid and Vapor Phases, and Applications
Swastik Kar

2020- Barrett Smith Doctoral Candidate, Northeastern University
Gelation in Confined Flows
Sara Hashmi

2020- Sevy Harris Doctoral Candidate, Northeastern University
Automatic Kinetic Monte Carlo Simulations for Heterogeneous Catalysis
Richard West

2016-2020 David Medina Cruz Ph.D., Northeastern University
Microbial Nano-Biofactories: A Nanometric Trojan Horse With Biomedical Applications
Sidi Bencherif

2016-2021 Emily Mazeau Ph.D., Northeastern University
Ongoing Developments in Automatic Generation of Microkinetic Models for Heterogeneous Catalysis using RMG
Richard West

2016-2021 Sai Krishna Sirumalla Ph.D., Northeastern University
Graph neural networks and high throughput quantum chemistry workflows for detailed kinetic modeling
Richard West

2016-2018 Yan Shen Ph.D., Northeastern University
Molecular Simulation Of Ionic Liquids And Deep Eutectic Solvents In The Bulk, Near Surfaces And Inside Nanopores
Francisco Hung

2021- Christopher Blais Doctoral Candidate, Northeastern University

Automatically Generating Catalytic Mechanisms for Alloys and Arbitrary Surface Facets

Richard West

2021-2022 Matthew Kim Ph.D., Northeastern University
Low-cost MnO_2 intercalation cathodes enabled by using bismuth as a pillaring agent
Joshua Gallaway

2021 Ting-Chen Lee M.S., Northeastern University
Application Of Reaction Mechanism Generator (RMG) For Modeling Heterogeneous Ammonia Oxidation
Richard West

2018-2020 Nathan Harms Ph.D., Northeastern University
Improving detailed kinetic models through automated transition state theory calculations
Richard West

2018-2020 Anh Phong Tran Ph.D., Northeastern University
Decision making by heterogeneous cell populations: immune-tumor interactions under metronomic chemotherapy and distributed computation in synthetic biology
Eduardo Sontag

2020 Chinaza Joy Okpechi M.S., Northeastern University
Silk Gelation Study
Gordon Institute for Engineering Leadership

2020 Jordan Rubio M.S., Northeastern University
Optimization of Electrode Formulation for Use in High Energy Battery Chemistries
Gordon Institute for Engineering Leadership

2019 Angela Isibor M.S., Northeastern University
Quantitative Analysis & Performance Improvement of Vapor Deposited Polymer Coatings on Inorganic surfaces
Gordon Institute for Engineering Leadership

2019 Justin Crisafulli M.S., Northeastern University
Increasing the Speed to Market for Neurological Therapeutics by Evaluating the Chromatographic Separations
Gordon Institute for Engineering Leadership

2018-2019 Rubaiyet Abedin Ph.D. Northeastern University
Computational Studies Of Mixtures Of Refrigerants, Ionic Liquids And Deep Eutectic Solvents For Absorption Refrigeration Systems And Absorption Power Cycle
Francisco Hung

2018-2019 Arthur Gonzales Ph.D. Northeastern University
Multiscale Molecular Modeling Of Rosette Nanotubes
Hicham Fenniri

2018-2019 Bohan Zhang Ph.D. Northeastern University

Preparation of nanoparticles by green synthesis and a study on their antibacterial and anticancer properties

Thomas Webster

2008-2012 Russell Burnett Ph.D. University of Delaware
Predicting liquid-phase thermodynamic properties using COSMO-SAC
Stanley Sandler

1999-2003 Jan Boshoff Ph.D. University of Delaware
Configurational Diffusion in Glassy, Amorphous Polymers: Effects of Polymer Structure and Dynamics on Permeation via Molecular Simulation
Norman Wagner

1991-1996 Sanjeev Rastogi Ph.D. University of Delaware
Nonequilibrium Brownian Dynamics of Colloidal Suspensions
Advisor: Norman Wagner

1991-1994 Rajesh Khare Ph.D. University of Delaware
Molecular simulations of phenyl ring flip motion in polystyrene
Michael Paulaitis

