

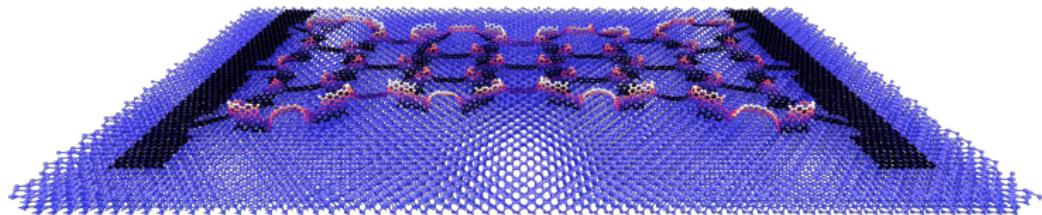
# Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

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# Outline

- ① Introduction
- ② Creating a graphene Kirigami system
- ③ Pilot study
- ④ Kirigami configuration search
- ⑤ Summary and outlook

# Thesis overview

## System preview

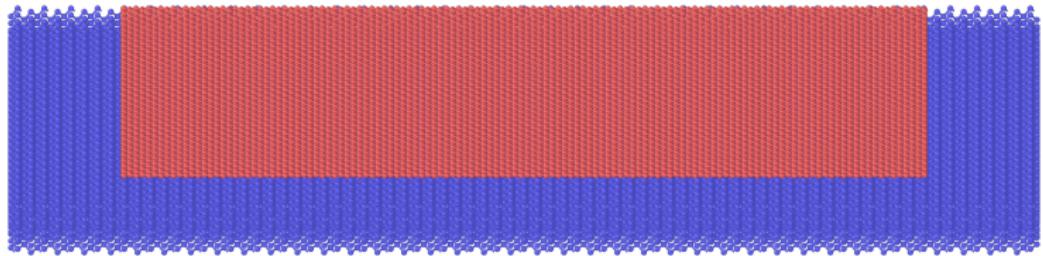


Figure: System of choice: Graphene sheet (red) on a silicon substrate (blue).

# Thesis overview

- ① **Sheet modification:** Atomic-scale cuts and stretching
- ② **Forward simulation:** Simulate system and measure friction
- ③ **Accelerated search:** Use machine learning to search for new designs

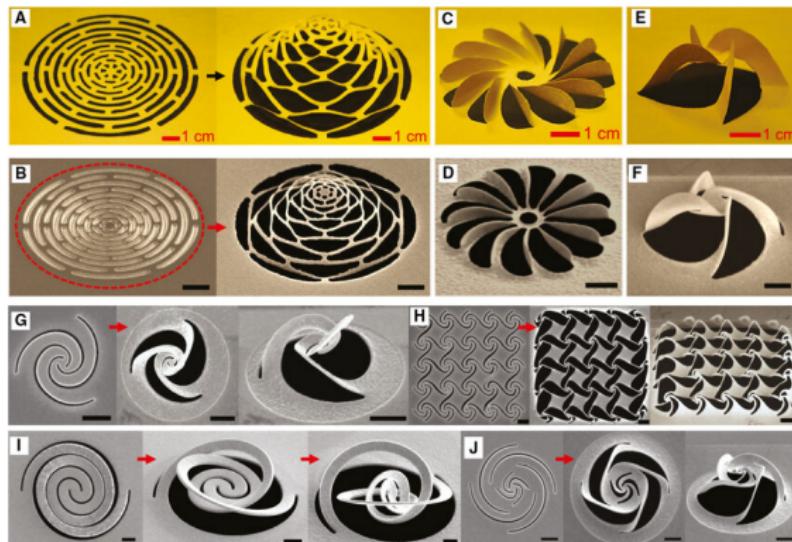
## Main research question

Can we control the friction of a nanoscale Kirigami sheet with pattern design and straining of the sheet?

# Motivation

## Kirigami

- Kirigami: Variation of origami with cuts permitted
- Designs: Macroscale → nanoscale

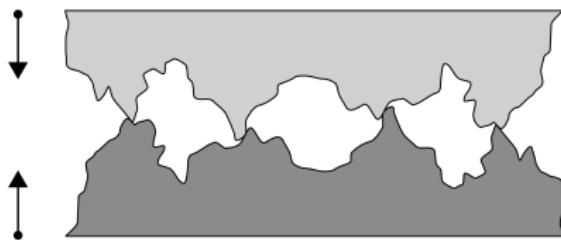


**Figure:** Example of macroscale Kirigami designs implemented on a microscale using a focused ion beam. Black scale bars:  $1 \mu\text{m}$ . Reproduced from [1].

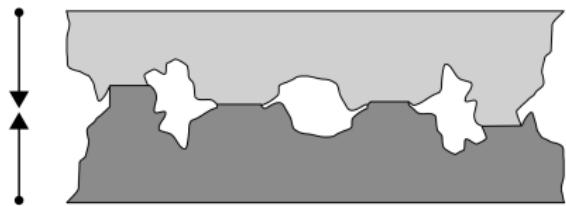
# Motivation

## Out-of-plane buckling

- Out-of-plane buckling
- Surface properties are important for friction
  - Asperity theory: Contact area



(a) Small load.



(b) High load.

**Figure:** Qualitative illustration of microscopic asperity deformation under increasing load.  
Reproduced from [2].

# Creating a graphene Kirigami system

① Introduction

② Creating a graphene Kirigami system

③ Pilot study

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⑤ Summary and outlook

# System setup

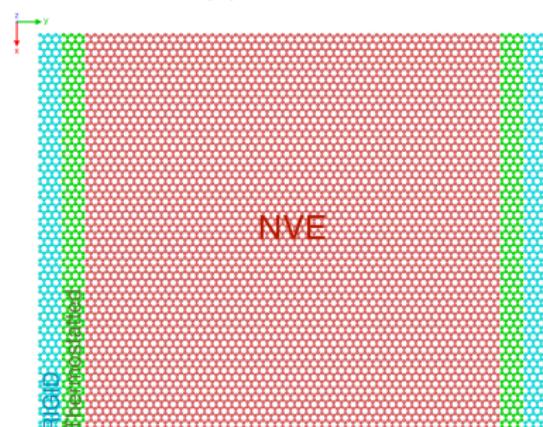


## Regions

- Red:  $NVE$
- Green: Thermostat  $NVT$
- Blue: Rigid

## System size

- Atoms  $\sim 60,000$
- Sheet  $\sim 130 \times 165 \text{ \AA}$



(b) Top view.

