

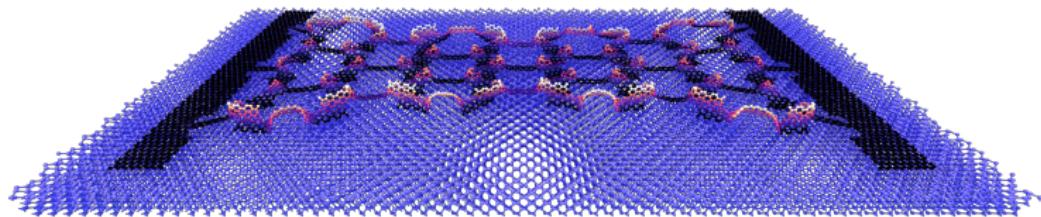
Predicting Frictional Properties of Graphene Kirigami Using Molecular Dynamics and Neural Networks

Designs for a negative friction coefficient

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University of Oslo

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Outline

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Thesis overview

Motivation

② Creating a graphene Kirigami system

System setup

Kirigami design

③ Pilot study

Friction metrics

Out-of-plane buckling

Strain profiles

Negative friction coefficient

④ Kirigami configuration search

Machine learning

Accelerated search for new designs

⑤ Summary and outlook

Thesis overview

System preview

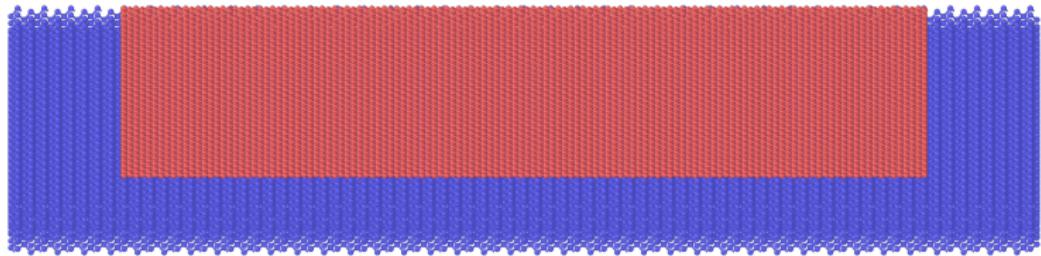


Figure: System of choice: Graphene sheet (red) on a silicon substrate (blue).

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

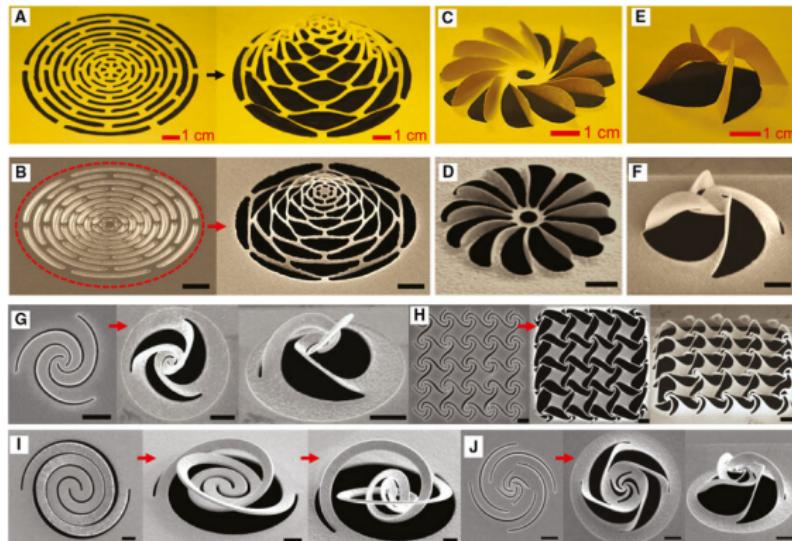
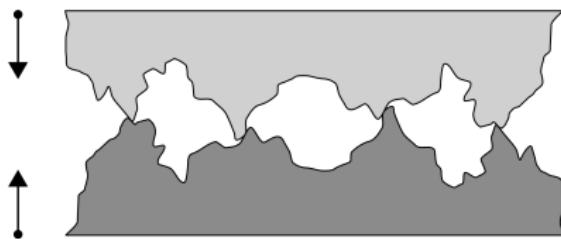


Figure: Example of macroscale Kirigami designs implemented on a microscale using a focused ion beam. Black scale bars: $1 \mu\text{m}$. Reproduced from [1].

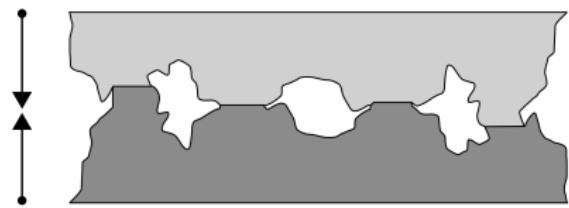
Motivation

Out-of-plane buckling

- Out-of-plane buckling
- Surface properties are important for friction
 - Asperity theory: Contact area
 - Frenkel–Kontorova models: Commensurability



(a) Small load.



(b) High load.