Undergraduate Research Supervision
(Period, Name, Institution, *Project title*)

2023 Kanishk Jain, Christopher Ramirez, Katharine Dixon, Kenji Goto-Hardy, David O'Leary ChE, Northeastern University
Capstone: Low Lifetime Cost Ionic Liquid Solvents for Carbon Capture

2023 Grace O'Dwyer, Matthew Goffin, Rachel Joseph, Andrew Carr ChE, Northeastern University
Capstone: Ionic Liquid Absorbents for Carbon Capture

2023- Daniel DeLong ChE, Northeastern University
Carbon Capture using Novel Ionic Liquids

2022-2023 Matthew O'Rourke MIE, Northeastern University
Rheo-Raman of Liquid Crystalline Polymer Solutions

2022 Paris Charbonneau ChE, Northeastern University
Honors Early Research Award: Nanoscale Mechanics of Anti-Ballistic Armors

2021-2022 Kara Lui MIE, Northeastern University
Honors Early Research Award: Mechanochemistry of 2D polymerization

2021-2022 Richard Osgood ChE, Northeastern University
Honors Early Research Award: Nanoscale Mechanics of Anti-Ballistic Armors

2021-2022 Chaitanya Peety ChE, Northeastern University
Honors Early Research Award: Nanoscale Mechanics of Anti-Ballistic Armors

2021-2022	Ani Parekh *Synthesis of Novel Monomers for 2D Graphitic Polymers*	Chem, Northeastern University
2021-2022	Audrey Murphy *Synthesis of Novel Monomers for 2D Graphitic Polymers*	Chem, Northeastern University
2022	Tanishka Kucheria *Kinetics of 2D Polymerizations*	ChE, Northeastern University
2022-	Neil Dungca *Undergraduate Program for Leaders In Future Transformation (UPLIFT) Research, Center for STEM Education: 2D Polymers*	ChE, Northeastern University
2020-2021	Olivia Taylor, Jeffrey Yao, Katherine Spengler, Avi Natan *Capstone: Ferroelectric Polymers for Solid State Refrigeration*	ChE, Northeastern University
2020-2021	Shreyas Ravichandar *Undergraduate Program for Leaders In Future Transformation (UPLIFT) Research, Center for STEM Education 2D Polymerization*	ChE, Northeastern University
2020-2021	Max Gildemeister *Two Dimensional Polymerization Kinetics*	ChE, Northeastern University
2020-2021	Taryn Sparacino *Two Dimensional Polymerization Kinetics*	ChE, Northeastern University
2020-2021	Sarah Benson *Artificial Antibiotics*	ChE, Northeastern University
2018-2021	Isabella Barber *Biomolecular Air Cathodes*	ChE, Northeastern University
2018-2021	Emily DiPietro *Rheo-Raman Molecular Dynamics*	ChE, Northeastern University
2018-2021	Liam Gordon *Biomolecular Air Cathodes*	ChE, Northeastern University
2018-2021	Eduardo Semidey *Biomolecular Air Cathodes*	ChE, Northeastern University
2019-2021	Ana Sobrino *Honors Early Research Award: Biomolecular Air Cathodes*	ChE, Northeastern University
2019-2021	Landon Wade *Rheo-Raman Molecular Dynamics*	ChE, Northeastern University
2021	Evan Otash *Honors Early Research Award: Nanoscale Mechanics in Antiballistic Materials*	ChE, Northeastern University