# Sheet Kirigami

## Indexing

$$M \in \mathbb{Z}_2^{62 \times 106}, \quad \text{Combinations} = 2^{6572} = 10^{1978}$$

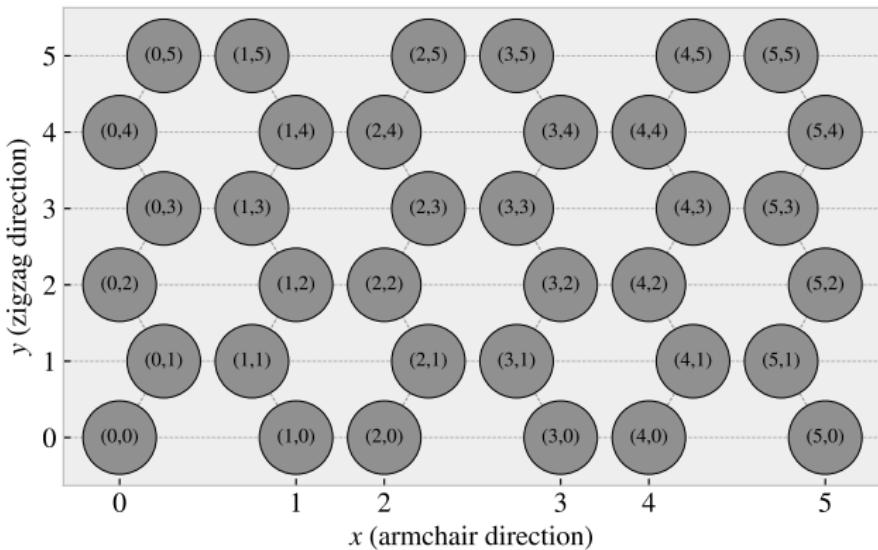
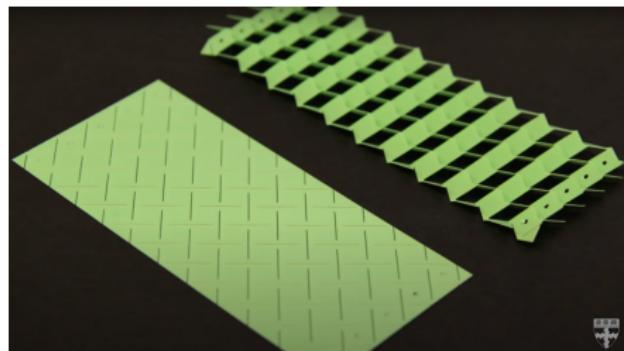


Figure: Graphene atom site indexing.

# Sheet Kirigami

Macroscale inspiration



(a) Tetrahedron: Alternating perpendicular cuts producing a tetrahedron-shaped surface buckling when stretched. Reproduced from [3].

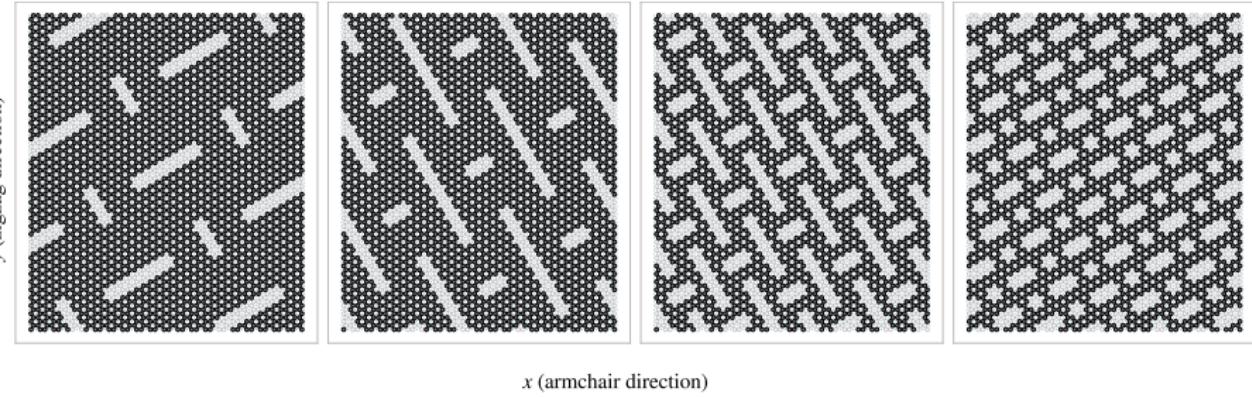
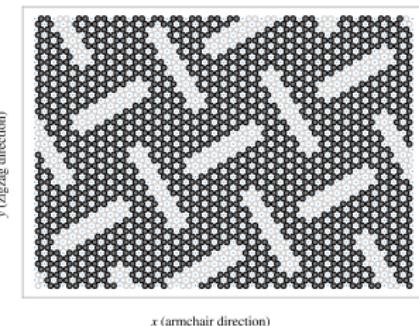
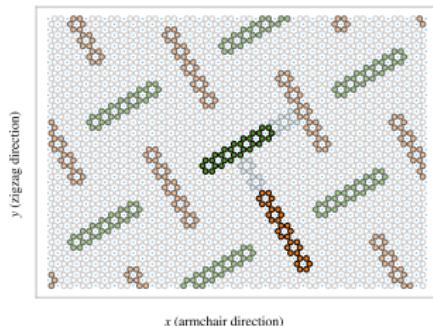


(b) Honeycomb: Scotch<sup>TM</sup> Cushion Lock<sup>TM</sup> [4] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [4].

