Thomas E. Gartner III

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ACADEMIC AND PROFESSIONAL APPOINTMENTS

Assistant Professor, Lehigh University, Bethlehem, PA (08/2023 - Present)
Department of Chemical & Biomolecular Engineering

Assistant Professor, Georgia Institute of Technology, Atlanta, GA (01/2022 - 07/2023)
School of Chemical & Biomolecular Engineering

Postdoctoral Research Associate, Princeton University, Princeton, NJ (08/2019 - 12/2021)
Chemistry in Solution and at Interfaces (CSI) Center, Department of Chemistry
Advisors: Pablo Debenedetti, Athanassios Panagiotopoulos, Roberto Car, Salvatore Torquato

Graduate Student Researcher, University of Delaware, Newark, DE (08/2014 - 07/2019)
Department of Chemical & Biomolecular Engineering
Advisor: Arthi Jayaraman

Process Engineer, Applied Materials, Inc., Sunnyvale, CA (06/2011 - 07/2014)
Chemical-Mechanical Planarization (CMP) Division

EDUCATION

University of Delaware (08/2014 - 07/2019)
Ph.D. in Chemical & Biomolecular Engineering GPA: 4.0/4.0

University of California, Berkeley (08/2007 - 05/2011)
Bachelor of Science with Honors in Chemical & Biomolecular Engineering GPA: 3.71/4.0

SELECT HONORS AND AWARDS

Woody Faculty Fellow 2022-2023
Georgia Tech School of Chemical & Biomolecular Engineering

DARPA Riser 2022
DARPA Forward Conference Series

Finalist, APS Division of Polymer Physics Frank J. Padden Jr. Award 2019
APS March Meeting 2019

1st Place, AIChE Area 8A Excellence in Graduate Polymer Research Symposium 2018
AIChE 2018 Annual Meeting

Fraser and Shirley Russell Teaching Fellowship 2018
University of Delaware Department of Chemical & Biomolecular Engineering

1st Place, AIChE MESD Graduate Student Poster Competition 2017
AIChE 2017 Annual Meeting

Honorable Mention 2015
NSF Graduate Research Fellowship Program

Paul H. Schipper Fellowship 2015
University of Delaware Department of Chemical & Biomolecular Engineering

Robert L. Pigford Fellowship 2014
University of Delaware Department of Chemical & Biomolecular Engineering

President's Quality Award 2012
Applied Materials, Inc.