2021	Theodore Walinskas *Honors Early Research Award: Nanoscale Mechanics in Antiballistic Materials*	ChE, Northeastern University
2021	James Smalley *Nanoscale Mechanics in Antiballistic Materials*	ChE, Northeastern University
2021	Adam Switeck *Chemical Synthesis of Novel Monomers for 2D Polymers*	Chem, Northeastern University
2018-2019	Olivia Taylor *Computational Rheology*	ChE, Northeastern University
2018-2019	Alexis Dubbs *Computational Rheology*	ChE, Northeastern University
2018-2019	Christian Albertelli, Matt Honeyman,Ashley Dodge, Andy He, Theodore Rausch, *Capstone: Polyaramid 3-D Printing*	MIE, Northeastern University
2019	Angela Cuff *Polyaramid Fiber Mechanics*	ChE, Northeastern University
2019	Audrey Froelich *Polyaramid Fiber Mechanics*	ChE, Northeastern University
2019	Ahmed Al Hosani, Lauren Burke, Musa Mustafayev, Frankie Wai, Tim Orth *Capstone: Polymers for Solid State Refrigeration*	ChE, Northeastern University
2019	Joshua Lee, Mina Dolay, Emma Burke, Jake Tomlinson, Sam Zakrzewski *Capstone: Poly(lactic acid) from Potato Peels*	ChE, Northeastern University
2017	Maria Jennings *Development of Crosslinkable, Electrically-Conducting Hydrogels for Microbial Fuel Cell Air Cathods*	ChE, Northeastern University

Undergraduate Advising Activities

- Academic advisor for *ca.* 20-30 students each semester since 2016, as part of the Department of Chemical Engineering undergraduate advising program, meeting with advisees at least once per year with occasional follow-up as necessary
- Participated in *Chemeunity* lunches to help first year undergraduates become familiar with the Department of Chemical Engineering and opportunities at Northeastern University

SERVICE and PROFESSIONAL DEVELOPMENT

Service to the Department of Chemical Engineering

- Associate Chair for Research (2019-2022)

- Faculty Search Committee co-chair (2016-2022)
- Graduate Committee (2017- present)
- Awards Committee (2022- present)
- Lab Ops and Safety Manager Search Committee (2022)
- Formal mentoring to three diverse, junior faculty includes meeting regularly to share perspectives on research proposal writing, teaching techniques, student advising, research lab infrastructure, professional engagements, awards, and work-life balance.
- Graduate Candidate Day (2017, 2018, 2020)
- Tenure and Promotion Committee (2017-2019)

Service to the College of Engineering

- Graduation Ceremony Marshal (2017, 2018, 2019, 2022)
- Research Advisory Committee (2019-2022)
    - I initiated an effort to improve campus mail delivery effectiveness during COVID, participated in Tier One proposal reviews, and participated in the COE COVID-19 Research Coordination Task Force to help faculty perform on research programs during the pandemic (2020).
    - I proposed and composed the Shared Space Policy, which was adopted as a novel addition to the COE Space Policy (2020).
    - I brokered donations of industrial incubators, refrigerators, and freezers from Takeda, that were ultimately used for NU COVID testing and vaccination facilities as well as other research laboratories on campus. I pioneered a new process to monetize unwanted equipment through consignment sales using Cambridge Scientific Instruments. (2021)
    - I lead a task force appointed by the Senior Associate Dean for Research and Graduate Education to identify all barriers to research in the College of Engineering. Our survey received a 71% response rate from tenture/tenure-track faculty and a 53% total response rate across all researchers. Our analyses determined systematic barriers in proposal development, award management, producing impactful outcomes, funding opportunities, personnel management, and other classifications. We developed actionable recommendations to the College of Engineering Executive Committee how to reduce the systematic research barriers, specifically in new programming, modified policies, and support improvement. While the college research development team has already implemented several recommedations, others recommendations are being adopted across the university. (2021-2022)
- I sought and brokered donation of a NanoIR2 (atomic force microscope with in-situ vibrational spectroscopy at probe tip) from Schlumberger and installed the instrument in the Kostas Nanoscale Technology and Manufacturing Research Center as a shared resource. (2021)

Service to the University

- Research Policy Oversight Committee for Faculty Senate (2019-2022)
  I investigated the effectiveness and efficiency of NU-RES operations. I examined issues with shared research space within the University. I drafted the resolution that was passed unanimously by the Faculty Senate that encourages the Provost Office to work with college deans to require shared space charters in all instances of shared space within the University.
- Research Computing Advisory Council (2017-present)
  As a member appointed by the dean for the College of Engineering, I assisted the hiring of new leadership and formulation of new policies involving the use of the MGHPCC.
- Faculty Advisor to Gordon Institute of Engineering Leadership (2019-present)