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

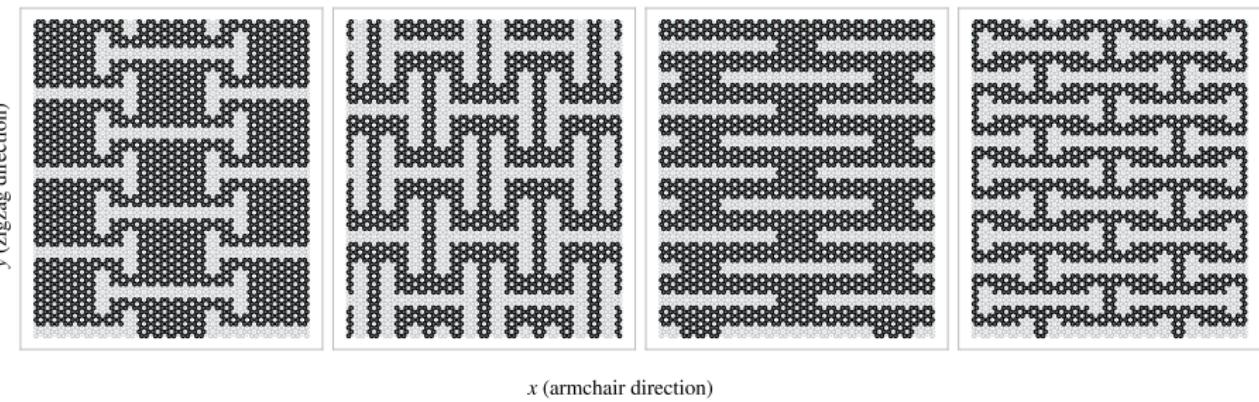
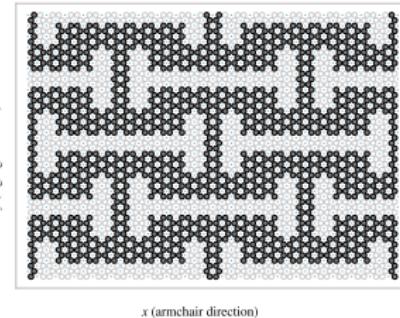
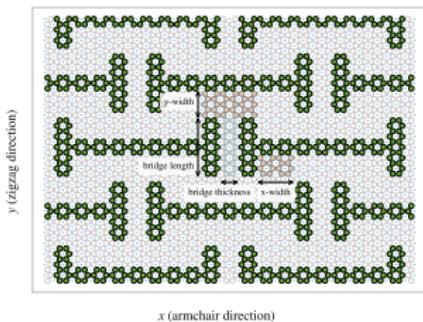
# Sheet Kirigami

## Tetrahedron patterns



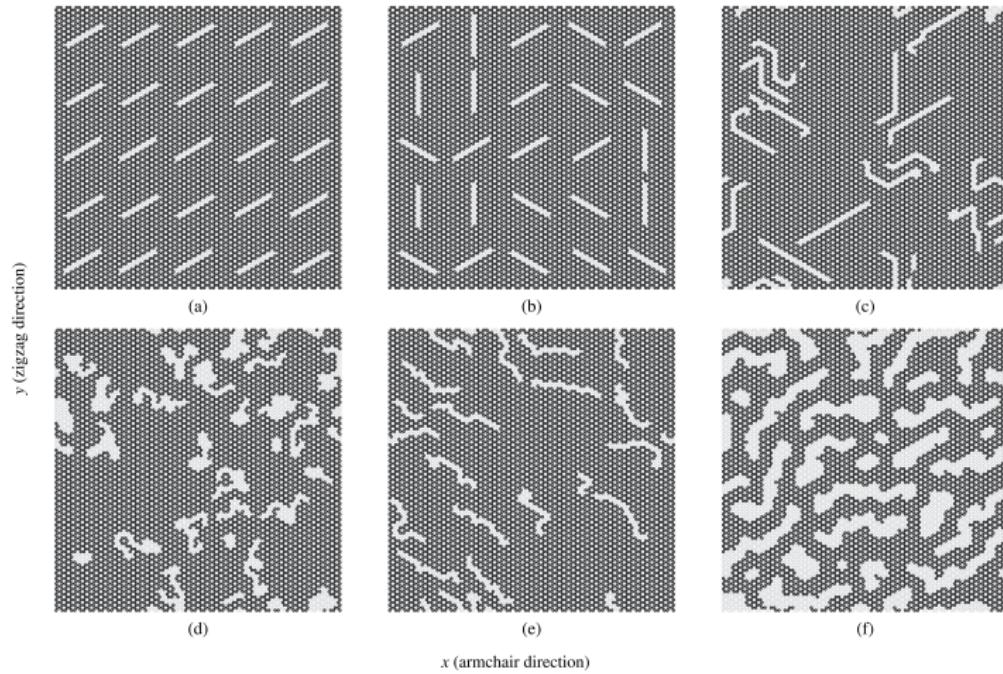
# Sheet Kirigami

## Honeycomb patterns



# Sheet Kirigami

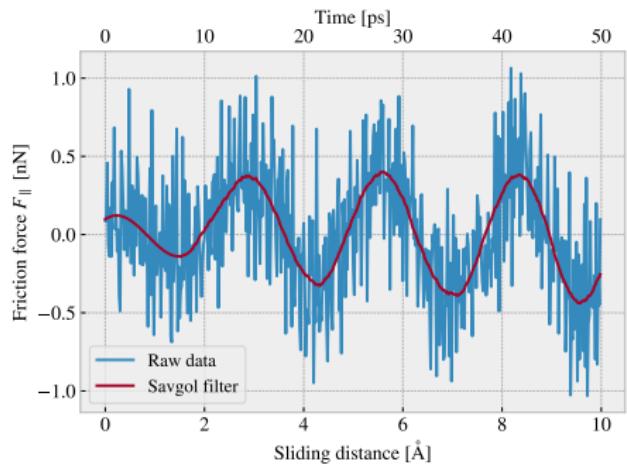
## Random walk patterns



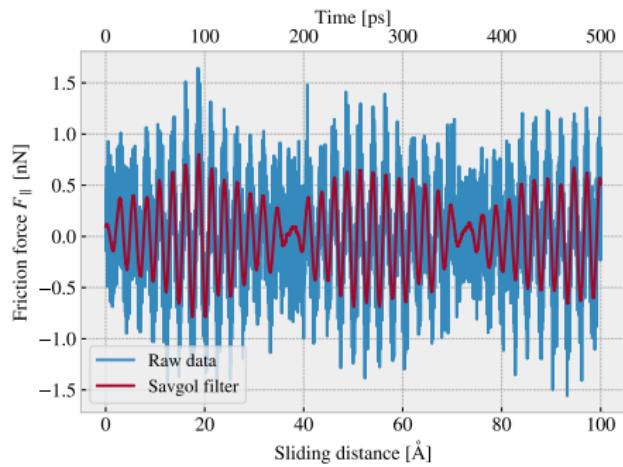
# Pilot study

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# Friction metrics



(a) 10  $\text{\AA}$  sliding.



