NATHAN REBELLO

Massachusetts Institute of Technology
77 Massachusetts Ave., Cambridge, MA 02139

+1 (972)-693-1431
nrebello@mit.edu
Personal Website LinkedIn GitHub

SUMMARY

Intersection of AI/ML, Materials Science, and Chemistry to support polymer informatics.

EDUCATION

Massachusetts Institute of Technology
Candidate for PhD Chemical Engineering; Minor in Artificial Intelligence; *expected completion, May 2023.*
Thesis: *Predicting Properties of Polymer Networks Using Analytical Theory and Data-Driven Approaches.*
Advisor: Prof. Bradley D. Olsen

The University of Texas at Austin
B.S. Chemical Engineering High Honors; Special Honors in Engineering; Minor in Economics; *May 2018.*
Thesis: *Influence of Counterion Chemical Structure on Ionic Conductivity in Polymerized Ionic Liquids.*
Advisor: Prof. Venkat Ganesan

RESEARCH EXPERIENCE

Massachusetts Institute of Technology
Research Assistant, Olsen Research Group *1/19-Present*
Interested in polymer molecular design, materials, machine learning, and inverse design. Developed machine learning tools to identify trends in polymer properties and accelerate the design of new polymers.

New Query Language for Stochastic Polymer Structures - Developing a line notation to query functional groups and stochastic patterns in stochastic polymers. Used with the database schema PolyDAT developed in this PhD, polymer informatics will enjoy the benefits that have advanced small molecule search in the era of artificial intelligence.

Predicting Soft-Matter Phases Using Machine Learning - Developed machine learning models based on the random forest approach to model and predict the phase behavior of block copolymers. This approach led to almost twice the accuracy as compared to physics-based methods, in particular, self-consistent field theory (SCFT). This work can be expanded for applications in drug delivery, electrolytes, and surfactants.

Material Design and Property Prediction - Leveraged advanced approximations of network topological theory and developed an innovative molecular editor that facilitates the engineering and mechanical property predictions of polydisperse polymer networks that are below full conversion, thereby reducing the cost, time and resources needed for expensive trial and error experiments.

Update to the famous Flory-Rehner Equation in Polymer Science - The Flory-Rehner and Bray-Merrill swelling theories are venerable theories for calculating the swelling of polymer networks. These were revised to include cyclic topological defects and validated against experiments.

The University of Texas at Austin
Undergraduate Research Assistant, Ganesan Research Group *2/16-8/18*
Modeled polymeric ionic liquids using long-time all-atom simulations to target high conductivity and high mechanical strength batteries.

TEACHING/MENTORING EXPERIENCE

Massachusetts Institute of Technology
Teaching Assistant *Fall 2021*

MIT - Duke Collaboration (Duke Muser Program) *01/20-05/20*
Mentored Anna Go and Angelo Guo, undergraduate students at Duke to develop code that translates between the BigSMILES line notation and graphical polymer representations in ChemDraw format.

INDUSTRY EXPERIENCE

Procter & Gamble, Cincinnati, OH
Personal Healthcare Research & Development Intern *5/17-8/17*
Modeled Global Vicks Manufacturing Processing using an algorithm that optimizes dissolution of active ingredients while simultaneously adapting system to output more formulations.