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

Creating a graphene Kirigami system

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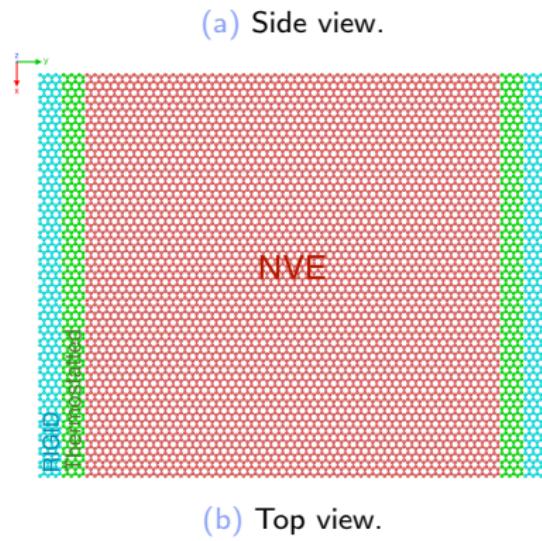


Regions

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

System size

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



Sheet Kirigami

Indexing

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

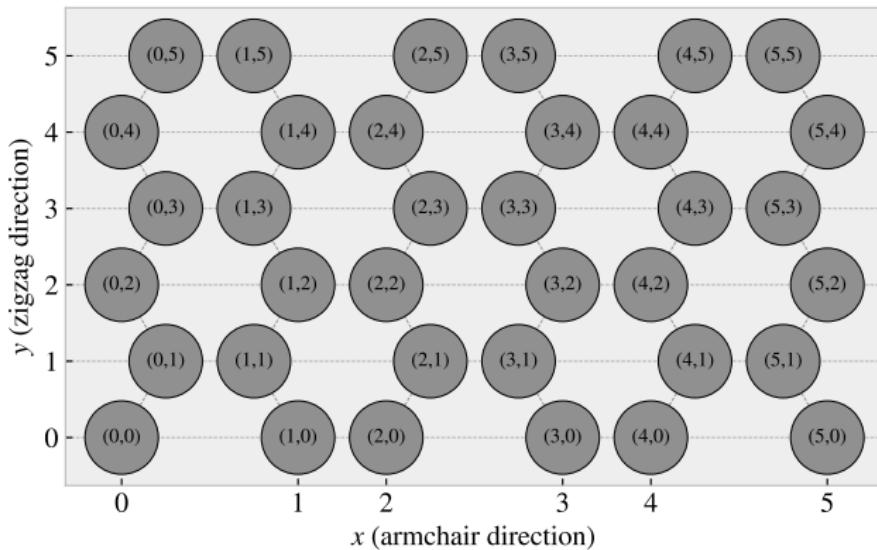


Figure: Graphene atom site indexing.

Sheet Kirigami

Indexing

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

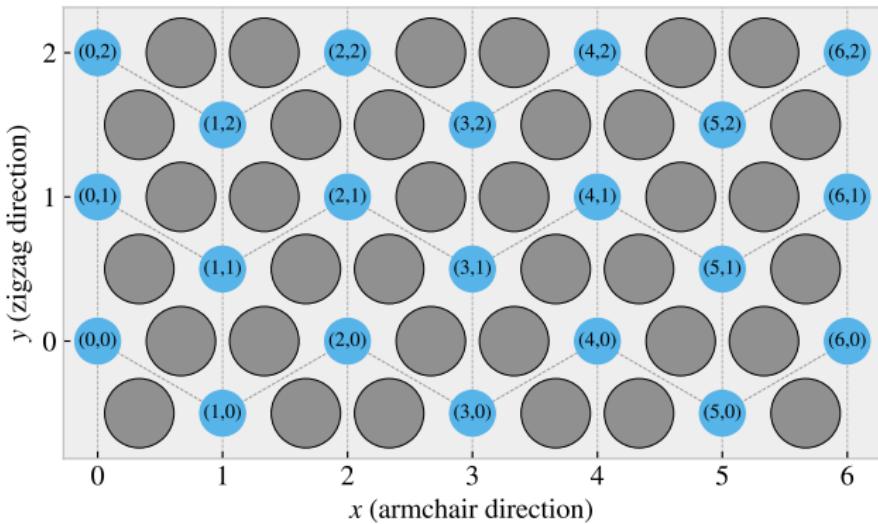
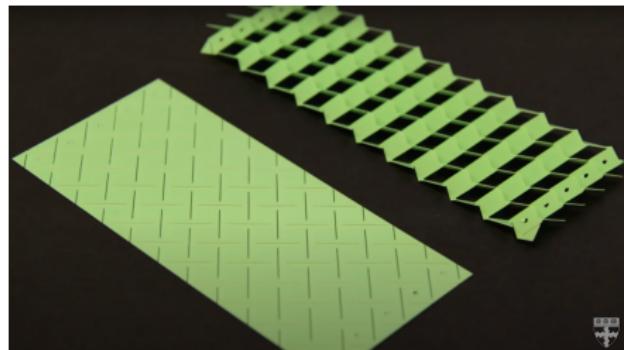


Figure: Graphene center element indexing.

Sheet Kirigami

Macroscale inspiration



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

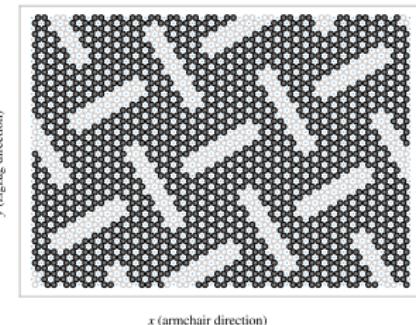
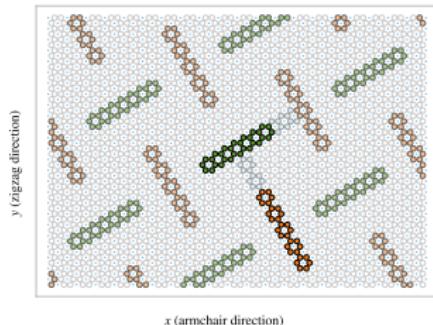


(b) Honeycomb: ScotchTM Cushion LockTM [4] producing a honeycomb-shaped surface buckling when stretched. Reproduced from [4].