(b) 100  $\text{\AA}$  sliding.

**Figure:** Friction force traces. The red line represents a Savgol filter.

# Out-of-plane buckling

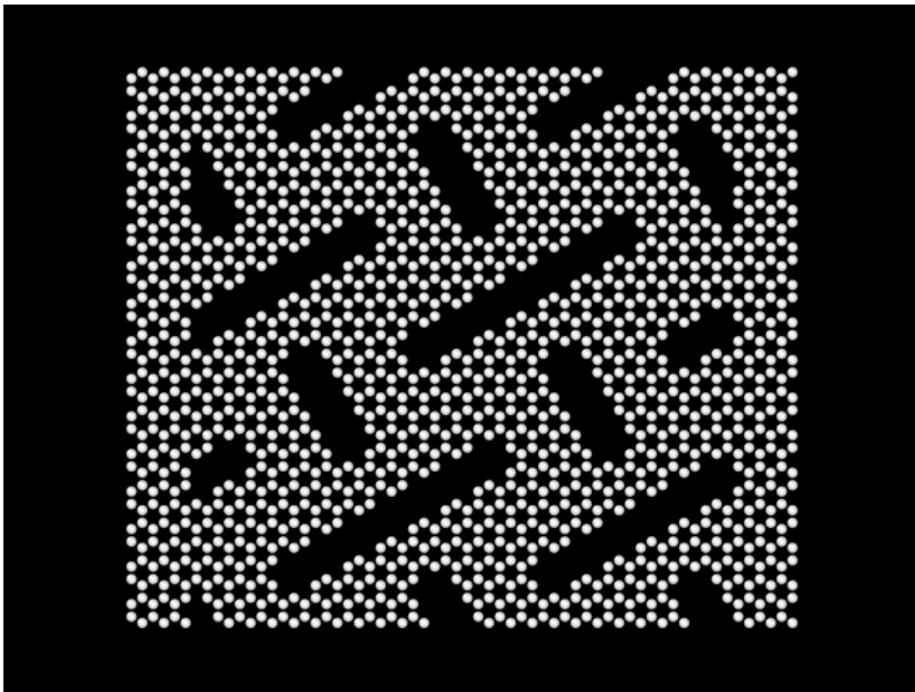
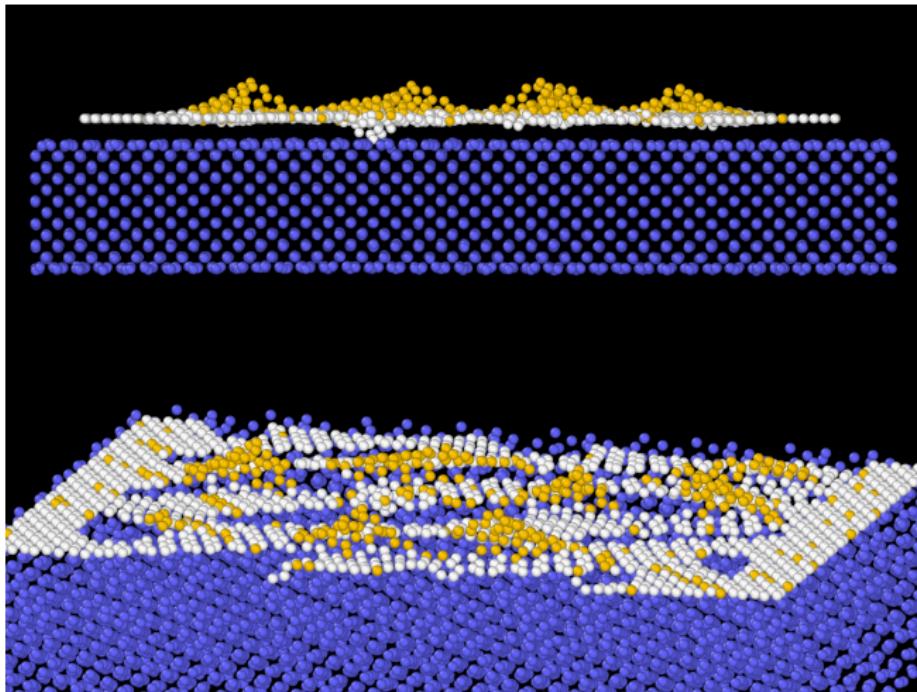


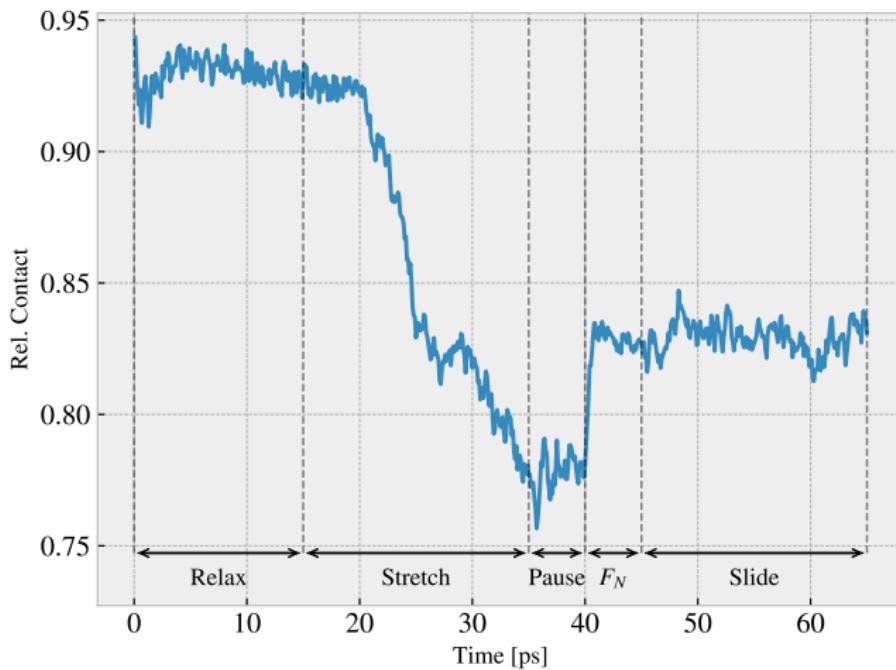
Figure: Kirigami sheet stretch in a vacuum.

