NATHAN REBELLO

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SUMMARY

Developing the tools, including stochastic subgraph search, data-centric infrastructure, and machine learning models, to support polymer informatics, accelerating the design and discovery of new polymers.

EDUCATION

Massachusetts Institute of Technology
Candidate for Ph.D. in Chemical Engineering; 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 with High Honors, Special Honors in Engineering. Minor in Economics.
Thesis: *Influence of Counterion Chemical Structure on Ionic Conductivity in Polymerized Ionic Liquids.*
Advisor: Prof. Venkat Ganesan

RESEARCH EXPERIENCE

Massachusetts Institute of Technology – Cambridge, MA
Graduate Research Assistant, Olsen Research Group *1/19-Present*
Creating the tools to support polymer informatics. Invented search syntax to query functional groups and patterns in stochastic macromolecular graphs for drug design and analytical chemistry. Developed universal polymer database schema closely aligned with experimental techniques to support data analytics.

The University of Texas – Austin, TX
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 EXPERIENCE

Massachusetts Institute of Technology – Cambridge, MA
Graduate Teaching Assistant *Fall 2021*

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.

PEER-REVIEWED 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. *In Progress.*
2. **Rebello, N.J.**; Beech, H. K.; Olsen, B. D. Adding the Effect of Topological Defects to the Flory-Rehner and Bray-Merrill Swelling Theories. *Submitted.*

3. 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**.
4. 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.
5. 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.
6. **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. 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**.
2. **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**.
3. 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.**
4. **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.**
5. 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**.
6. Walsh, D.J.; **Rebello, N.**; Introducing CRIPT and Demo. *Virtual Symposium on Polymer Data*, **January 2021.**
7. 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.**
8. 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.**
9. Liu, S.; Magliarditi, E.; **Rebello, N**. Advanced Scoliosis Detection with Deep Neural Nets. **MIT IAP 2019.**
10. 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.**
11. Keith, J.; **Rebello, N.;** Ganesan, V. Influencing Transport Properties in Polymerized Ionic Liquids through Ion Chemistry. *2018 AIChE Annual Meeting*, **Fall 2018**.
12. **Rebello, N.** How Counteranions Affect Transport Properties in Polymerized Ionic Liquids. Undergraduate Engineering Honors Thesis Symposium, University of Texas at Austin, Austin, TX, **Spring 2018**.
13. **Rebello, N.** Influence of Counterion Chemical Structure on Ionic Conductivity in Polymerized Ionic Liquids. Senior Thesis, University of Texas at Austin, Austin, TX, **2018**.

14. 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.**
15. **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**.
16. 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.**
17. 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.**
18. **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**.
19. **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.**
20. **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.**
21. 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.**
22. **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 Competition, UT Austin, 2016
- 2nd Place, Cockrell Engineering Poster Competition, UT Austin, 2015
- Engineering Honors Scholarship, Cockrell School of Engineering, UT Austin, 2014-2018
- American Airlines Federal Credit Union Scholarship, 2014-2015

SELECTED PROJECTS

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, Keras, NumPy, Pandas, SQL