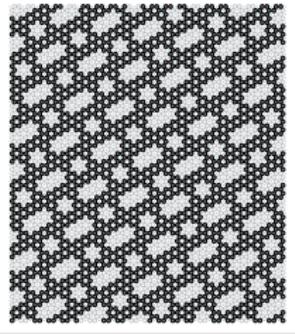
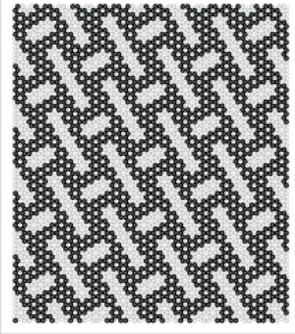
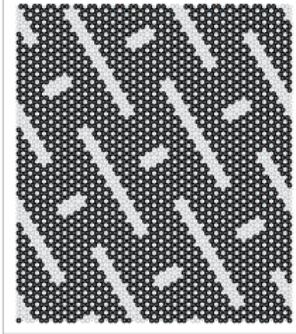
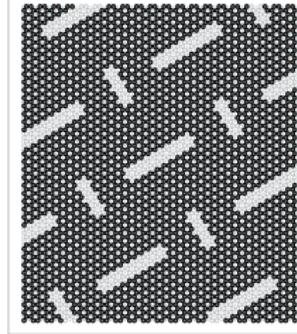
Figure: Macroscale kirigami cut patterns used as inspiration for the nanoscale implementation.

Sheet Kirigami

Tetrahedron patterns



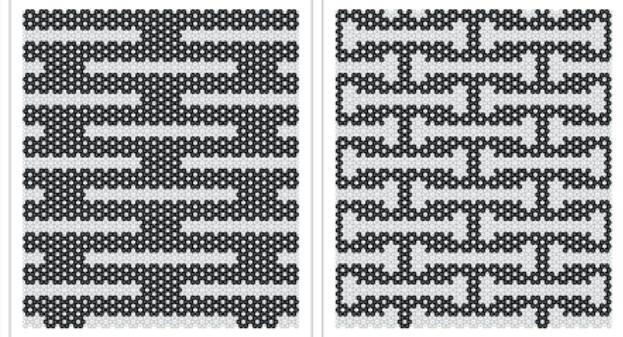
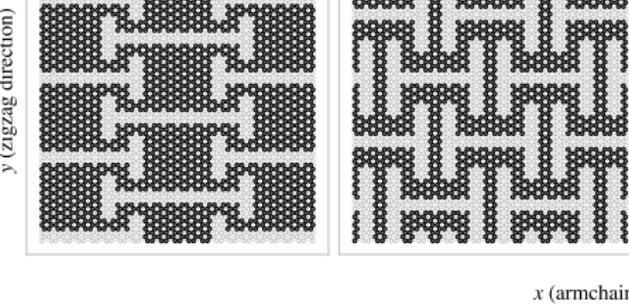
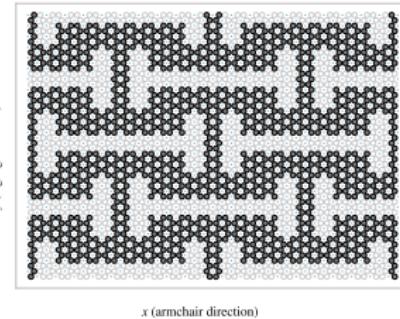
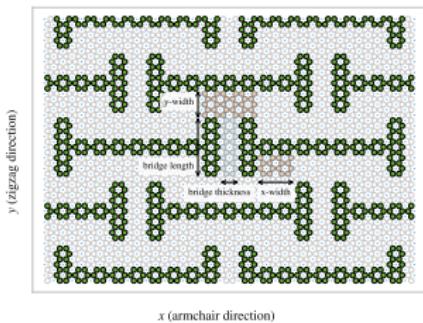
y (zigzag direction)



x (armchair direction)

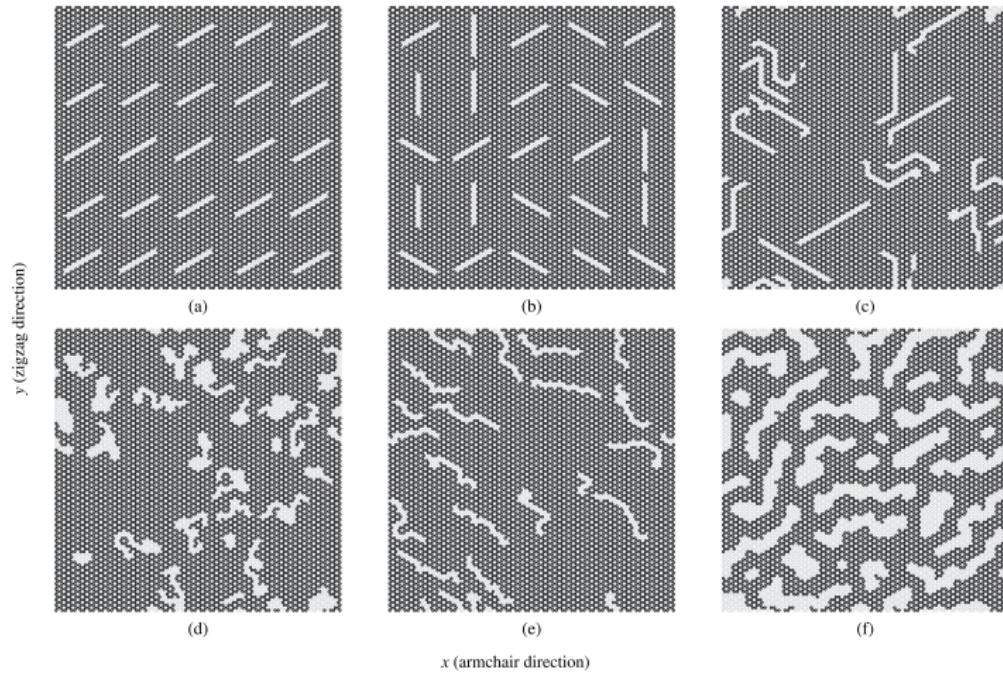
Sheet Kirigami

Honeycomb patterns



Sheet Kirigami

Random walk patterns



Pilot study

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Negative friction coefficient

