

# 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
- System setup

## ② Creating a graphene Kirigami system

- 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

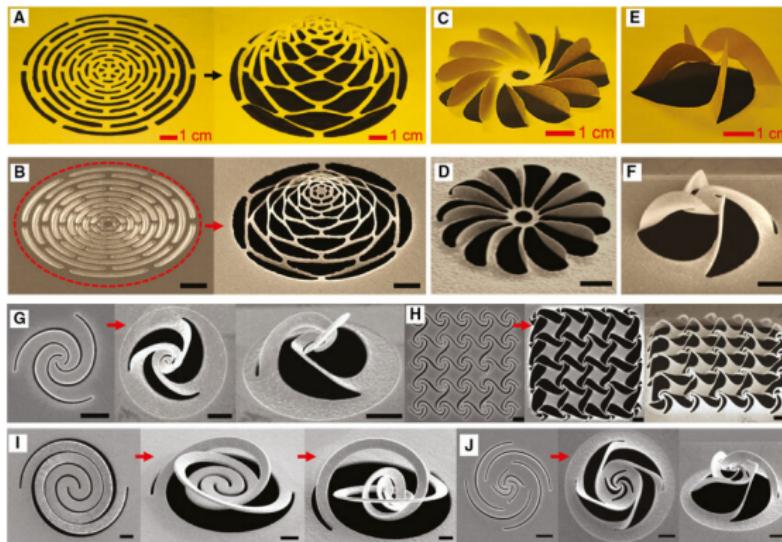
Three main parts

- 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
- Designs: Macroscale → nanoscale

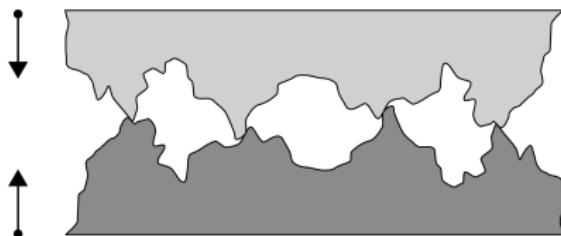


**Figure:** Example of macroscale Kirigami designs implemented on a nanoscale using a focused ion beam (FIB). Black scale bars:  $1 \mu\text{m}$ . Reproduced from [1].

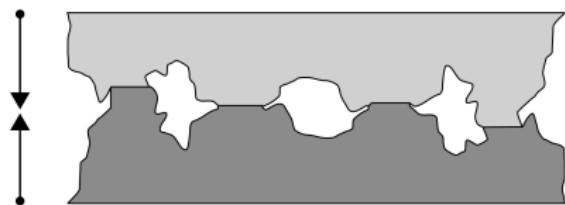
# Motivation

## Out-of-plane buckling

- Hanakata et al. [2, 3] found out-of-plane buckling with Kirigami designs
- Surface properties are predicted to be important for friction properties
  - Asperity theory: Contact area
  - Frenkel-Kontorova models: Commensurability



(a) Small load.

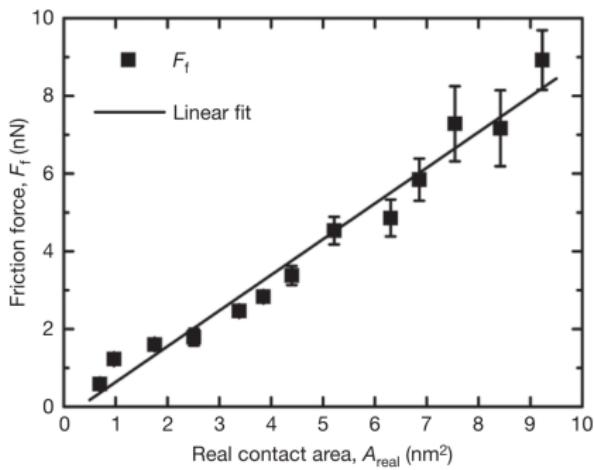


(b) High load.

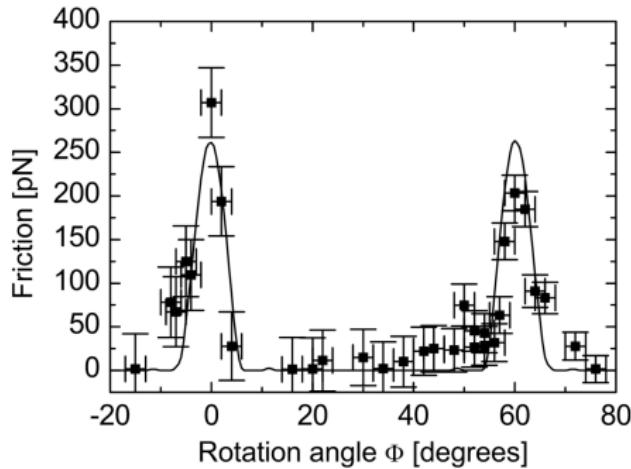
Figure: Reproduced from [4].

# Motivation

Contact area and commensurability



(a) Numerical MD results using an amorphous carbon tip and a diamond sample. Reproduced from [5] with permission from the Springer Nature.



(b) Experimental results of a graphene sheet sliding on graphite. Adapted from [6], reproduced from [7] with permission from the American Physical Society.