# Out-of-plane buckling



**Figure:** Kirigami stretch in contact with the substrate.

# Out-of-plane buckling



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

# Contact-strain profile

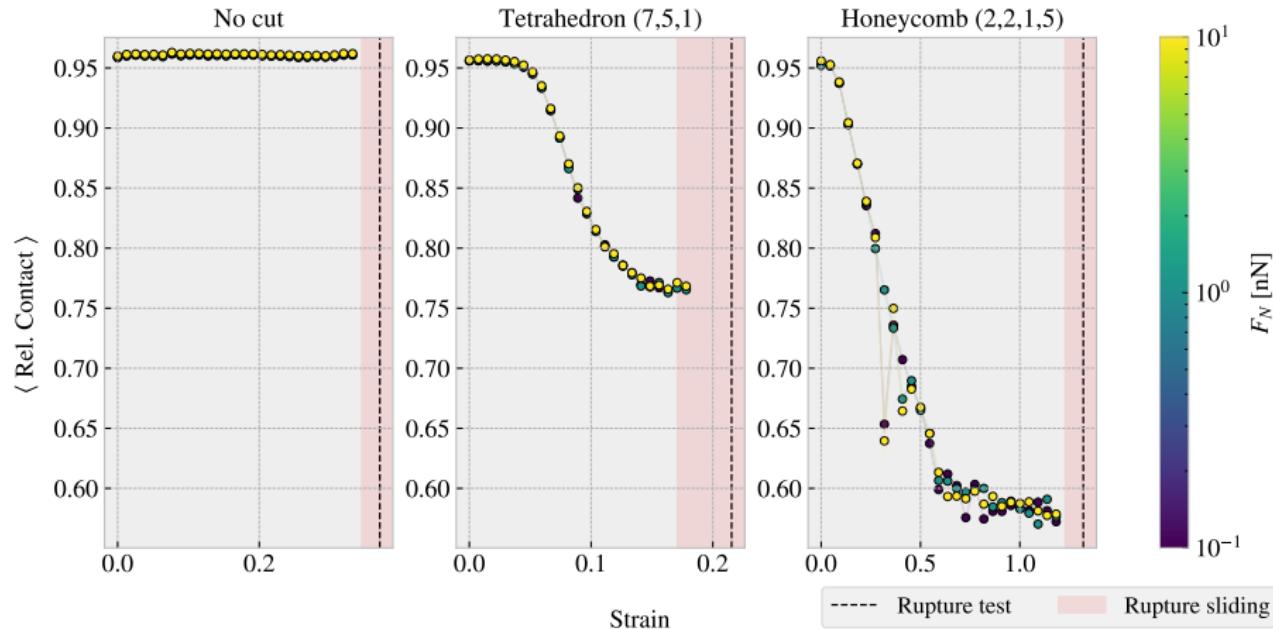


Figure: Contact-strain profile for  $F_N = \{0.1, 1, 10\}$  nN.

# Friction-strain profile

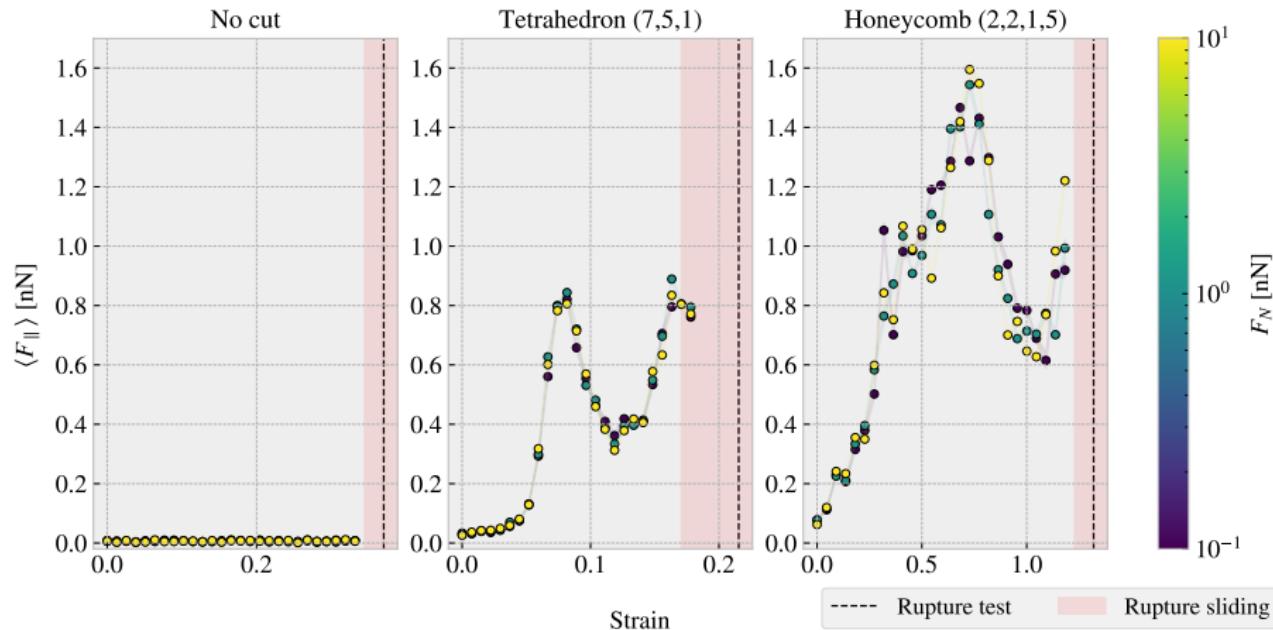
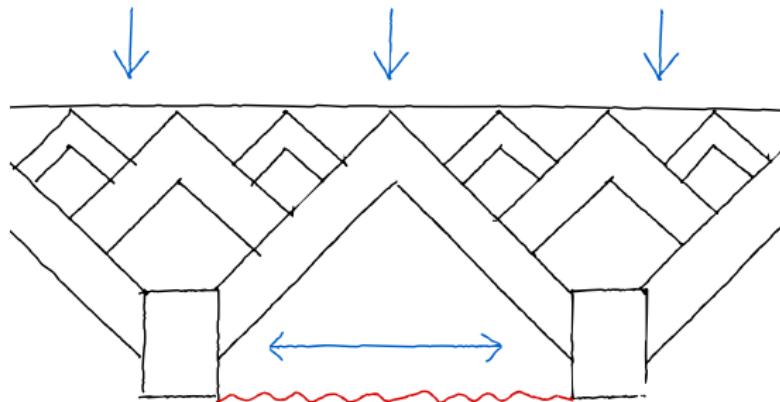