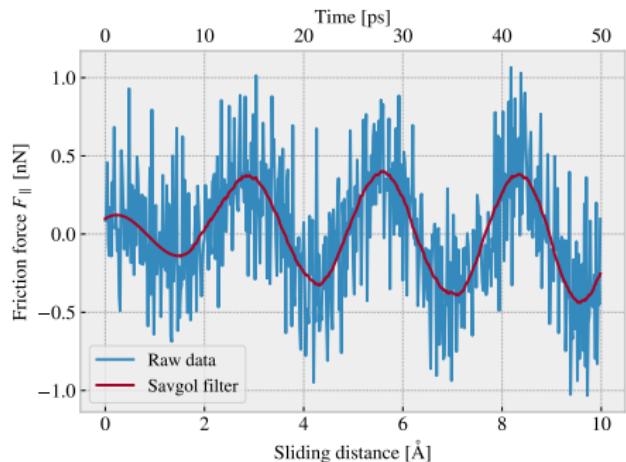
④ Kirigami configuration search

Machine learning

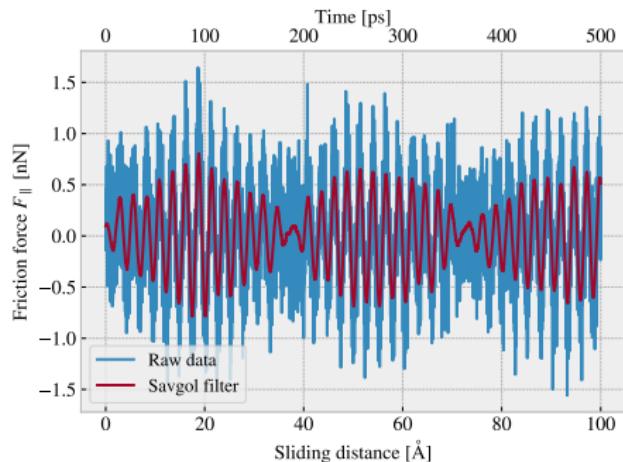
Accelerated search for new designs

⑤ Summary and outlook

Friction metrics



(a) 10 \AA sliding.



(b) 100 \AA sliding.

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

$T = 300 \text{ K}$, $v = 20 \text{ m/s}$, $K = \infty$.

Out-of-plane buckling

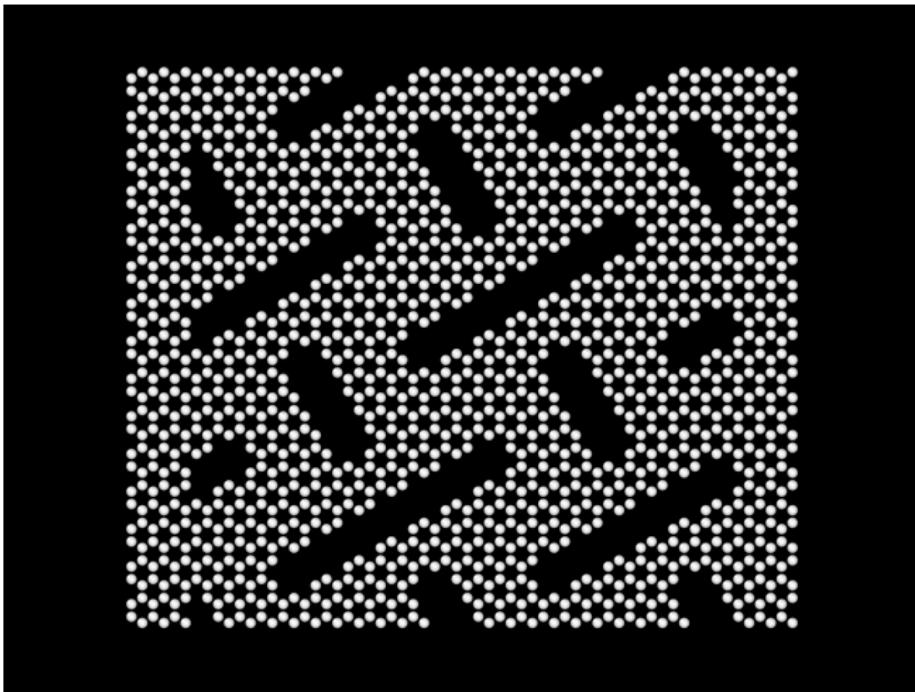


Figure: Kirigami sheet stretch in a vacuum.