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Kirigami

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Friction metrics

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## ④ Kirigami configuration search

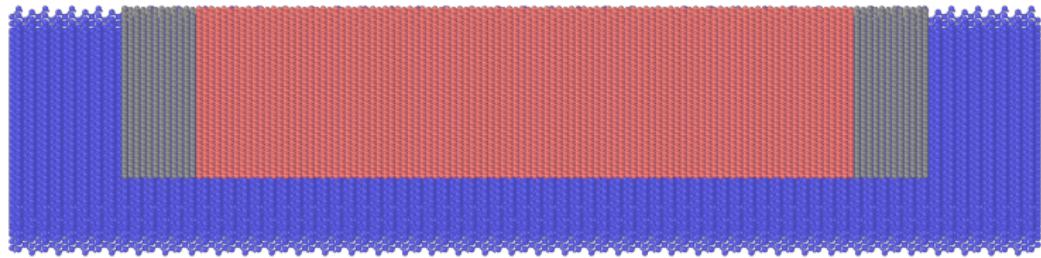
Machine learning

Accelerated search

## ⑤ Summary and outlook

# Creating a graphene Kirigami system

## System setup



**Figure:** Graphene sheet on a silicon substrate. Blue: Substrate, Red: Inner sheet, Grey: Pull blocks.

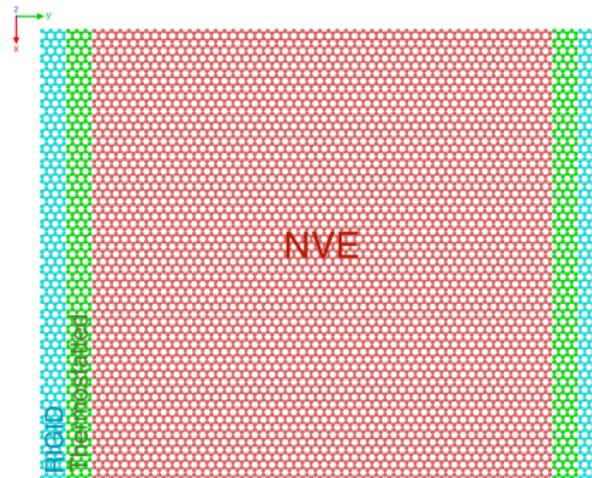
# Creating a graphene Kirigami system

System setup

System size = ???



(a) Side view.



(b) Top view.

# Creating a graphene Kirigami system

## Sheet Kirigami

Primitive lattice vectors

$$\mathbf{a}_1 = a \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right) \quad \mathbf{a}_2 = a \left( \frac{\sqrt{3}}{2}, \frac{1}{2} \right), \quad |\mathbf{a}_1| = |\mathbf{a}_2| = a = 2.46 \text{ \AA}.$$

Basis

$$\left\{ (0, 0), \frac{a}{2} \left( \frac{1}{\sqrt{3}}, 1 \right) \right\}.$$

Interatomic distance

$$\left\| \frac{a}{2} \left( \frac{1}{\sqrt{3}}, 1 \right) \right\| \approx 1.42 \text{ \AA}.$$

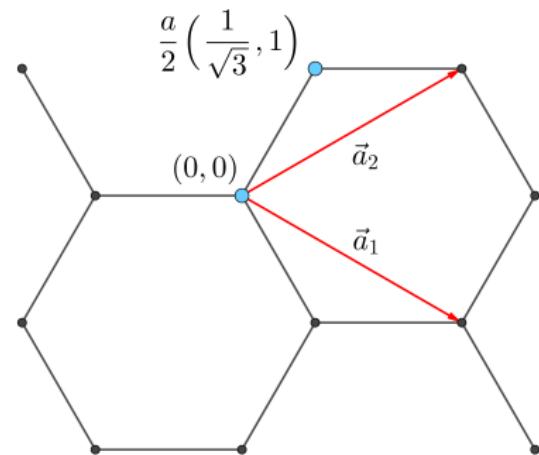


Figure: Graphene crystal structure.

# Creating a graphene Kirigami system

## Sheet Kirigami

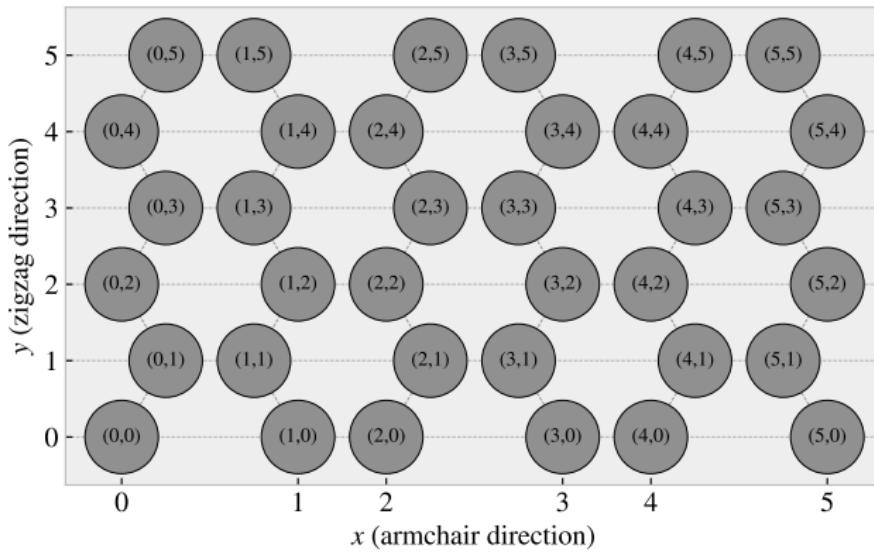


Figure: Graphene atom site indexing.

