# **Entao Yang**

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#### **EDUCATION**

University of Pennsylvania	Philadelphia, PA
Ph.D., Chemical & Biomolecular Engineering, Computational Science, GPA: 3.82/4.0	Expected May 2022
Master of Science in Engineering, GPA: 3.8/4.0	May 2018
Tianjin University	Tianjin, China
Bachelor of Engineering, Chemical Engineering, GPA: 3.79/4.0	July 2016
Nankai University	Tianjin, China
Bachelor of Economics, Finance	July 2016

#### RELEVANT EXPERIENCE

# PhD Researcher, Penn Institute for Computational Science

Jan.2017-Present

#### Understanding Longtime Deformation in Polymer Nanocomposites using Machine Learning

- Develop the Dynamical Decomposition Model in PNCs using machine learning (SVM, logistic regression, and clustering), which can predict PNCs' linear response limit under creep deformation from the structural information of pre-deformation samples. Manuscript is under review by *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 (since 1936). Manuscript is under review by *Physical Reviews Letters*

# Machine Learned Structuro-elasto-plastic (StEP) Model for Plasticity in Disordered Solids

 Develop a 3D and parallelizable version Structuro-elasto-plasticity (StEP) model incorporating thermal contributions, using the technique of machine learning, Monte Carlo method, Fourier transform, and coarse graining. StEP is the first elasto-plastic model involving structure information and is applicable in four different amorphous systems

### **Understanding Glassy Structure through Physics-informed Neural Network**

• Design a Physics-informed Neural Network and use it to extract a tensorial structural field in glassy materials. This is the first glassy structural metric being able to predict particle-level glassy dynamics with orientations.

# 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 has been published on *Soft Matter* 

# **Bound Layer Exchange in Polymer Nanocomposite Melts**

 Use systematic coarse grain techniques to develop implicit solvent model and study the polymer entanglement change with Monte Carlo method. 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 effect of dust dispersion mechanism and dust concentration on dust particle breakage and evaluate potential hazards of dust explosion. This work has been published on *Journal of Loss Prevention in the Process Industries* 

#### TECHNICAL SKILLS

- Mathematical modeling and data-driven modeling: develop three physical models (StEM, StEP model, and Dynamical Decomposition Model in PNCs) and one machine learning based algorithm (transfer-learned softness)
- Machine learning: Interpretable machine learning, transfer learning, physics-informed machine learning
- Coding language / framework: Python, PyTorch, C++, MySQL, Bash, OpenMP, Matlab, R

# LEADERSHIP EXPERIENCE

#### Treasurer of American Physical Society Chapter at University of Pennsylvania

Nov.2021-Present

• Serve as one of the first three officers in the new founded APS chapter at University of Pennsylvania with more than 80 members, including faculties, post-docs, and graduate students from seven departments.

#### 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 research labs from School of Engineering & Applied Science and School of Arts & Sciences at Penn.

#### 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

# HONORS & AWARDS

- American Physical Society Frank J. Padden Jr. Award 2022, Nomination
- Sigma Xi Grants in Aid of Research 2021, Principal Investigator (one of four in physics)
- Bertelsmann Technology Scholarship, Artificial Intelligence 2021
- Chinese Government Scholarship for Studying Abroad, 2016
- Silver Medal of 1st 'Excellence Cup' National Undergrad Chemical Experimental Design Competition, 2015

#### **PUBLICATIONS**

- Yang, E., & Riggleman, R. A. (2021). Role of Local Structure in the Enhanced Dynamics of Deformed Glasses. *Under review by Physical Review Letters*. Preprint: arxiv.org/abs/2108.06016.
- Yang, E., Pressly, J., Natarajan, B., Winey, K., & Riggleman, R. A. (2021). Understanding the Mechanism of Creep Suppression in Polymer Nanocomposites using Machine learning. *Under review by 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 CONFERENCE PRESENTATIONS (first and co-first author work only)

- Yang, E., & Riggleman, R. (2021). Modeling the bound polymer layer in polymer nanocomposites. *American Institute of Chemical Engineers Annual Meeting*
- Yang, E., Pressly, J., Natarajan, B., Winey, K., & Riggleman, R. (2021). Dynamical decomposition in model polymer nanocomposites under Creep. *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 due to Covid)*