Figure: Friction-strain profile for  $F_N = \{0.1, 1, 10\}$  nN.

# Negative friction coefficient

Coupling of load to sheet tension

$$F_t = T \cdot F_N, \quad T = 6$$



**Figure:** Working sketch for a nanomachine design translating applied load to a strain of the sheet (shown in red).

# Negative friction coefficient

Tetrahedron results

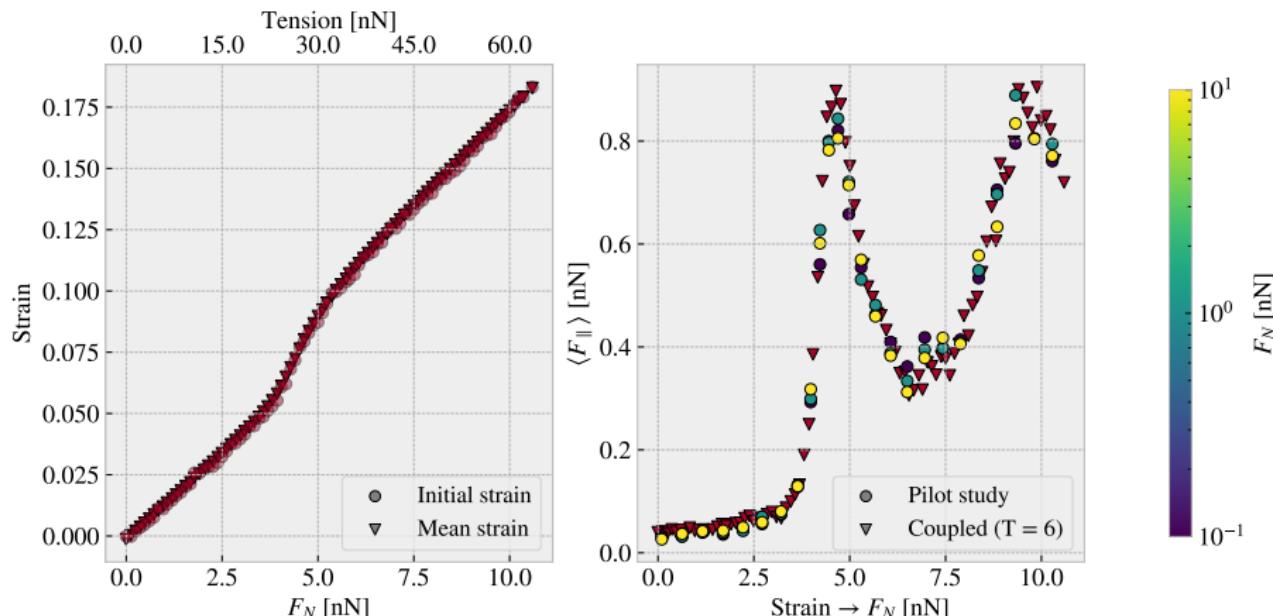


Figure: Tetrahedron (7, 5, 1)