# Creating a graphene Kirigami system

## Sheet Kirigami

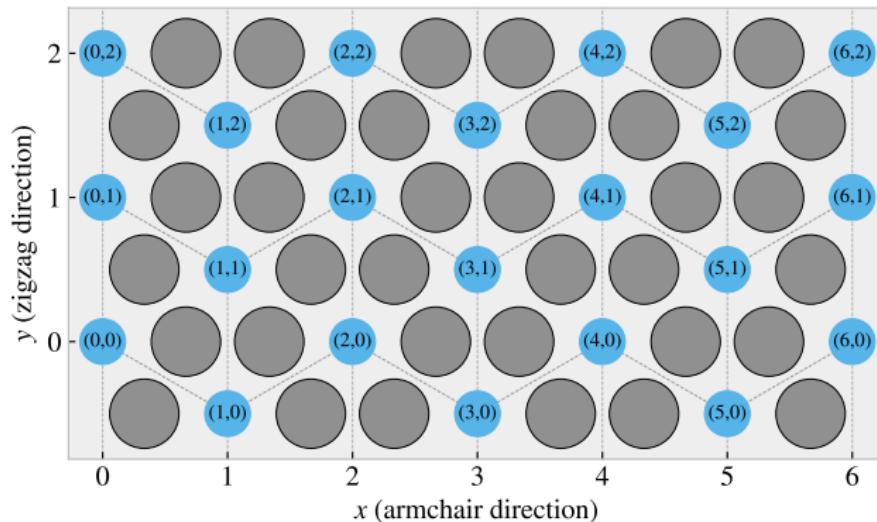
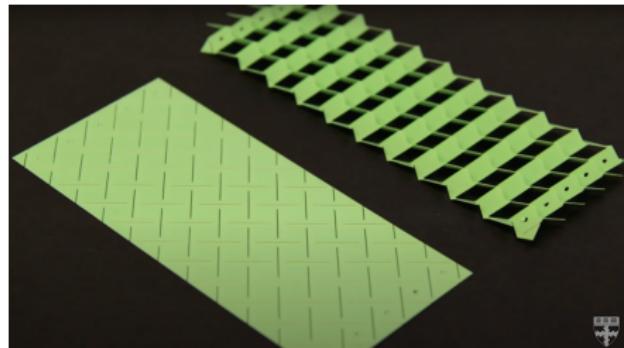


Figure: Graphene center element indexing.

# Creating a graphene Kirigami system

## Sheet Kirigami



(a) Tetrahedron: Alternating perpendicular cuts producing a tetrahedron-shaped surface buckling when stretched.  
Reproduced from [8].

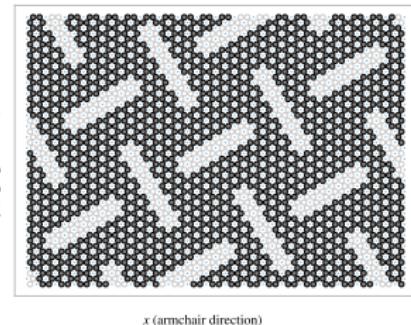
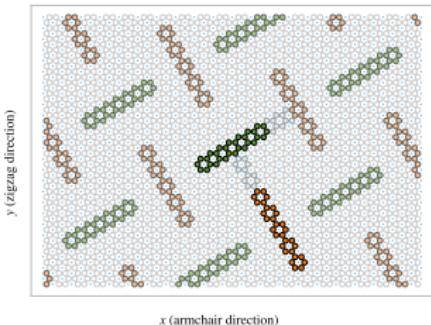


(b) Honeycomb: Scotch™ Cushion Lock™ [9] producing a honeycomb-shaped surface buckling when stretched.  
Reproduced from [9].

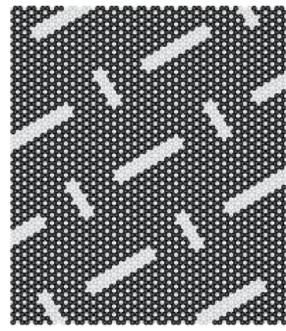
**Figure:** Macroscale kirigami cut patterns used as inspiration for the nanoscale implementation.

# Creating a graphene Kirigami system

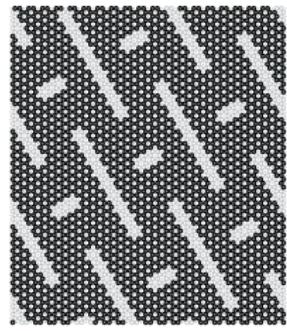
## Sheet Kirigami



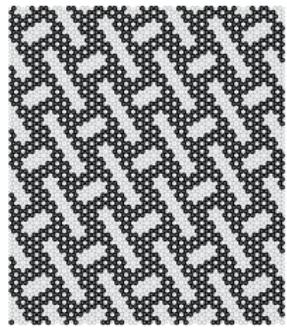
(9, 3, 4)



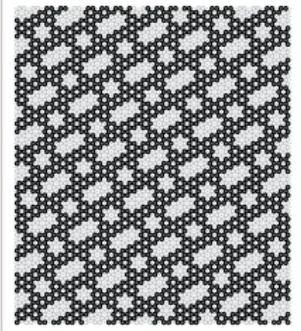
(3, 9, 3)



(3, 5, 1)

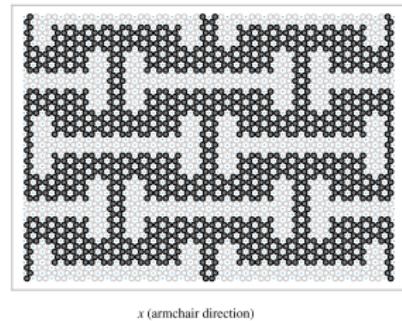
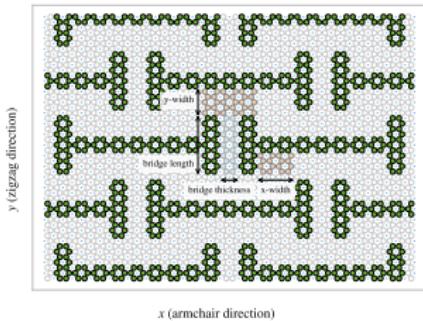