PUBLICATIONS AND PATENTS

1. P.M. Piaggi,* **T.E. Gartner, III**,* R. Car, P.G. Debenedetti, "Melting curves of ice polymorphs in the vicinity of the liquid-liquid critical point," arXiv:2302.08540 **[cond-mat.stat-mech]**; **Equal contributions*
2. **T.E. Gartner, III**, P.M. Piaggi, R. Car, A.Z. Panagiotopoulos, P.G. Debenedetti, "Liquid-liquid transition in water from first principles,"*** Phys. Rev. Lett.,* **2022**, *129*, 255702; ***featured as a PRL Editors' Suggestion; link to feature article in Physics magazine about this work*
3. **T.E. Gartner, III**, K.M. Hunter, E. Lambros, A. Caruso, M. Riera, G.R. Medders, A.Z. Panagiotopoulos, P.G. Debenedetti, F. Paesani, "The Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model," *J. Phys. Chem. Lett.,* **2022**, *13*, 3652-3658
4. **T.E. Gartner, III**, "Linking amorphous ice and supercooled liquid water," *Proc. Natl. Acad. Sci. U.S.A.,* **2021,** 118 (34), e2112191118
5. **T.E. Gartner, III**, S. Torquato, R. Car, P.G. Debenedetti, "Manifestations of metastable criticality in the long-range structure of model water glasses," *Nat. Commun.*, **2021**, *12*, 3398
6. M. Muniz,* **T.E. Gartner, III**,* M. Riera, C. Knight, S. Yue, F. Paesani, A.Z. Panagiotopoulos, "Vapor-liquid equilibrium of water with the MB-pol many-body potential,"*** J. Chem. Phys.*, **2021**, *154*, 211103; **Equal contributions; **featured in AIP Scilights*
7. **T.E. Gartner, III**, L. Zhang, P.M. Piaggi, R. Car, A.Z. Panagiotopoulos, P.G. Debenedetti, "Signatures of a liquid-liquid transition in an *ab initio* deep neural network model for water," *Proc. Natl. Acad. Sci. U.S.A.,* **2020,** *117* (42), 26040-26046
8. **T.E. Gartner, III**,* C.M. Heil,* A. Jayaraman, "Surface composition and ordering of binary nanoparticle mixtures in spherical confinement," *Mol. Syst. Des. Eng.*, **2020,** *5*, 864-875; **Equal contributions*
9. M. Xiao,* Z. Hu,* **T.E. Gartner, III**,* X. Yang, W. Li, A. Jayaraman, N.C. Gianneschi, M.D. Shawkey, A. Dhinojwala, "Experimental and theoretical evidence for molecular forces driving surface segregation in photonic colloidal assemblies," *Sci. Adv.,* **2019**, *5*, eaax1254; **Equal contributions*
10. H. Kuang, **T.E. Gartner, III**, M.D. de Mello, J. Guo, X. Zuo, M. Tsapatsis, A. Jayaraman, E. Kokkoli, "ssDNA-amphiphile architecture used to control dimensions of DNA nanotubes," *Nanoscale,* **2019**, *11* (42), 19850-19861
11. **T.E. Gartner, III**, F.M. Haque, A.M. Gomi, S.M. Grayson, M.J.A. Hore, A. Jayaraman, "Scaling exponent and effective interactions in linear and cyclic polymer solutions: theory, simulations, and experiments," *Macromolecules,* **2019**, *52* (12), 4579-4589
12. **T.E. Gartner, III**, A. Jayaraman, "Modeling and Simulations of Polymers: A Roadmap,"*** Macromolecules,* **2019**, *52* (3), 755-786; ***Journal cover article, featured in ACS Editors' Choice, journal's #1 most-read article in Nov. 2019-Sept. 2021*
13. T.B. Martin, **T.E. Gartner, III**, R.L. Jones, C.R. Snyder, A. Jayaraman, "Design and implementation of *py*PRISM: a polymer liquid-state theory framework," *Proc. of the 17th Python in Science Conf. (SCIPY 2018)*, **2018**, 129-136
14. T.B. Martin, **T.E. Gartner, III**, R.L. Jones, C.R. Snyder, A. Jayaraman, "*py*PRISM: a computational tool for liquid-state theory calculations of macromolecular materials," *Macromolecules,* **2018**, *51* (8), 2906-2922
15. **T.E. Gartner, III**, A. Jayaraman, "Macromolecular 'size' and 'hardness' drives structure in solvent-swollen blends of linear, cyclic, and star polymers," *Soft Matter,* **2018**, *14*, 411-423
16. **T.E. Gartner, III**,* M.A. Morris,* C.K. Shelton,* J.A. Dura, T.H. Epps, III, "Quantifying lithium salt and polymer density distributions in nanostructured ion-conducting block polymers," *Macromolecules,* **2018**, *51* (5), 1917-1926; **Equal contributions*

17. **T.E. Gartner, III**, T. Kubo, Y. Seo, M. Tansky, L.M. Hall, B.S. Sumerlin, T.H. Epps, III, "Domain spacing and composition profile behavior in salt-doped cyclic vs linear block polymer thin films: a joint experimental and simulation study," *Macromolecules,* **2017**, *50* (18), 7169-7176
18. M.A. Morris,* **T.E. Gartner, III**,* T.H. Epps, III, "Tuning block polymer structure, properties, and processability for the design of efficient nanostructured materials systems,"** *Macromol. Chem. Phys.,* **2017**, *218* (5), 1600513; **Equal contributions; **Journal cover article, in journal's top-20 most-read articles 2016-2018*
19. **T.E. Gartner, III**, T.H. Epps, III, A. Jayaraman, "Leveraging Gibbs ensemble molecular dynamics and hybrid Monte Carlo/molecular dynamics for efficient study of phase equilibria," *J. Chem. Theory Comput.,* **2016**, *12* (11), 5501-5510
20. V.V. Hardikar, Z. Wang, D.M. Gage, **T.E. Gartner, III**. Chemical mechanical polishing process and slurry containing silicon nanoparticles. United States Patent Application No. US 14/143,262. **2013**, Dec 30.
21. H. Wu, H. Pan, M.A. Green, D. Dietderich, **T.E. Gartner, III**, H.C. Higley, M. Mentink, D.G. Tam, F.Y. Xu, F. Trillaud, X.K. Liu, L. Wang, and S.X. Zheng, "The resistance and strength of soft solder splices between conductors in MICE coils," *IEEE Trans. Applied Superconductivity*, **2011**, *21* (3), 1738-1741

