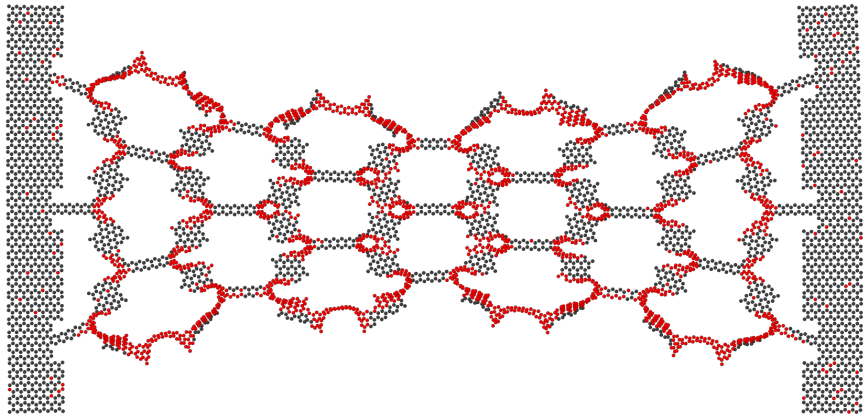

UiO : Fysisk institutt
Det matematisk-naturvitenskapelige fakultet

Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

Mikkel Metzsch Jensen

Juni 02, 2023

Outline

Overview

Three main parts

1. **Sheet kirigami**: Alter a graphene sheet using atomic scale cuts and stretching
2. **Forward simulation**: Calculate the frictional properties of the sheet using MD simulations
3. **Accelerated search**: Use machine learning to replace the MD simulations and perform an accelerated search for new designs

Can we control the frictional properties of a graphene sheet using this technique?

UiO : Fysisk institutt

Det matematisk-naturvitenskapelige fakultet