Out-of-plane buckling

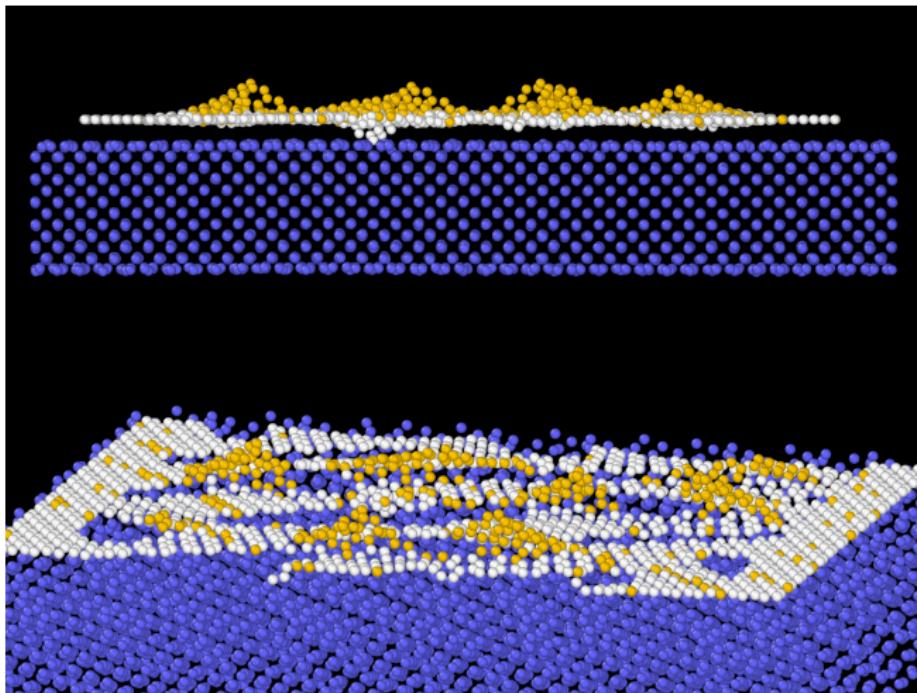


Figure: Kirigami stretch in contact with the substrate.

Out-of-plane buckling

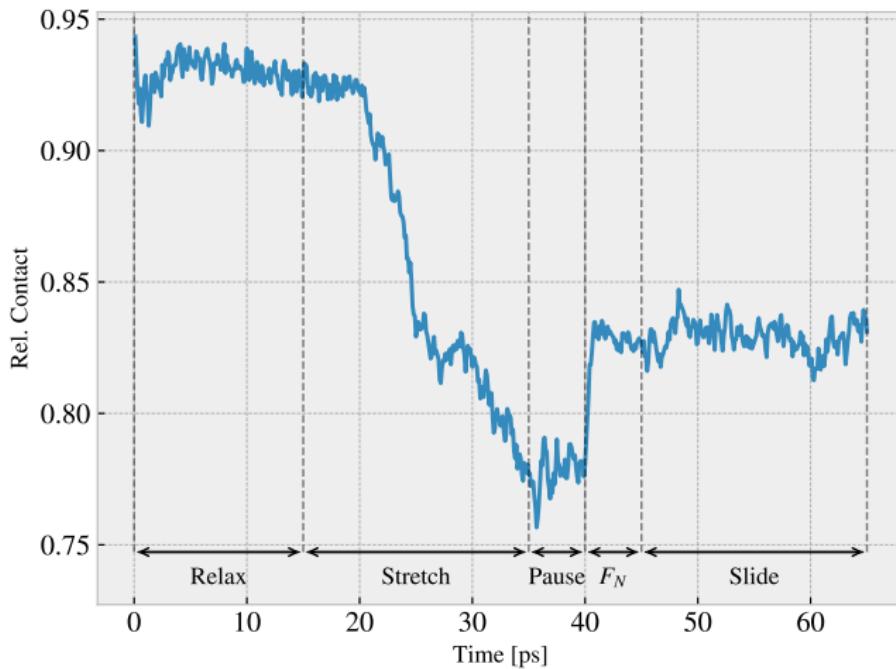


Figure: Contact area approximation: Number of C–Si bonds within a threshold distance of 110% the LJ interaction equilibrium distance.

Contact-strain profile

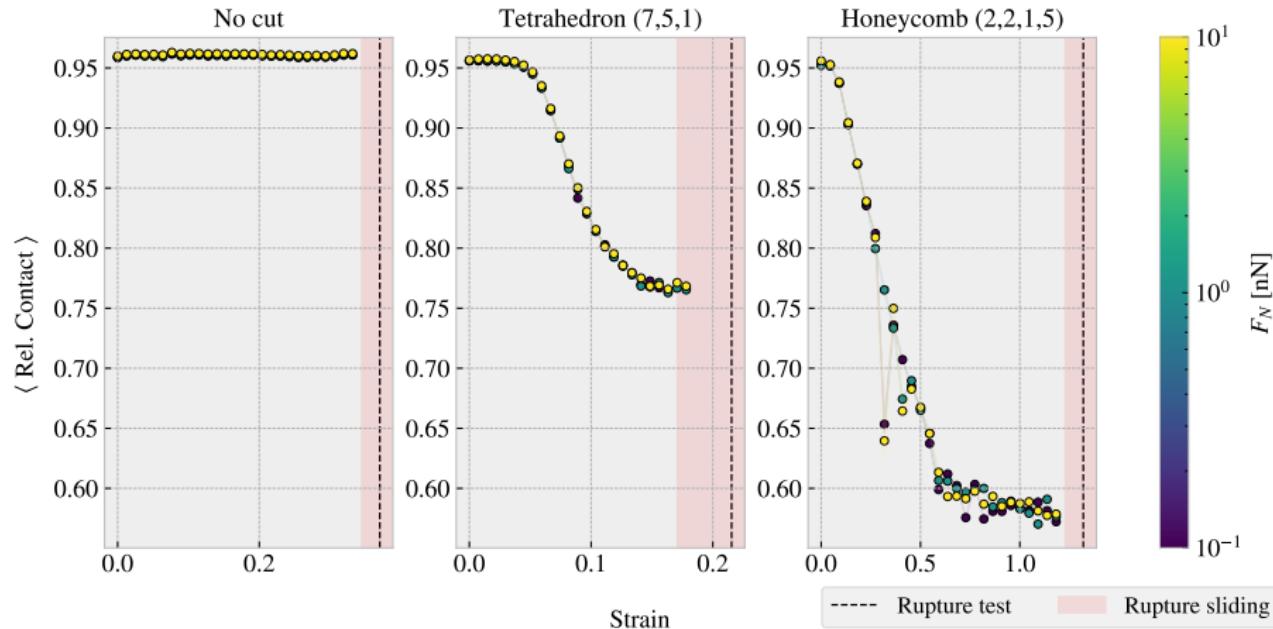


Figure: Contact-strain profile for $F_N = \{0.1, 1, 10\}$ nN.