(3, 1, 1)

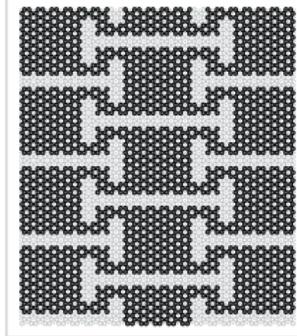


# Creating a graphene Kirigami system

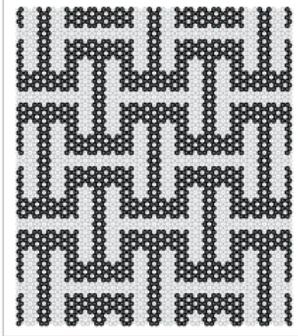
## Sheet Kirigami



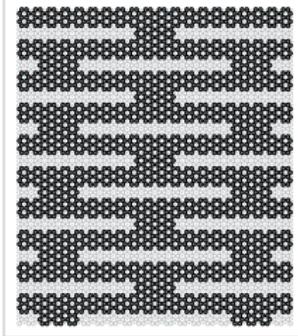
(1, 1, 5, 5)



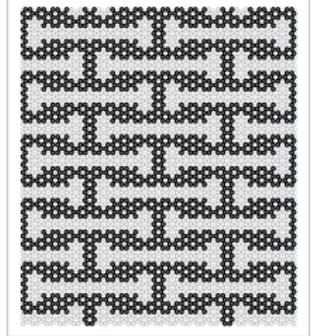
(1, 2, 1, 9)



(2, 2, 3, 1)



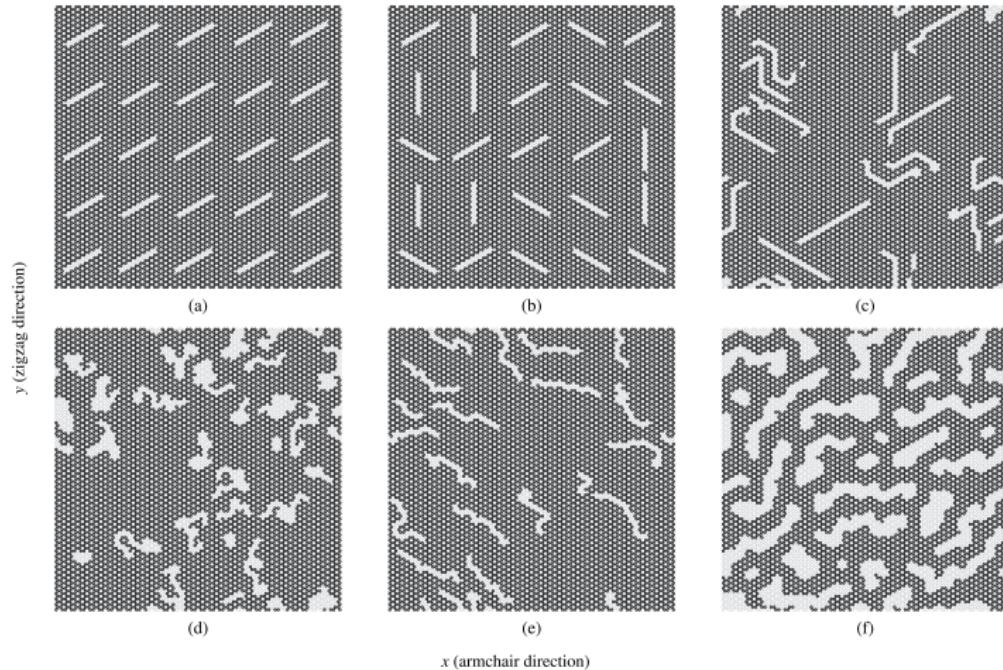
(2, 1, 1, 3)



# Creating a graphene Kirigami system

## Sheet Kirigami

### Random walk



# Creating a graphene Kirigami system

MD simulation

Introduction to MD simulation. Something about newtons equations and Langevin maybe?

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# Pilot study

## Friction metrics

- Friction metrics?
- Stick slip?

