

Fall 2024: MSE760 Final Project Proposal

Quick Introduction:

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Project Title:

Data-Driven Atom-Level Explanation of Polymer Properties

Link to the git repo for the project:

<https://github.com/jhyang13/UWMadison-MSE760-MolecularModeling>

Problem Statement:

Understanding the relationship between the molecular structure of polymers and their macroscopic mechanical properties, such as Young's modulus, is crucial for advancing polymer design and applications. Traditional representations like SMILES lack topology details (e.g., branching or cross-linking), making it challenging to explain how molecular units influence the mechanical properties.

Motivation/Rationale:

Polymers are integral to countless applications due to their versatility and mechanical properties. Despite progress, there remains a gap in linking atomic-level structural features to macroscopic mechanical properties, especially for complex polymer architectures. This study aims to bridge this gap using machine learning (ML) and molecular dynamics (MD) simulations to interpret the atom-level impact on mechanical behavior.

Explain how you contemplate going about it:

Data Preparation:

- Utilize PoLyInfo database ^[1] to extract homopolymer data
- Focus on polymers with documented Young's modulus values

Machine Learning Implementation:

- Convert polymer structures into SMILES format
- Train a single-task ML model to predict Young's modulus
- Conduct atom-level impact analysis by iteratively removing atoms and observing changes in predictions

Validation through MD Simulations:

- Build polymer models using Materials Studio
- Perform relaxation and tensile experiments in LAMMPS to compute Young's modulus
- Compare results with ML predictions to assess consistency

Interpretation and Analysis:

- Apply SHAP values to identify key substructures affecting mechanical properties
- Highlight discrepancies between SHAP and atom-level ML predictions

Reference:

[1] Otsuka, Shingo, et al. "PoLyInfo: Polymer database for polymeric materials design." 2011 International Conference on Emerging Intelligent Data and Web Technologies. IEEE, 2011.