Friction-strain profile

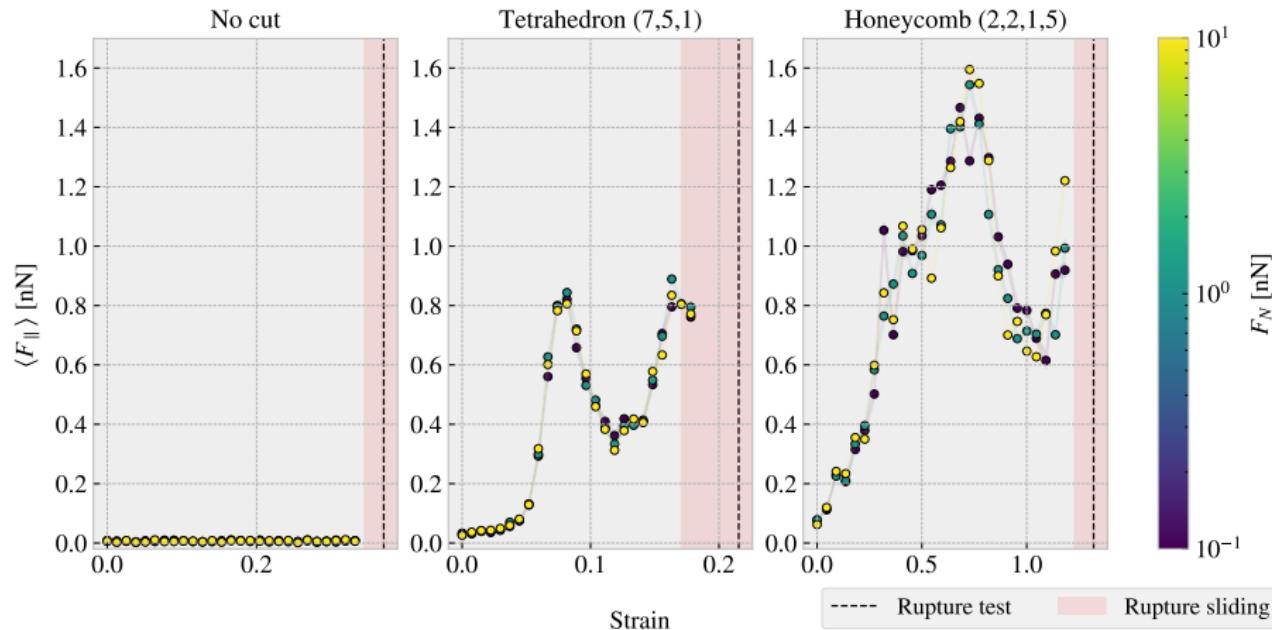


Figure: Friction-strain profile for $F_N = \{0.1, 1, 10\}$ nN.

Negative friction coefficient

Coupling of load to sheet tension

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

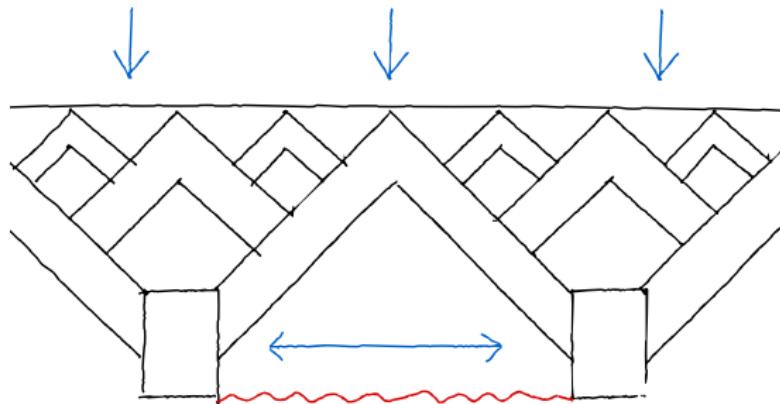


Figure: Working sketch for a nanomachine design translating applied load (from the top of the figure) to a straining of the graphene sheet (shown in red).