# Negative friction coefficient

## Honeycomb results

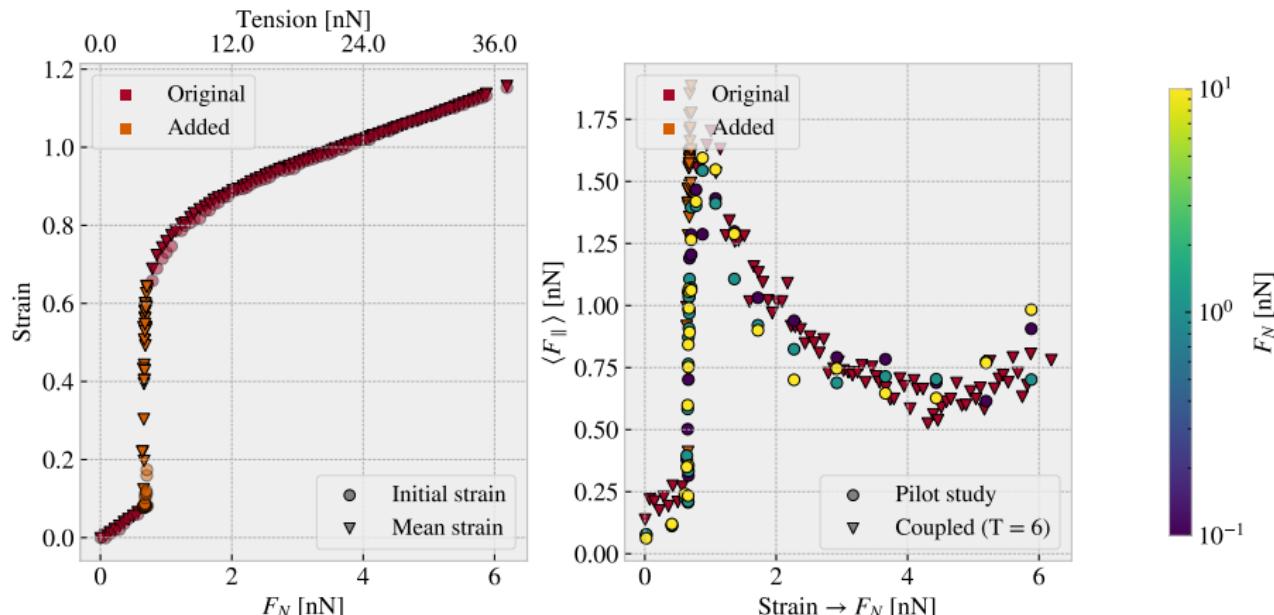
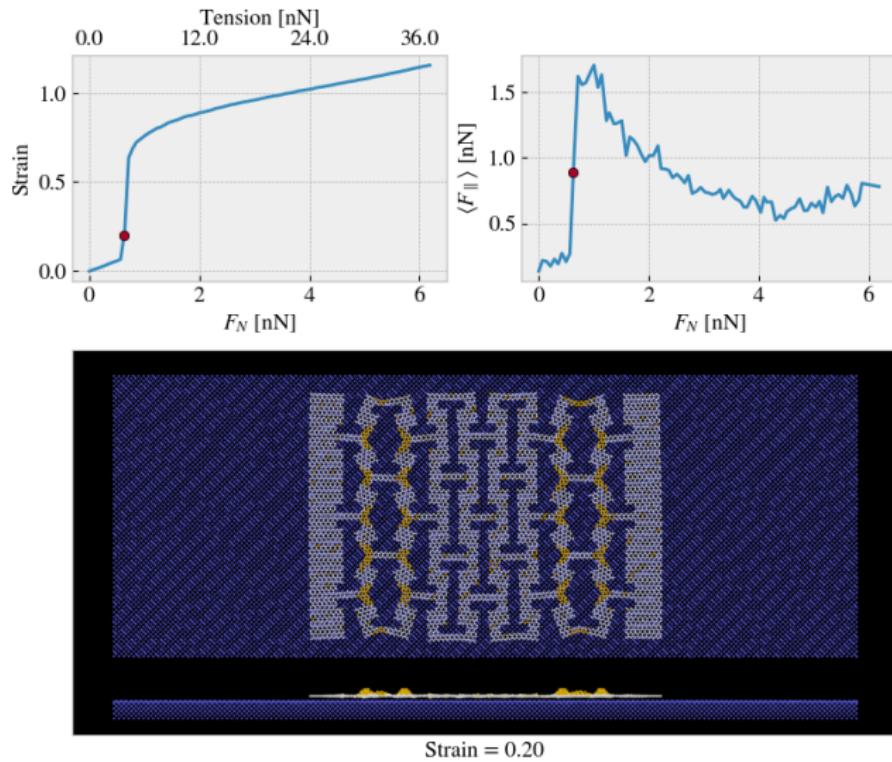


Figure: Honeycomb (2, 2, 1, 5)

# Negative friction coefficient

## Honeycomb deformations



# Kirigami configuration search

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# Machine learning

## Dataset

- 216 Kirigami configurations ( $\sim 10,000$  data points)

## Machine learning

- Input: Kirigami configuration, strain and load
- Output: Mean  $F_{\text{fric}}$ , max  $F_{\text{fric}}$ , contact area, porosity, rupture, rupture strain

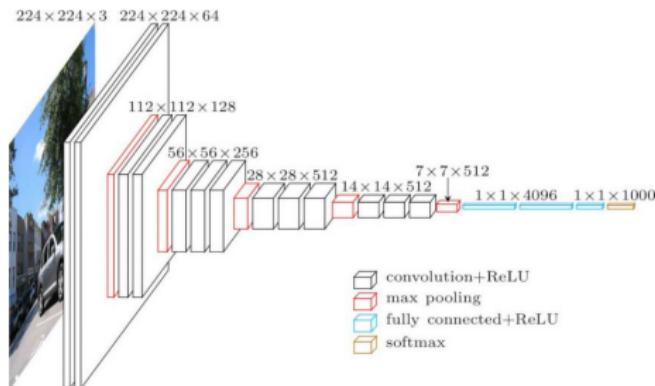


Figure: Convolutional network architecture. Reproduced from [5].

# Properties of interest

- (1)  $\min F_{\text{fric}}$ , (2)  $\max F_{\text{fric}}$ , (3)  $\max \Delta F_{\text{fric}}$ , (4) max drop.

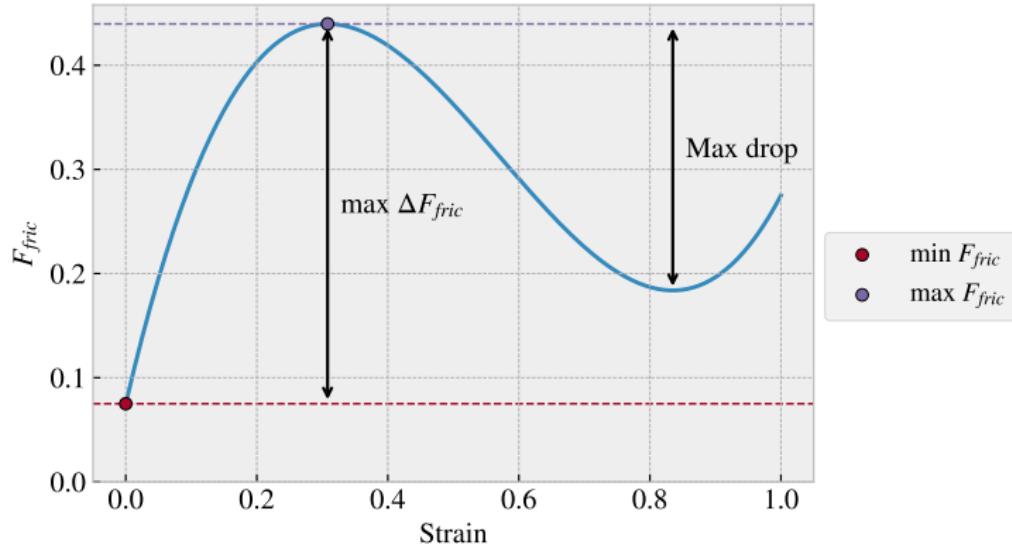


Figure: Properties of interest.