PUBLICATIONS

1. **Rebello, N.J.**; Lin, T.S.; Olsen, B. D. NERD: A Multiscale Tool to Design Polymer Networks and Quantify Elasticity with Reaction Detection. *Working Paper.*
2. **Rebello, N.J.**; Lin, T.-S.; Olsen, B.D. BigSMARTS: A Line Notation to Search Polymers. *Working Paper.*
3. Lin, T.-S.; Lee, G.H.; **Rebello, N.J.**; Olsen, B.D. Canonical BigSMILES: A Canonical Language for Polymer Indexing and Search I. Linear Polymers. *Working Paper.*
4. Zou, W.; Tupper, A.; **Rebello, N.J.**; Ranasinghe, D.S.; Green, W.H.; Couch, C.; Olsen, B.D. Multiscale modeling and characterization of radical-initiated modification of molten polyolefins. *Working Paper*.
5. **Rebello, N.J.**; Arora, A. Mochigase, H., Lin, T.-S., Audus, D.J., Olsen, B.D. BCDB: The Block Copolymer Phase Behavior Database. *Submitted to Journal of Chemical Information and Modeling.*
6. Arora, A.; Lin, T.S.; **Rebello, N.J.**; Av-Ron, S.; Mochigase, H.; Olsen, B.D. A Random Forest Predictor for Diblock Copolymer Phase Behavior. *Submitted.to ACS Macro Letters.*
7. **Rebello, N.J.**; Beech, H. K.; Olsen, B. D. Adding the Effect of Topological Defects to the Flory-Rehner and Bray-Merrill Swelling Theories. *ACS Macro Letters,* **2021**, *10, xxx, 531-537.*
8. Lin, T. S.; **Rebello, N.J.**; Beech, H. K.; Wang, Zi; El-Zaatari, B.; Lundberg, D.; Johnson, J.; Kalow, J.; Craig, S.; Olsen, B. D. PolyDAT: a generic data schema for polymer characterization. *Journal of Chemical Information and Modeling*, **Spring 2021**.
9. Keith, J. R.; **Rebello, N.J.**; Cowen, B. J.; Ganesan, V., Influence of counterion structure on conductivity of polymerized ionic liquids. *ACS Macro Letters* **2019,** *8* (4), 387-392.
10. Lee, W.; Park, S.; Kim, Y.; Sethuraman, V.; **Rebello, N.**; Ganesan, V.; Ryu, D. Y., Effect of grafting density of random copolymer brushes on perpendicular alignment in PS-b-PMMA thin films. *Macromolecules* **2017,** *50* (15), 5858-5866.
11. **Rebello, N.**; Sethuraman, V.; Blachut, G.; Ellison, C. J.; Willson, C. G.; Ganesan, V., Influence of topographically patterned angled guidelines on directed self-assembly of block copolymers. *Physical Review E* **2017,** *96* (5), 052501.