Negative friction coefficient

Tetrahedron results

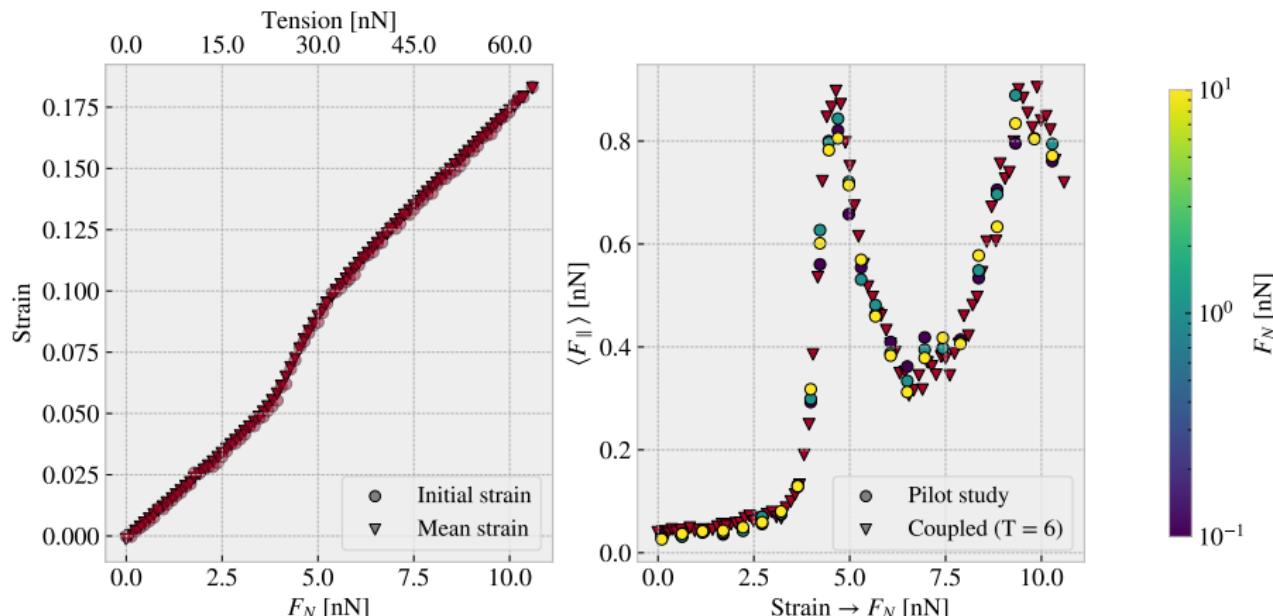


Figure: Tetrahedron (7, 5, 1)

Negative friction coefficient

Honeycomb results

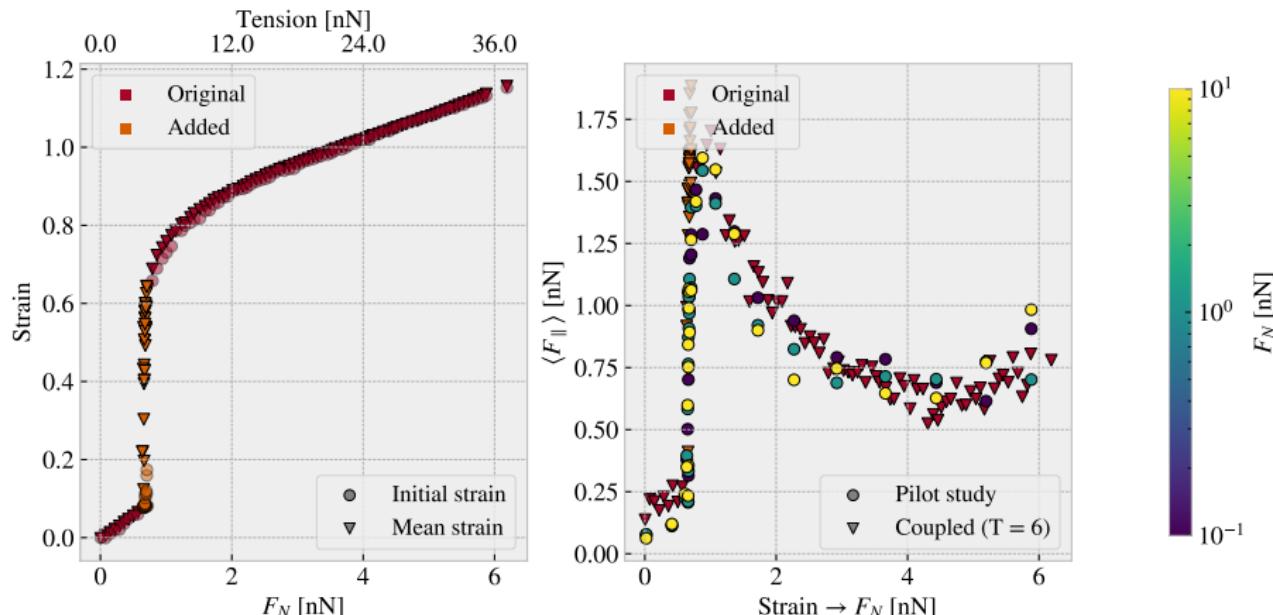


Figure: Honeycomb (2, 2, 1, 5)

