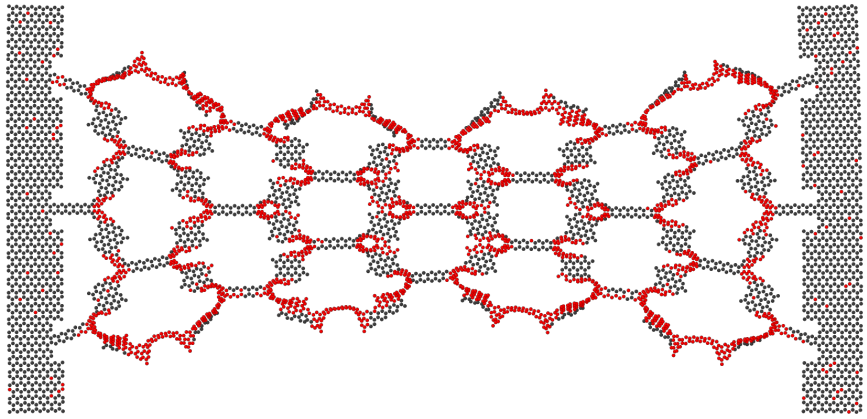

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Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

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Outline

1. **Introduction**
   - Thesis overview
   - Motivation
2. **Creating a graphene Kirigami system**
   - System setup
   - Kirigami
3. **Pilot study**
   - Friction metrics
   - Out-of-plane buckling
   - Friction-strain profiles
   - Negative friction coefficient
4. **Kirigami configuration search**
   - Machine learning
   - Accelerated search
5. **Summary and outlook**

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?

Motivation

- Kirigami: Variation of origami with cuts permitted
- Macroscale designs $\rightarrow$ nanoscale

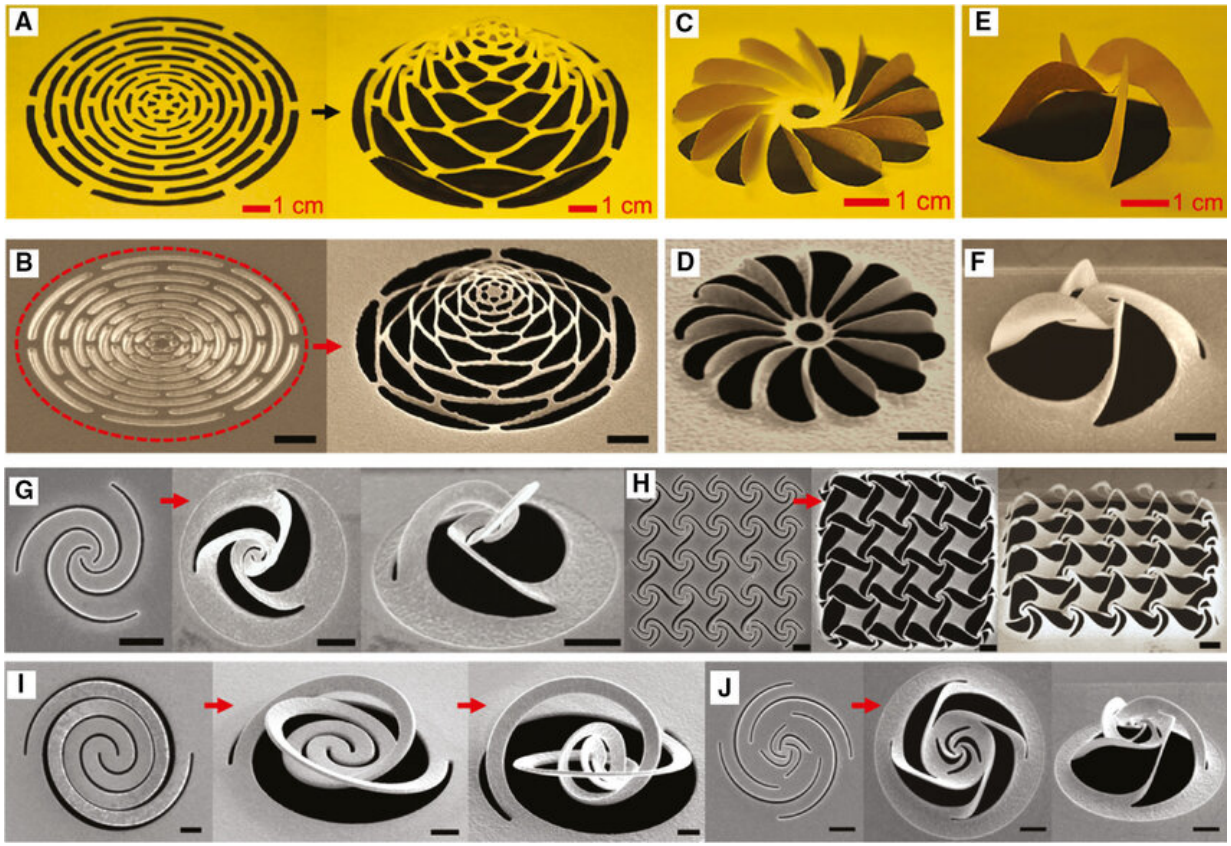

Figure: Example of macroscale Kirigami designs implemented on a nanoscale using a focused ion-beam (FIB). Black scale bars: 1 μm. Reproduced from [Li and Zhiguang, 2018].

References

Li, J. and Zhiguang, L. (2018).
Focused-ion-beam-based nano-kirigami: From art to photonics.
Nanophotonics, *7*.

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