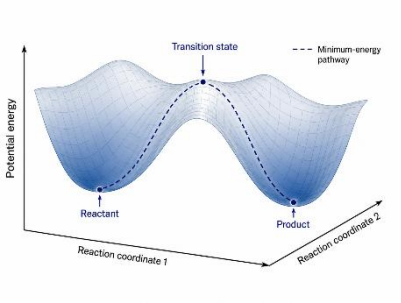
Delta-Learning Refinement of PBE-Based Machine-Learning Interatomic Potentials for Light-Induced Polymerization

Project Description



3D printing is a promising advanced additive manufacturing technique and has attracted increasing interest in recent years. However, the underlying molecular mechanisms, such as the curing process from liquid precursors to a solid polymer network, remain insufficiently understood. In this project, we focus on light-induced polymerization, which is a key process in photopolymerization-based 3D printing.

Molecular dynamics (MD) simulations provide a powerful tool to investigate the microscopic mechanisms of polymerization processes. Several reactive force fields have been developed for photo-polymerization systems and have provided useful insights into the associated physicochemical processes. However, these methods still suffer from limitations in accurately describing reaction energetics and reaction pathways.

Machine-learning interatomic potentials (MLIPs) have shown great potential in reconstructing high-dimensional potential energy surfaces (PESs), which form the foundation of accurate and efficient MD simulations. In this project, we aim to develop and refine a MLIP framework for light-induced polymerization by correcting a PBE-based MLIP using higher-level density functional theory (DFT) data. The refined model will be used to investigate the physical, chemical, and thermodynamic mechanisms involved in the polymerization process.

Objectives

1. Perform DFT calculations using different exchange-correlation functionals and compare their performance in describing representative reaction pathways.

2. Construct a correction dataset based on higher-accuracy DFT calculations for key configurations along the polymerization reaction pathway.

3. Develop a delta-learning framework to refine a PBE-based machine-learning interatomic potential.

4. Evaluate the accuracy and computational efficiency of the refined MLIP in representative MD simulations.

Desired Qualifications

Bonus points will be given for:

* Familiarity with density functional theory or other first-principles methods.
* Basic knowledge of molecular dynamics simulations.
* Interest in AI for science and machine-learning potential development.
* Experience with Python, Linux, or high-performance computing.
* Strong time-management skills and a proactive mindset.

Application

If interested, please send an email to [yingfei.cao@tum.de] with:

* A brief introduction of your background and motivation.
* Your transcript of records.