- Co-host/moderator to "NU Saving Lives: COVID-19 Idea Exchange – Critical Care Devices and Personal Protective Equipment" sponsored by Office of Provost for Research Development, 17 April 2020

Service to the Discipline

- AIChE Institute Awards Committee Chair (2023-2026)
- AIChE Annual Meeting Area 8a Session Chair *Transport Phenomena in Polymers* (2020-2023)
- ACS Northeast Regional Meeting (NERM) 2023 Treasurer
- Editorial Board MDPI Journal: Thermo (https://www.mdpi.com/journal/thermo)
- Covetics Workshop, Organizer, Northeastern University, November 18-19, 2019
- Safety inspector, competition judge at the Northeast Regional Chem-E-Car Competition at Worcester Polytechnic Institute March 26, 2017
- AIChE Awards Committee, 2017-2020

Service to the Broader Community

- Which is the best COVID-19 mask? Northeastern Global News (https://news.northeastern.edu/2021/12/23/best-covid-mask/)
- How to make a homemade mask that is as good as an N95, India New England News, (https://indianewengland.com/how-to-make-a-homemade-mask-that-is-as-good-as-an-n95/)
- Not All Masks Are Created Equal (https://silverarch.io/blog/not-all-masks-are-created-equal)
- What makes for the best COVID-19 mask? (https://medicalxpress.com/news/2021-12-covid-mask.html) (2021)
- Top Performers Among Common Fabrics Tested to Block Virus-Like Particles (https://www.sciencenewsservice.com/particles) (2020)
- Omicron update: Best mask to reduce your risk of a COVID-19 infection – experts weigh in (https://www.express.co.uk/life-style/health/1542353/Omicron-update-face-mask-n95-fit-filtration-function-covid-19) (2020)
- R.M. Bliss, "Common Fabrics Tested to Block Virus-Like Particles", Science News Service, 4 June 2020
- Here's what could make your homemade mask work as well as an N95 (https://news.northeastern.edu/2020/07/08/what-goes-into-a-homemade-mask-that-can-stop-the-coronavirus) (2020)
- Interview on the importance of wearing masks during COVID pandemic https://fb.watch/1-7YMhiuUn/ , see clip at time 16:39 (2020)
- Vision Amazonica para la Sostenibilidad Integral (VASI) on the identification of common fabrics that can effectively protect peoples in the Brazilian Amazon and Ecuador against COVID transmission (2020)
- USDA, Food Safety and Inspection Service, Consulted on the use of safe alternatives to N95 masks during food inspections (2020)

Select Journal Paper and Book Reviews

- ACS Applied Materials & Interfaces
- ACS Applied Nano Materials
- ACS Nano
- Advanced Materials
- Advanced Science

- Cambridge University Press
- Fluid Phase Equilibria
- Global Challenges
- Industrial & Chemical Engineering Research
- Interface Focus
- Journal of Molecular Liquids
- Langmuir
- Macromolecules
- Nano Letters

Ad Hoc Reviewer

- NSF CBET Review Panelist
- NSF Science and Technology Centers Panelist
- Army Research Office (ARO) Review Panelist

Professional Development

- *Runway to Broader Impacts Peer Learning Community* (2022-2023) Research Development Office, Northeastern University
- *Establishing a Research Program in STEM* (2022) ADVANCE Office Faculty Development workshop, Northeastern University
- *Transforming Teaching with Microsoft Teams Community of Practice* (Fall 2022) Center for Advancing Teaching and Learning Through Research (CATLR), Northeastern University
- *National Research Mentoring Network*, Mentor Training Workshop, 1 Feb 2019
- *Exploring SAIL: A Full-Day Immersion Experience*, Self-Authored Integrated Learning, April 11, 2018, Center for Advancing Teaching and Learning Through Research (CATLR), Northeastern University