Centre for AI-Fundamentals
RAEng Google DeepMind Summer Internship Programme 2025

Project proposal

Project Title	Generative modelling to predict mechanochemical reactivity in polymers
Lead supervisor	Niamh Fox
Project Description	**Summary** The use of polymers has become ubiquitous in our lives, from the structural component in many consumer products to the active component in functional devices such as solar cells and as additives in to control the properties of coatings and adhesives. However, during processing polymers are exposed to large mechanical forces which can tear them apart, similar to snapping an over stretched elastic band. In polymer mechanochemistry, mechanical forces can be harnessed to trigger chemical reactions by embedding force-sensitive molecules known as mechanophores within polymer chains. Mechanophores have been designed to demonstrate changes in optical properties, release of drug species and reactions that are forbidden by other activation methods. The discovery of new mechanophores is largely driven by experimental synthesis and physical testing, which are time-consuming and resource-intensive. Computational simulations, such as Constrained Geometries Simulate External Force (CoGEF), have become valuable for predicting which bonds break under mechanical tension. However, these simulations are limited to molecules that have already been designed by chemists, leaving vast unexplored chemical space. This project aims to leverage generative machine learning models to explore this chemical space, predicting new mechanophore structures based on known examples. Using a curated library of existing mechanophores, the student will convert chemical structures into SMILES strings and develop a Variational Autoencoder (VAE) model to generate novel mechanophore candidates. This approach not only accelerates the discovery process but also uncovers new structural motifs that could lead to innovative functionalities.

Objectives

1. Curate data set of known mechanophores
2. Convert chemical structures into SMILES strings and compute molecular descriptors
3. Build and train a basic diffusion model to learn from known mechanophores
4. Generate new potential mechanophore structures
5. Evaluate the plausibility of generated structures

Workplan

Week 1 and 2: Literature review on mechanochemistry and AI-molecule driven molecule generation. Set up software tools (e.g. RDKit, Pytorch)

Week 3: Select and clean data set from literature source. Convert to SMILES and compute descriptors

Week 4: Develop and train basic Diffusion model using the dataset from week 3

Week 5: Generate new molecular structures and evaluate their chemical validity

Week 6: Refine the model, tune hyperparameters, and analyse generated molecules

Week 7: Document findings and prepare visualisations, write project report, report findings at group meeting

Learning outcomes

Skills developed:
Computational Chemistry: Understanding molecular representations (SMILES, fingerprints) and using RDKit for molecular manipulation.

Chemical understanding: A basic understanding of the structure-activity relationships for mechanophores.

Machine Learning: Developing and training a diffusion model using Python libraries (Pytorch).