INVITED PRESENTATIONS

1. **T.E. Gartner, III**, Simulation and theory approaches toward thermodynamic and structural understanding of polymer solutions of varying architecture, (Invited talk) ACS Southwest Regional Meeting 2022
2. **T.E. Gartner, III**, Machine learning-enhanced molecular simulations for molecules and materials, (Invited talk) Lehigh University ChBE Department Seminar 2022
3. **T.E. Gartner, III**, M.J.A. Hore, A. Jayaraman, Solvent quality and polymer concentration effects in linear and cyclic polymer solutions, (Invited award talk) APS March Meeting 2019
4. **T.E. Gartner, III**, A. Jayaraman, Understanding the interplay between polymer architecture and solvent quality through coarse-grained molecular simulation and liquid state theory, (Invited award talk) AIChE Annual Meeting 2018

CONTRIBUTED PRESENTATIONS

1. Z. Feng, **T.E. Gartner, III**, Development of a machine learning-based closure relation for polymer integral equation theory, (Poster) APS March Meeting 2023
2. S. Kumari, **T.E. Gartner, III**, Developing machine learning interaction potentials for polyolefins, (Poster) APS March Meeting 2023
3. **T.E. Gartner, III**, P.M. Piaggi, R. Car, A.Z. Panagiotopoulos, P.G. Debenedetti, Properties and Phase Behavior of Supercooled Water from First Principles, (Talk) AIChE Annual Meeting 2021
4. **T.E. Gartner, III**, L. Zhang, P.M. Piaggi, R. Car, A.Z. Panagiotopoulos, P.G. Debenedetti, First principles simulations of the liquid-liquid transition in water using deep neural networks, (Talk) APS March Meeting 2021
5. **T.E. Gartner, III**, S. Torquato, R. Car, P.G. Debenedetti, Long-range structure in simulations of glassy water exhibits evidence of metastable criticality, (Poster) APS March Meeting 2021
6. **T.E. Gartner, III**, L. Zhang, P.M. Piaggi, R. Car, P.G. Debenedetti, A.Z. Panagiotopoulos, Liquid-Liquid Phase Transition in Water from a Machine-Learning First Principles Force Field, (Talk) AIChE Annual Meeting 2020; *Link to YouTube video of the talk*
7. **T.E. Gartner, III**, R. Car, S. Torquato, P.G. Debenedetti, Long-Range Structural Features in the Amorphous Ices Could be a Signature of Criticality in Supercooled Liquid Water, (Talk) AIChE Annual Meeting 2020; *Link to YouTube video of the talk*

8. **T.E. Gartner, III**, C.M. Heil, A. Jayaraman, Structural development during emulsion assembly of binary particle mixtures: simulation and experiment,* (Talk) AIChE Annual Meeting 2019; **Selected as an AIChE "Best Presentation of the Session"*
9. **T.E. Gartner, III**, A. Jayaraman, Combining Molecular Simulation, Liquid State Theory, and Gibbs Ensemble Techniques to Study the Structure, Thermodynamics, and Phase Behavior of Polymer-Solvent Mixtures, (Poster) AIChE Annual Meeting 2018
10. **T.E. Gartner, III**, A. Jayaraman, Controlling macromolecular structure and thermodynamics through solvent processing and polymer architecture: theory and simulation, (Poster) GRC Polymer Physics 2018
11. **T.E. Gartner, III**, A. Jayaraman, Understanding linear and cyclic polymer chain conformations and thermodynamics in solution, (Talk) APS March Meeting 2018
12. **T.E. Gartner, III**, P. Ammu, A. Jayaraman, Multiscale simulation study of synthetic melanin nanoparticle self-assembly, (Poster) APS March Meeting 2018
13. **T.E. Gartner, III**, A. Jayaraman, Solvent effects on the structure and thermodynamics of polymer blends with varying architectures, (Talk) AIChE Annual Meeting 2017
14. **T.E. Gartner, III**, H. Kuang, E. Kokkoli, A. Jayaraman, Influence of molecular design on the self-assembly of single-stranded DNA amphiphiles, (Poster) AIChE Annual Meeting 2017
15. **T.E. Gartner, III**, A. Jayaraman, Gibbs ensemble-based molecular simulation methods for predicting structure and thermodynamics of polymer films during solvent vapor annealing, (Talk) ACS Fall Meeting 2017
16. **T.E. Gartner, III**, T.H. Epps, III, A. Jayaraman, Gibbs ensemble simulations of the solvent swelling of polymer films, (Poster) APS March Meeting 2017
17. **T.E. Gartner, III**, C.K. Shelton, M.A. Morris, A. Jayaraman, T.H. Epps, III, Salt distribution, domain spacing, and interfacial characteristics in lithium ion-doped block polymer electrolyte films, (Talk) APS March Meeting 2017
18. **T.E. Gartner, III**, T.H. Epps, III, A. Jayaraman, Utilizing Gibbs ensemble molecular dynamics and hybrid Monte Carlo/molecular dynamics simulations for efficient study of polymer-solvent phase equilibria, (Talk) ACS Fall Meeting 2016
19. **T.E. Gartner, III**, T.H. Epps, III, A. Jayaraman, Development of simulation methods in the Gibbs ensemble to predict polymer-solvent phase equilibria, (Talk) APS March Meeting 2016