# Pilot study

## Out-of-plane buckling

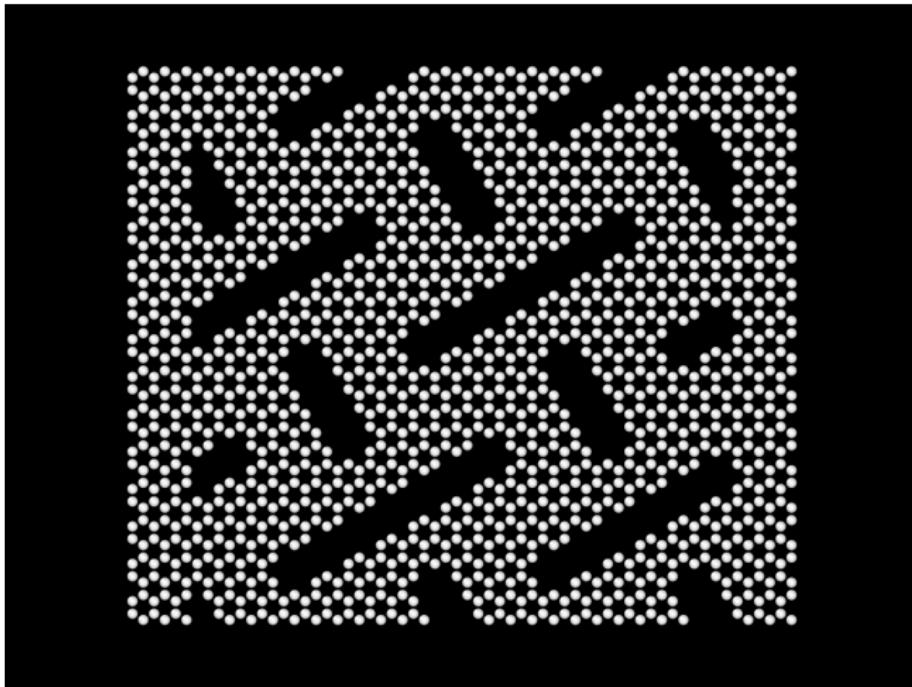


Figure: Kirigami sheet stretch in vacuum. Small tetrahedron pattern.

# Pilot study

## Out-of-plane buckling

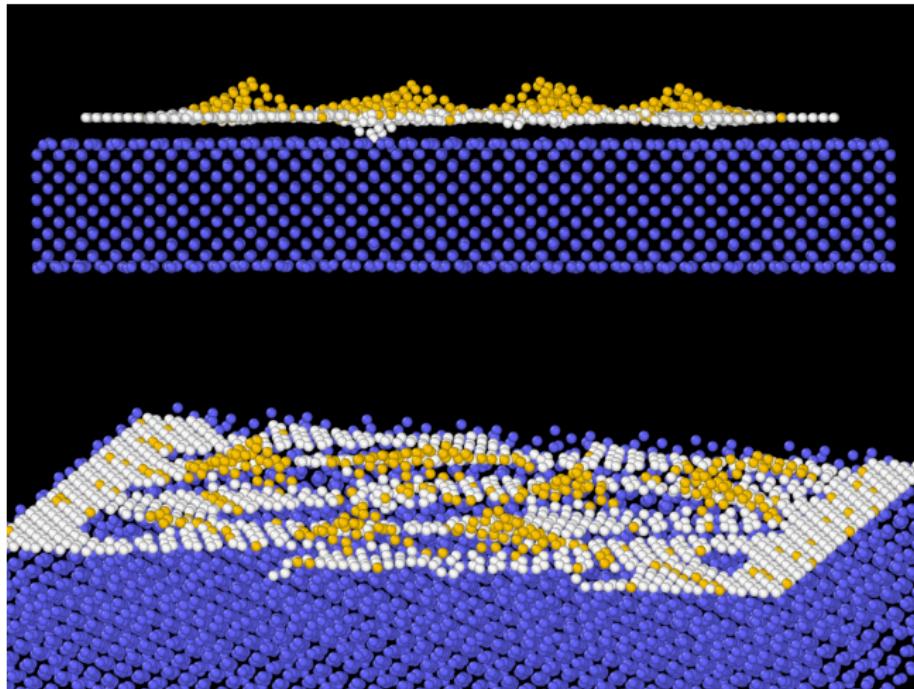
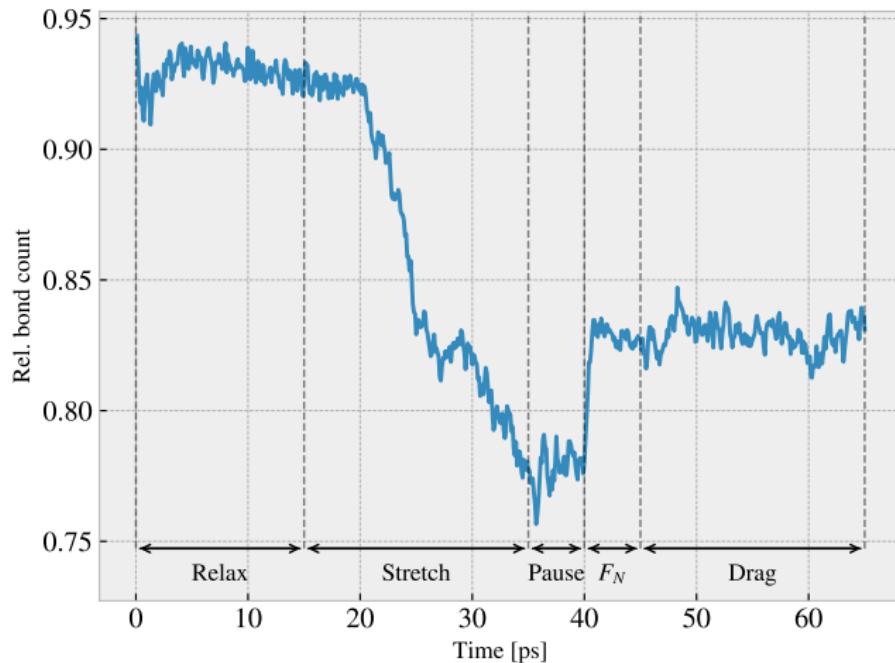


Figure: Kirigami stretch in contact with Si-substrate.