PRESENTATIONS AND CONFERENCES

1. **Rebello, N.**; Lin, TS.; Olsen, B.D. BigSMARTS: A chemical search grammar for macromolecules. *Abstract of Papers of the American Chemical Society* 261: CINF, **April 2021.**
2. Zou, W.; Tupper, A.; **Rebello, N.**; Ranasinghe, D.; Green, W.; Olsen, B.D.; Couch, C. Predicting the flow of polymers under melt processing: from reaction kinetics to viscoelasticity. *Bulletin of the American Physical Society*, **Spring 2021**.
3. **Rebello, N.**; Arora, A.; Lin, TS.; Av-Ron, S.; Olsen, B.D. Prediction of Block Copolymer Phase Behavior using Machine Learning. *Bulletin of the American Physical Society*, **Spring 2021**.
4. Lin, T.S..; Walsh, D.; **Rebello, N.**; Kroenlein, K.; Audus, D.; Olsen, B.D. A Hierarchical Model for Polymer Data. *Bulletin of the American Physical Society*, **Spring 2021.**
5. **Rebello, N.**; Lin, TS.; Olsen, B.D. BigSMARTS: A Structurally-Based Line Notation for Macromolecule Search, Classification, and Reactions. *Bulletin of the American Physical Society*, **Spring 2021.**
6. Beech, H.K.; **Rebello, N.**; Olsen, B.D. Updating classical swelling theory with loops: experiments and real elastic swelling theory. *Bulletin of the American Physical Society*, **Spring 2021**.
7. Walsh, D.J.; **Rebello, N.**; Introducing CRIPT (**C**ommunity **R**esource for **I**nnovation in **P**olymer **T**echnology) and Demo. *Virtual Symposium on Polymer Data*, **January 2021.**
8. Zou, W.; Tupper, A.; **Rebello, N.**; Joo, W.; Ranasinghe, D.; Lin, TS.; Ji, G.; Khan, S.; Olsen, B.D.; Gopalan, K.; Coach, C. From quantum mechanics to viscoelasticity: A multiscale modeling and characterization of radical initiated modification of polyolefin in molten state. *Bulletin of the American Physical Society*, **Spring 2020.**
9. Zou, W.; Sourakov, A.; **Rebello, N.**; Lin, T.S.; Olsen, B.D.; Johnson, J. Unveiling the effects of molecular topology on the viscoelasticity of entangled polymers under gelation. *Bulletin of the American Physical Society*, **Spring 2020.**
10. Liu, S.; Magliarditi, E.; **Rebello, N**. Advanced Scoliosis Detection with Deep Neural Nets. **MIT IAP 2019.**
11. Lee, W.; Park, S.; Sethuraman, V.; **Rebello, N.**; Ganesan, V.; Ryu, D.Y. Microdomain Orientation of Self-Assembled Block Copolymer Vertically to the Substrate by Polymer Brush Grafting. *International Symposium on Directed Self-Assembly*, **Fall 2018.**
12. Keith, J.; **Rebello, N.;** Ganesan, V. Influencing Transport Properties in Polymerized Ionic Liquids through Ion Chemistry. *2018 AIChE Annual Meeting*, **Fall 2018**.
13. **Rebello, N.** How Counteranions Affect Transport Properties in Polymerized Ionic Liquids. Undergraduate Engineering Honors Thesis Symposium, The University of Texas at Austin, **May 2018**.
14. **Rebello, N.** Influence of Counterion Chemical Structure on Ionic Conductivity in Polymerized Ionic Liquids. Senior Thesis, The University of Texas at Austin, **2018**.
15. Lee, W.; Park, S.; Sethuraman, V.; **Rebello, N.**; Ganesan, V.; Ryu, D.Y. Perpendicular Orientation of PS-b-PMMA Microdomains Controlled by the Grafting Density of P (S-r-MMA) Brushes. *Bulletin of the American Physical Society*, **Spring 2018.**
16. **Rebello, N.**; Sethuraman, V.; Blachut, G.; Ellison, C. J.; Willson, G.; Ganesan, V. Parametric Conditions for the Directed Self Assembly of Block Copolymers using a Topographically Patterned Angled Substrate and Grafted Brush. *Bulletin of the American Physical Society*, **Spring 2017**.
17. Lee, W.; Park, S.; Kim, Y.; Sethuraman, V.; **Rebello, N.**; Ganesan, V.; Ryu, D.Y. Perpendicular Alignment of Symmetric Diblock Copolymer Thin Film Controlled by the Grafting Density of Random Copolymer Brush. *Korean Chemical Engineering Society*, **Spring 2017.**
18. Lee, W.; Park, S.; Kim, Y.; Sethuraman, V.; **Rebello, N.**; Ganesan, V.; Ryu, D.Y. Perpendicular Orientation of Block Copolymer by Random Copolymer Brush: The Effect of Grafting Density. *Korea Polymer Society*, **Spring 2017.**

