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

Designs for a negative friction coefficient

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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?



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