# Pilot study

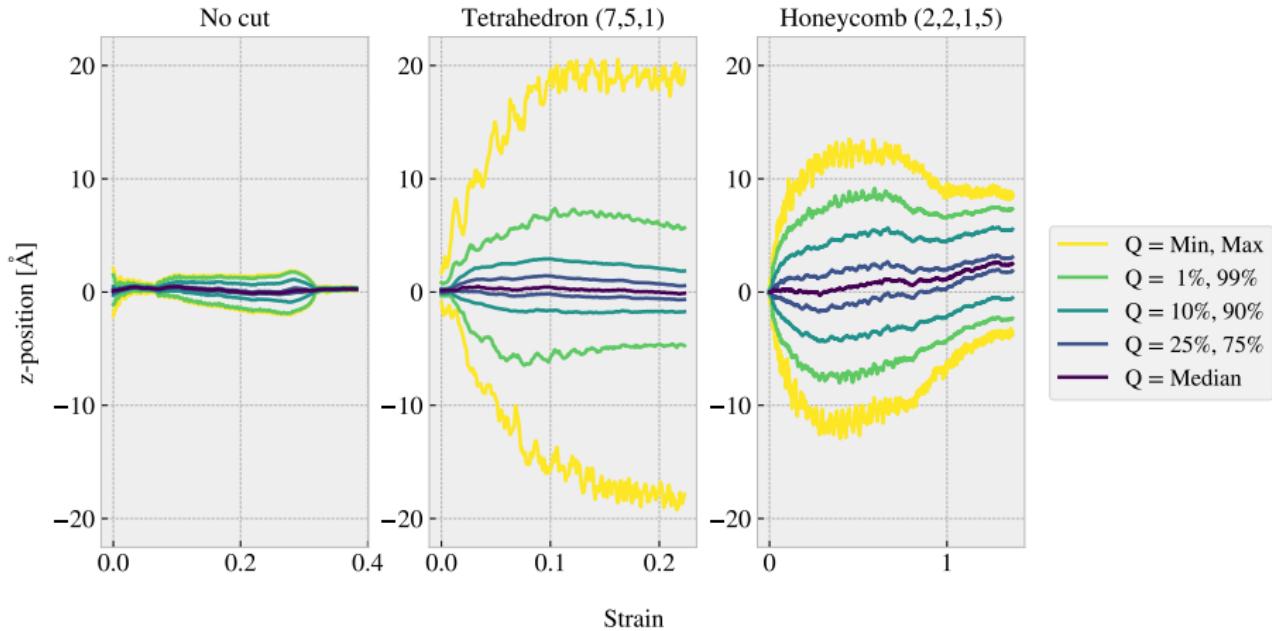
## Out-of-plane buckling



**Figure:** Contact area approximation: Number of C-Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

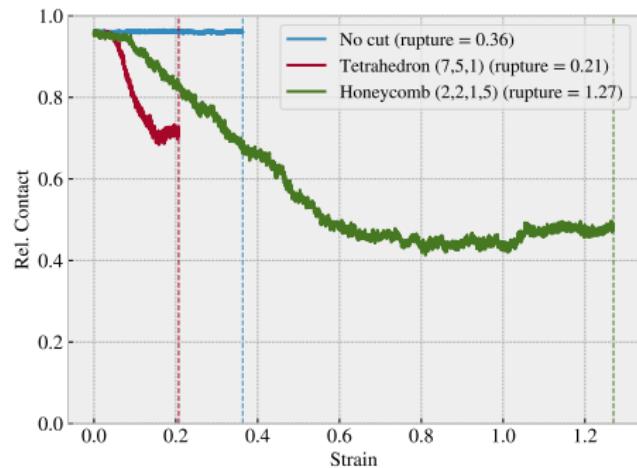
# Pilot study

## Out-of-plane buckling



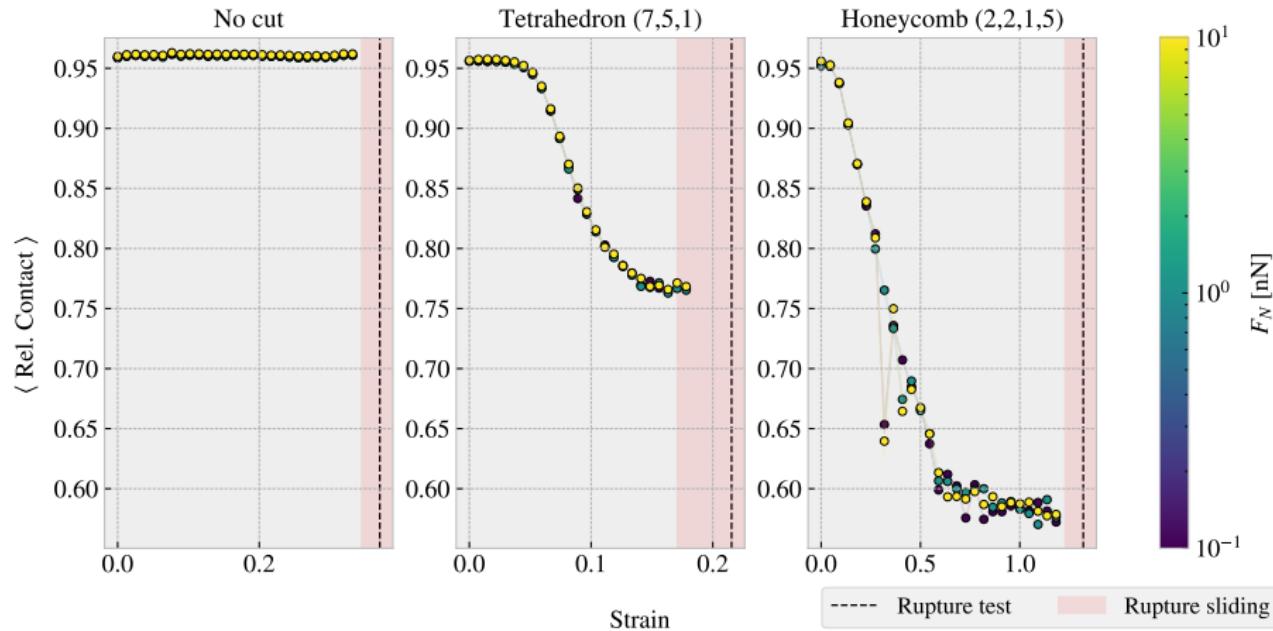
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## Out-of-plane buckling



