Entao Yang

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EDUCATION

Doctor of Philosophy, *University of Pennsylvania* Philadelphia, PA

Major in Chemical & Biomolecular Engineering, GPA: 3.82/4.0 Degree Expected May.2022

- Developed three physical models and one machine learning algorithm, connecting polymer dynamics to its microscopic structure in polymer glass and polymer nanocomposites under external load

Bachelor of Engineering, *Tianjin University* Tianjin, China

Major in Chemical Engineering, GPA: 3.79/4.0 Sep.2012-Jul.2016

- Thesis: Effect of dust dispersion on particle integrity and explosion hazards

Dual Bachelor of Economics, *Nankai University* Tianjin, China

Major in Finance Jan.2014-Jul.2016

- Thesis: Effects of Two-child policy on Chinese saving rate

RESEARCH EXPERIENCE

Graduate Researcher*, *University of Pennsylvania Jan.2017-Present

Understanding Longtime Deformation in Polymer Nanocomposites

- Collaborate with industry partners and investigate the effect of nanoparticle (NP) size, dispersion state, and polymer-NP interactions on polymer nanocomposites (PNCs) creep suppression through molecular dynamics simulation
- Develop a Dynamical Decomposition Model in PNCs using machine learning, which can predict PNCs' linear response limit under creep deformation from the structural information of pre-deformation samples. This work has been submitted to *Proceedings of the National Academy of Sciences*
- Propose a transfer-learned softness (a machine-learned structural field) which connects softness in the heterogenous system to the well-dispersed system for the first time and enable training on small scale (5-10%) data sets
- Build up a Structure-dependent Eyring Model (StEM) using machine learning, connecting the activation volume in the original Eyring model, to a polymer structure property for the first time
- Use StEM to prove the glassy dynamical enhancement due to external stress is heterogenous, which explains the narrower relaxation time distribution observed in both experiments and simulations. This work has been submitted to *Physical Reviews Letters*

Strain Localization in Polymer Nanopillars

- Study effect of NP attractive strength on strain localization position in tensile-deformed polymer nanopillars and connect it to a machine-learned microscopic structural property. This work shows how minor change of local polymer density can affect shear band formation and is published on *Soft Matter*

Structuro-elasto-plastic (StEP) model for plasticity in disordered solids

- Develop a 3D version of Structuro-elasto-plasticity (StEP) model incorporating thermal contributions, which is the first elasto-plastic model involving structure information and applicable in four different amorphous systems
- Use StEP model to reproduce shear banding and brittle-to-ductile transition in tensile-deformed polymer pillars at different temperatures

Bound Layer Exchange in Polymer Nanocomposite Melts

- Model the aging process of NP's bound layer in polymer solution and evaluate the effect of NP sizes, interaction strength, and polymer chain length
- Use systematic coarse grain techniques to develop implicit solvent model and study the polymer entanglement change during the solvent evaporation process. This work has been accepted by AICHE 2021 for an oral presentation

Research Intern*, *Mary Kay O'Connor Process Safety Center Jan.2016-May.2016

Effect of dust dispersion on particle integrity and explosion hazards

- Quantify the effect of dust dispersion mechanism and dust concentration on dust particle breakage and evaluate the potential hazards of dust explosion

PROFESSIONAL SKILLS

- **Mathematical modeling and data-driven modeling**: develop three physical models (StEM, StEP model, and Dynamical Decomposition Model in PNCs) and one machine learning algorithm (transfer-learned softness)
- **Molecular dynamics simulation**: LAMMPS
- **Machine learning**: Interpretable machine learning, transfer learning, and deep learning
- **Coding language**: C++, Python, SQL, R, Matlab
- **Parallel computation**: OpenMP

LEADERSHIP EXPERIENCE

Co-chair of 12th Penn CBE Graduate Student Symposium Jan.2021-Present

- Lead a committee of 14 current Ph.D. students and prepare for the symposium with 15 oral presentations and 30 posters from all CBE research labs

Co-founder of Penn Graduate Poker Group Mar.2019-Present

- Organize monthly live poker tournament (Texas hold 'em) involving faculty members and graduate students at University of Pennsylvania. Event has been moved to online after pandemic

PUBLICATIONS

- **Yang, E**., & Riggleman, R. A. (2021). Stress-induced dynamical enhancement in model polymer nanocomposites. *Manuscript in preparation*.
- **Yang, E**., & Riggleman, R. A. (2021). Structure-dependent Eyring model (StEM) in polymer glass. *Submitted to Physical Review Letters*.
- **Yang, E**., Pressly, J., Natarajan, B., Winey, K., & Riggleman, R. A. (2021). Dynamical decomposition in model polymer nanocomposites under creep. *Submitted to Proceedings of the National Academy of Sciences*.
- **Yang, E**., Ivancic, R. J., Lin, E. Y., & Riggleman, R. A. (2020). Effect of polymer-nanoparticle interaction on strain localization in polymer nanopillars. *Soft matter*, 16(37), 8639-8646.
- Bagaria, P., Zhang, J., **Yang, E.**, Dastidar, A., & Mashuga, C. (2016). Effect of dust dispersion on particle integrity and explosion hazards. *Journal of Loss Prevention in the Process Industries*, 44, 424-432.
- Tong, Y., Wang, Z., **Yang, E.**, Pan, B., Dang, L., & Wei, H. (2016). Insights into cocrystal polymorphic transformation mechanism of ethenzamide–saccharin: a combined experimental and simulative study. *Crystal Growth & Design*, 16(9), 5118-5126.
- Tong, Y., Wang, Z., **Yang, E.**, Pan, B., Jiang, J., Dang, L., & Wei, H. (2016). Determination and correlation of solubility and solution thermodynamics of ethenzamide in different pure solvents. *Fluid Phase Equilibria*, 427, 549-556.
- Feng, Y., **Yang, E.**, Dang, L., & Wei, H. (2015). Liquid–liquid phase equilibrium for ternary mixtures of formamide (or ethylene glycol, or monoethanolamine)+indole+2-methylnaphthalene at 308.15 K. *Fluid Phase Equilibria*, 398, 10-14.

SELECTED CONFERENCES

- **Yang, E**., & Riggleman, R. (2021). Modeling the bound polymer layer in polymer nanocomposites. *American Institute of Chemical Engineers Annual Meeting (Accepted)*
- **Yang, E**., Pressly, J., Natarajan, B., Winey, K., & Riggleman, R. (2021). Dynamical decomposition in model polymer nanocomposites under Creep. *American Physical Society March Meeting*
- Pressly, J., **Yang, E**., Bailey, E., Denby, T., Natarajan, B., Winey, K., & Riggleman, R. (2021). Effect of polymer-nanoparticle interaction strength on viscoelastic creep attenuation in polymer nanocomposites. *American Physical Society March Meeting*
- Zhang, G., Xiao, H., Ivancic, R., **Yang, E.**, Riggleman, R., Durian, D., & Liu, A. (2021). Structuro-elasto-plasticity (StEP) model for plasticity in disordered solids. *American Physical Society March Meeting*
- Xiao, H., Zhang, G., Ivancic, R., **Yang, E.**, Riggleman, R., Durian, D., & Liu, A. (2021). Modeling shear band formation in amorphous solids using a structuro-elasto-plasticity (StEP) model. *American Physical Society March Meeting*
- **Yang, E**., Pressly, J., Bailey, E., Natarajan, B., Mohan, A., Winey, K., & Riggleman, R. A. (2020). Suppression of creep in model polymer nanocomposites. *American Physical Society March Meeting (Meeting cancelled)*