19. **Rebello, N.**; Sethuraman, V.; Blachut, G.; Ellison, C. J.; Willson, G.; Ganesan, V. Quantifying the Self Assembly of Block Copolymers into Perpendicular Lamellae using a Trapezoidal Guideline, *Cockrell School of Engineering Poster Exhibition*, **Spring 2017**.
20. **Rebello, N.**; Sethuraman, V.; Blachut, G.; Ellison, C. J.; Willson, G.; Ganesan, V. Directed Self-Assembly of Block Copolymers into Perpendicular Domains using a Trapezoidal Guideline. *Chemical Engineering Poster Competition,* **Fall 2016.**
21. **Rebello, N.**; Sethuraman, V.; Pandav, G.; Ellison, C. J.; Willson, G.; Ganesan, V. Development of Lamellae using Self Assembly of Block Copolymers for Lithography Application. *Cockrell Undergraduate Engineering Research Poster Competition,* **Spring 2016.**
22. Moaseri, E.; Stover, R.; Gourisankar, S.; Isaac, G.; **Rebello, N.**; Truskett, T.; Johnston, K. Formation of Biodegradable Gold Nanoclusters with high-NIR Absorbance for Biomedical Imaging. *89th ACS Colloid Surface Science Symposium 2015,* **Summer 2015.**
23. **Rebello, N.**; Stover, R.; Gourisankar, S.; Isaac, G.; Truskett, T.; Sokolov, K.; Johnston, K. Essential Prevention of Protein Adsorption onto Gold Nanoclusters in Undiluted Fetal Bovine Serum. *Cockrell Undergraduate Engineering Research Poster Competition,* **Spring 2015.**

AWARDS AND HONORS

- Fannie and John Hertz Foundation Fellowship Semifinalist, 2019
- MIT IAP 2019 – "Exercises in amazement: Discovering deep learning" Project Winner http://news.mit.edu/2019/discovering-deep-learning-mit-iap-course-0315
- Graham F. Carey Undergraduate Scholarship in Computational Science, UT Austin, 2017
- University Co-op George H. Mitchell Scholarship - Academic Excellence, UT Austin, 2017
- 1st Place, Undergraduate Chemical Engineering Poster Competition, UT Austin, 2016
- Summer Research Fellowship, Chemical Engineering Dept., UT Austin, 2016
- 2nd Place, Cockrell Engineering Poster Competitions, UT Austin, 2015, 2016
- Engineering Honors Scholarship, Cockrell School of Engineering, UT Austin, 2014-2018
- American Airlines Federal Credit Union Scholarship, 2014-2015

SELECTED PROJECTS

MIT 6.871[J]: Machine Learning for Healthcare *February – May 2021*

MIT 6.882: Structured Models for Artificial Intelligence *September – December 2020*
Developed action-planning models to control autonomous intelligent agents in "Search and Rescue" domains. Metrics include success rate, time to produce actions, node expansions etc. Techniques incorporated the A* search algorithm with relaxation heuristics, PDDLs, belief states, planning and acting with partial observability via logical inference, constraint satisfaction problems and POMDPs.

MIT 6.036: Introduction to Machine Learning *September – December 2019*
Developed and trained machine learning models, including deep recurrent neural networks, convolutional neural networks, Markov decision processes, and reinforcement learning with agent-environment interaction. Key concepts cover over-fitting, classification, recommender problems, and regularization.

MIT 6.S191: Introduction to Deep Learning *January – February 2019*
Proposed idea of using convolutional neural networks to analyze x-ray images of scoliosis patients, detect features taken in early x-rays indicative that the condition will worsen, and classify the severity at time *t*. Awarded a GPU from NVIDIA for the practicality of the idea.

SKILLS AND TECHNOLOGIES

Programming: Python, C/C++, MATLAB, Fortran, JavaScript
Machine Learning: Deep Learning (ANN/RNN/LSTM/CNN), Reinforcement Learning (POMDPs)
Data Engineering + Mining: PyTorch, TensorFlow, scikit-learn, Kera, NumPy, Pandas, SQL

LEADERSHIP AND SERVICE:

- Volunteer; NetPals; Outreach program with seventh graders using interactive activities; *2021-Present*
- Website Designer; MIT: Olsen Research Group; *2020-Present*
- Audiovisual Technology Chair; MIT Housing (Sidney Pacific); Responsible for the development, maintenance, and direction of Sidney-Pacific electronic audio/visual equipment; *2019-Present*
- Volunteer; City Wide Club; Serving the poor and needy in the Houston area; *2010-2018*