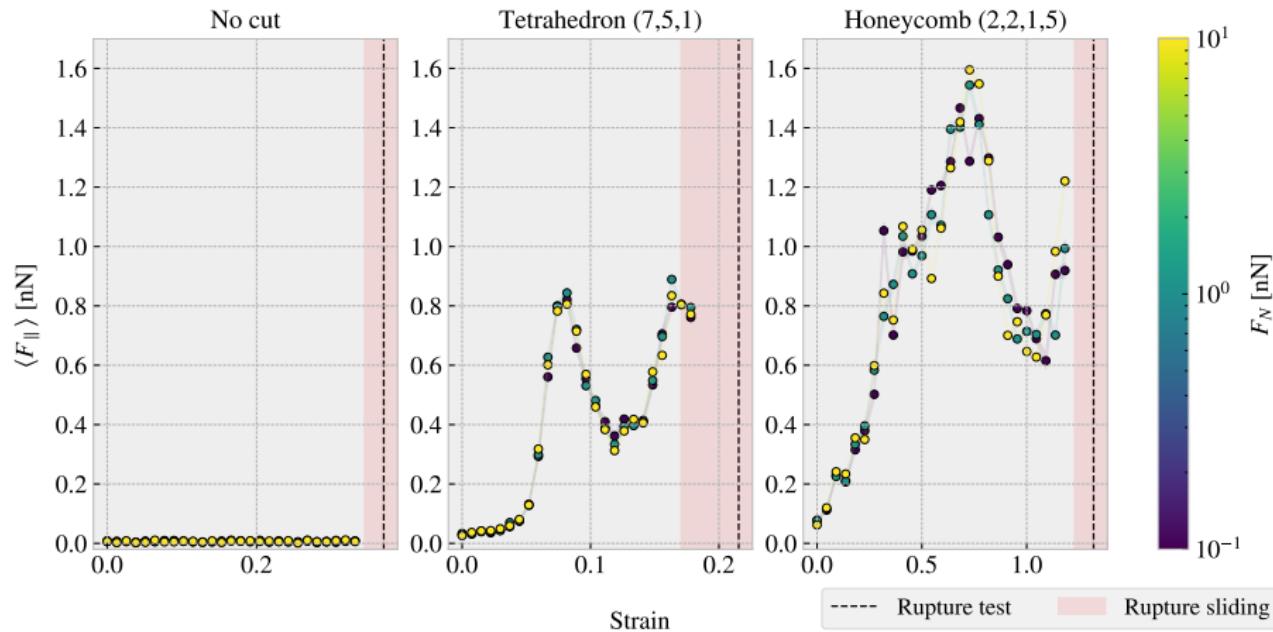
# Pilot study

## Friction-strain profiles



# Pilot study

## Friction-strain profiles

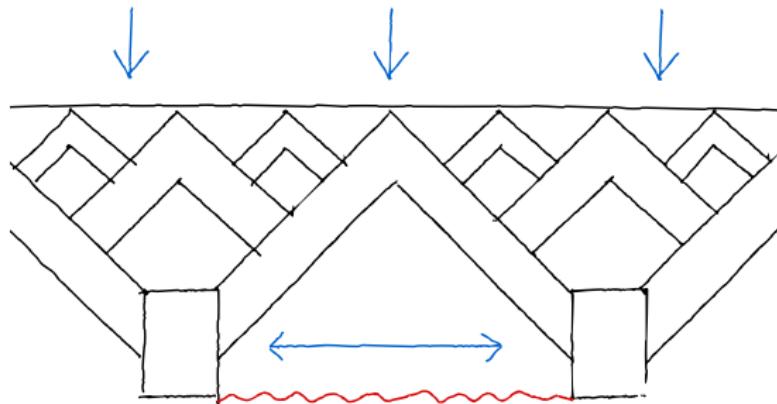


# Pilot study

Negative friction coefficient

Load to sheet tension coupling

$$F_t = TF_N, \quad T = 6$$



# Pilot study

Negative friction coefficient

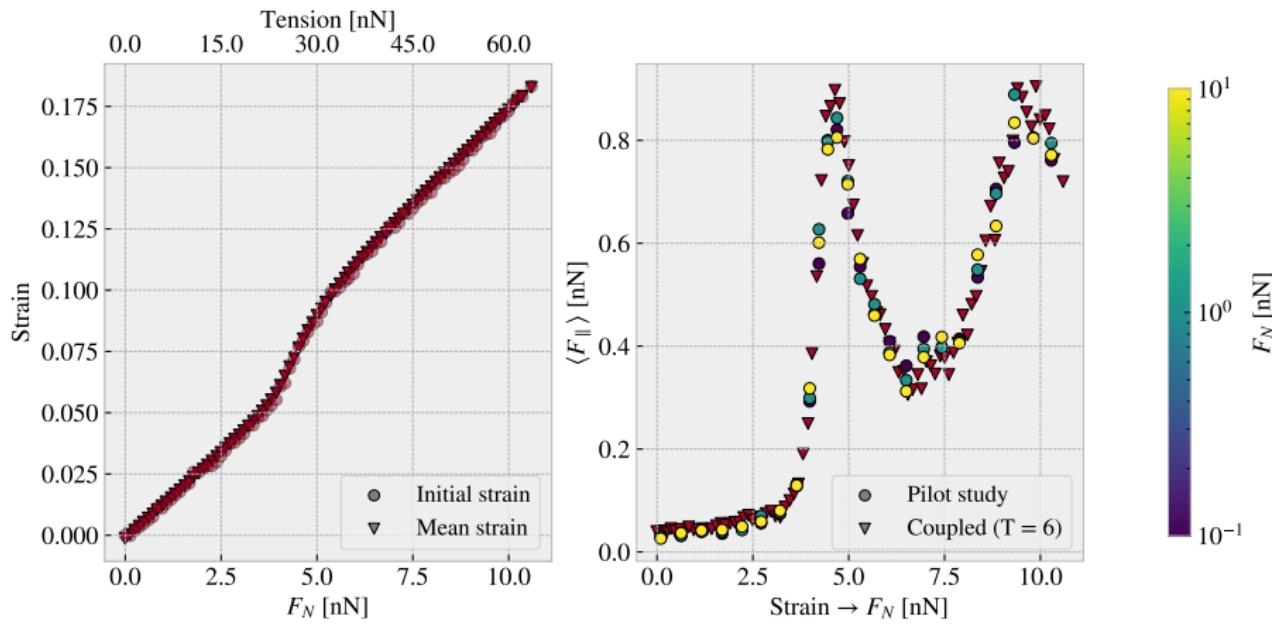


Figure: Tetrahedron (7, 5, 1)

# Pilot study

Negative friction coefficient

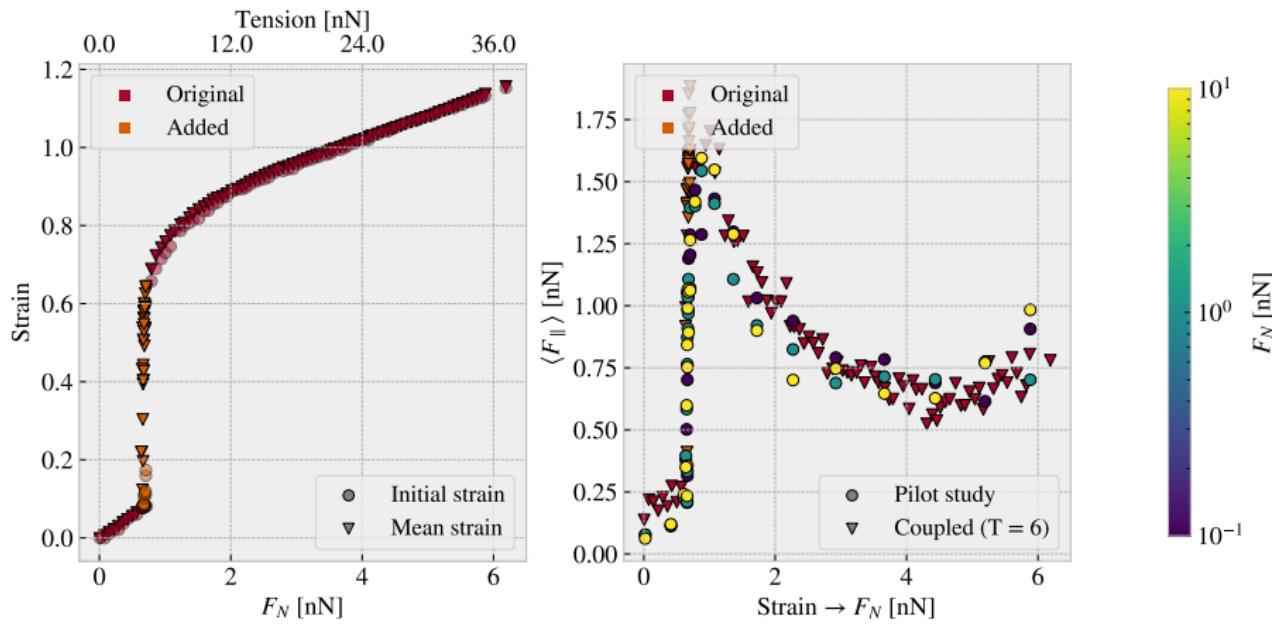


Figure: Honeycomb (2, 2, 1, 5)

# Pilot study

Negative friction coefficient

Honeycomb stretch simulation topview

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# References

- [1] J. Li and L. Zhiguang, "Focused-ion-beam-based nano-kirigami: from art to photonics", *Nanophotonics* **7**, 10.1515/nanoph-2018-0117 (2018).
- [2] P. Z. Hanakata, E. D. Cubuk, D. K. Campbell, and H. S. Park, "Accelerated search and design of stretchable graphene kirigami using machine learning", *Phys. Rev. Lett.* **121**, 255304 (2018).
- [3] P. Z. Hanakata, E. D. Cubuk, D. K. Campbell, and H. S. Park, "Forward and inverse design of kirigami via supervised autoencoder", *Phys. Rev. Res.* **2**, 042006 (2020).
- [4] W. Commons, *File:asperities.svg — wikimedia commons, the free media repository*, (2023)  
<https://commons.wikimedia.org/w/index.php?title=File:Asperities.svg&oldid=659167170> (visited on 02/03/2023).
- [5] Y. Mo, K. T. Turner, and I. Szlufarska, "Friction laws at the nanoscale", *Nature* **457**, 1116–1119 (2009).
- [6] M. Dienwiebel, N. Pradeep, G. S. Verhoeven, H. W. Zandbergen, and J. W. Frenken, "Model experiments of superlubricity of graphite", *Surface Science* **576**, 197–211 (2005).