CONTRIBUTIONS TO FUNDED PROPOSALS

Active Funding

1. Georgia Tech Renewable Bioproducts Institute, "Unraveling the physical chemistry of polyolefin-cellulose interfaces," (Thomas Gartner, PI; Natalie Stingelin, Co-PI) 10/2022 - 9/2026, $300,000

Prior Funding

2. NSF, DMR-CMMT 1609543, "Development of molecular simulation techniques for probing solvent effects in polymer films during solvent vapor annealing," (Arthi Jayaraman, PI) 9/2016 - 8/2019, $307,257
3. NSF, XSEDE Allocation MCB100140, "Molecular simulations of polymer blends and solutions with varying polymer architecture," (Arthi Jayaraman, PI) 4/2017 - 6/2018, $55,000 approx. value
4. NSF, XSEDE Allocation MCB100140 Renewal, "Molecular simulations of polymer blends and solutions with varying polymer architecture," (Arthi Jayaraman, PI) 7/2018 - 6/2019, $487,856 approx. value
5. DOE, BES-CSGB NERSC Allocation m3538, "Computational Chemical Science Center: Chemistry in Solution and at Interfaces," (Roberto Car, PI) 1/2020 - 1/2021

TEACHING AND MENTORSHIP EXPERIENCE

Instructor, Georgia Institute of Technology
Undergraduate Chemical Engineering Thermodynamics I (ChBE 2130A) (Spring 2022)
Undergraduate Chemical Engineering Thermodynamics I (ChBE 2130A) (Spring 2023)

Department Teaching Fellow, University of Delaware, Newark, DE
Molecular Modeling and Simulations of Soft Materials (Spring 2019)

Teaching Assistant, University of Delaware, Newark, DE
Undergraduate Chemical Engineering Thermodynamics II (Spring 2016)
Introduction to Polymer Science and Engineering (Fall 2016)

Mentor, Philadelphia Futures, Philadelphia, PA (11/2017 - Present)
Sponsor-a-Scholar Program

SERVICE AND AFFILIATIONS

Faculty Mentor, Mentoring for the Professoriate (01/2022 - Present)
School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

Contributor, Materials and Polymer Science Pedagogical Materials Page (08/2022 - Present)
Computer Aids for Chemical Engineering, https://cache.org/

Representative, DOE Basic Energy Sciences Early Career Network (09/2019 - 12/2021)
Chemistry in Solution and at Interfaces (CSI) Center, Princeton University

Representative, Diversity, Equity, Climate and Inclusion (DECI) Committee (01/2021 - 12/2021)
Department of Chemical & Biological Engineering, Princeton University

Member, PNAS Journal Club Panel (11/2020 - 12/2021)

Organizer and Host, Molecular Simulation with Machine Learning Workshop (07/2020)
Chemistry in Solution and at Interfaces (CSI) Center, Princeton University

Outreach Coordinator, University of Delaware Colburn Club (09/2015 - 09/2016)
Member, Colburn Club Outreach Group (03/2015 - 06/2019)

Reviewer: *PNAS, Nature Communications, JACS, Macromolecules, ACS Polymers Au, ACS Macro Letters, Soft Matter, Journal of Chemical Physics, Physical Chemistry Chemical Physics, NPJ Computational Materials, Journal of Materials Science, Journal of Membrane Science, European Physical Journal Plus, Swiss National Supercomputing Centre, ERC Consolidator Grant Program*

Member: American Physical Society, American Chemical Society, American Institute of Chemical Engineers

Organizer/Session Chair:
- APS March Meeting 2023, DPOLY: *Physics-informed design of recycled, upcycled, and sustainable polymers* and *Recent advances in polymer recycling, upcycling, and sustainability*
- AIChE Annual Meeting 2023, Area 8A: *Excellence in Graduate Polymer Research*

- AIChE Annual Meeting 2022, Area 8A: *Polymer Simulations*
- 33rd IUPAP Conference on Computational Physics (2022): *Soft Matter, Polymers, and Biological Physics*
- AIChE Annual Meeting 2020, Area 8A: *Polymer Thermodynamics and Self-Assembly: Predicting Properties*