# Accelerated search for new designs

Two search approaches

- ① Extended dataset search

Tetrahedron:  $1.35 \times 10^5$ , Honeycomb:  $2.025 \times 10^6$ , Random walk:  $10^4$

- ② Genetic algorithm

- Survival of the fittest

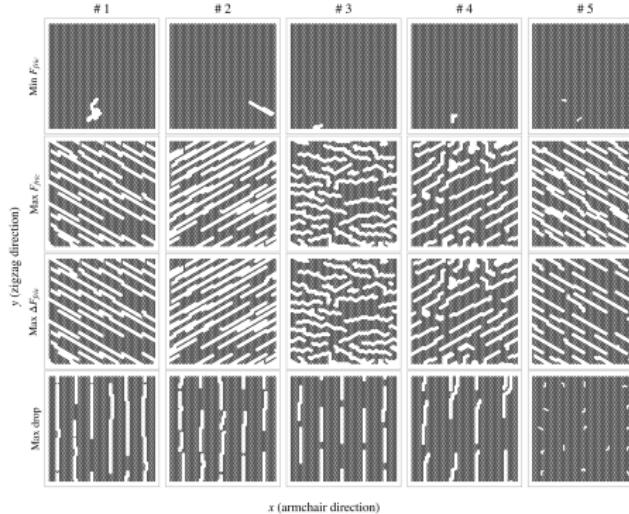
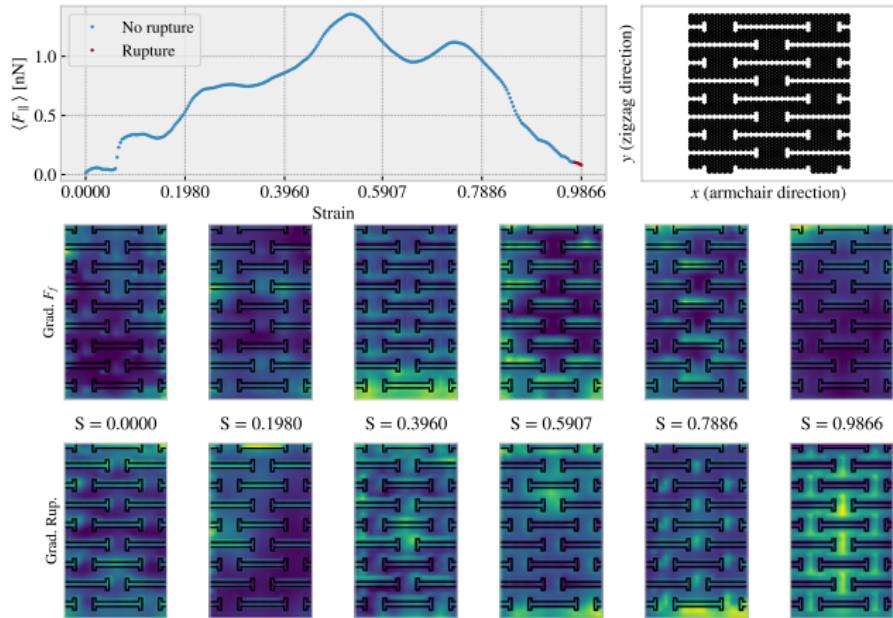


Figure: Top 5 candidates for random walk extended dataset accelerated search.

# Accelerated search

## Grad-CAM



**Figure:** Honeycomb (3, 3, 5, 3). Top: Friction-strain curve and configuration. Bottom: Grad-CAM analysis.

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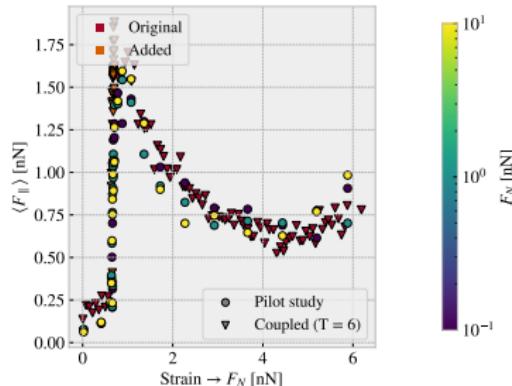
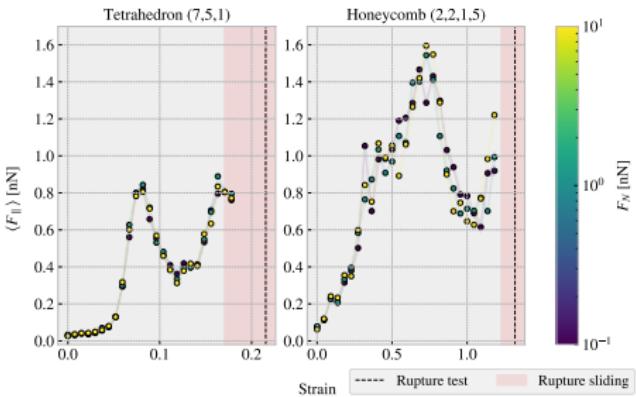
# Summary and outlook

## Key findings

- Non-monotonous friction-strain
- Negative friction coefficient
- Machine learning needs more data

## Further studies

- Underlying mechanism
  - Commensurability hypothesis
- Friction-strain relationship at different physical conditions
- Edge and thermostat effects
- Improve dataset with active learning





Mikkel Metzsch Jensen



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Kirigami Using Molecular Dynamics and  
Neural Networks

Designs for a negative friction coefficient

# 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).
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- [3] L. Burrows, *New pop-up strategy inspired by cuts, not folds*, (Feb. 24, 2017)  
<https://seas.harvard.edu/news/2017/02/new-pop-strategy-inspired-cuts-not-folds>.
- [4] *Scotch cushion lock protective wrap*,  
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- [5] Neurohive, *VGG16 — Convolutional Network for Classification and Detection*, (2018) <https://neurohive.io/en/popular-networks/vgg16/> (visited on 05/07/2023).