Negative friction coefficient

Honeycomb deformations

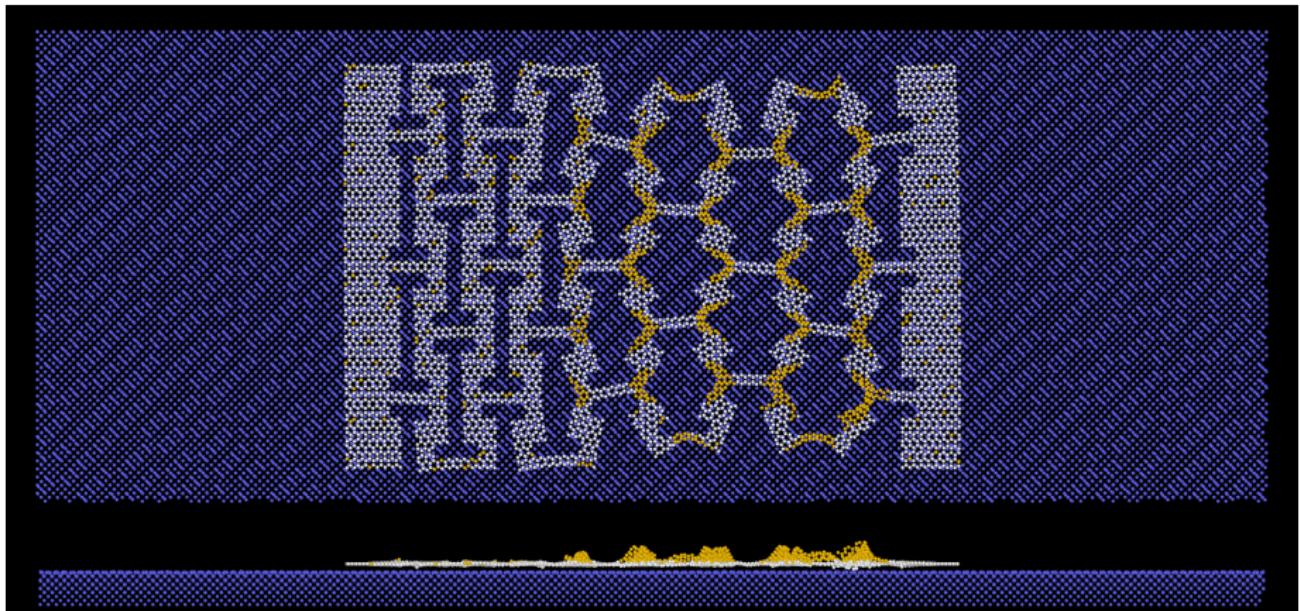


Figure: Honeycomb (2, 2, 1, 5) stretch.

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_{fric} , max F_{fric} , contact area, porosity, rupture, rupture strain

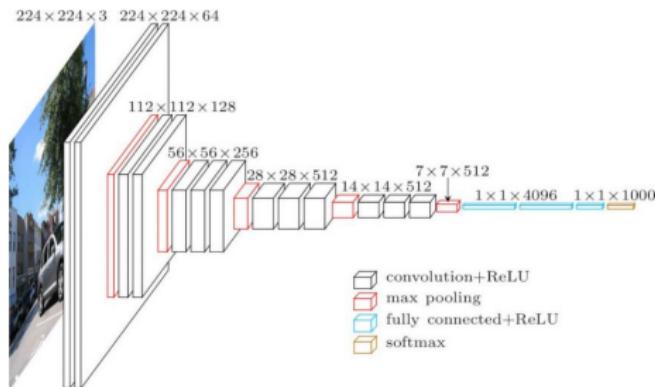


Figure: Convolutional network architecture. Reproduced from [5].

Machine learning

Results

- Good validation performance
- R^2 score

Properties of interest

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

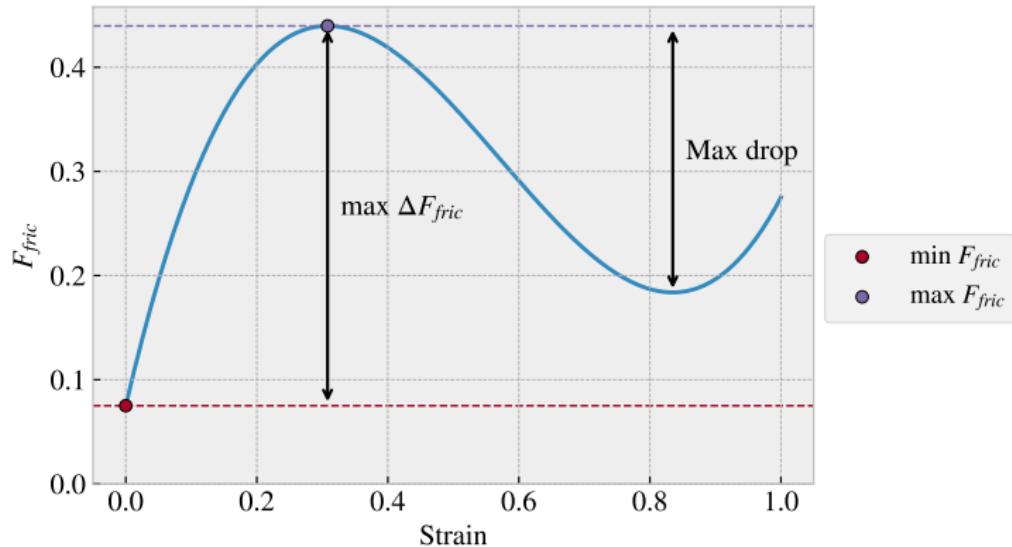


Figure: Properties of interest.

Accelerated search for new designs

Two search approaches

① Extended dataset search

Tetrahedron: 1.35×10^5 , Honeycomb: 2.025×10^6 , Random walk: 10^4

② Genetic algorithm

- Survival of the fittest

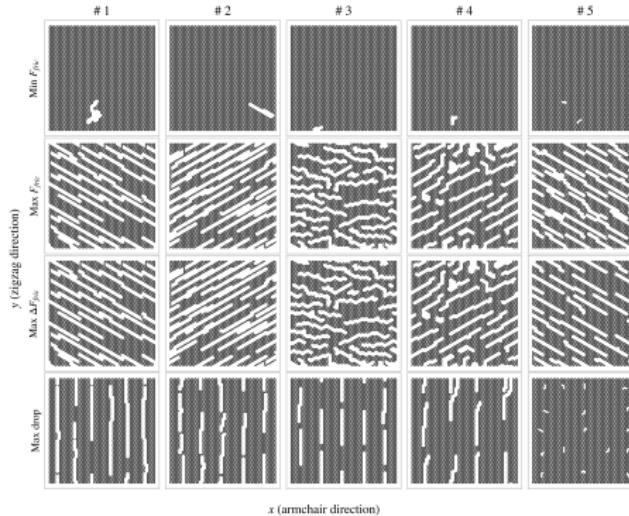


Figure: Top 5 candidates for random walk extended dataset accelerated search.

Accelerated search

Grad-CAM

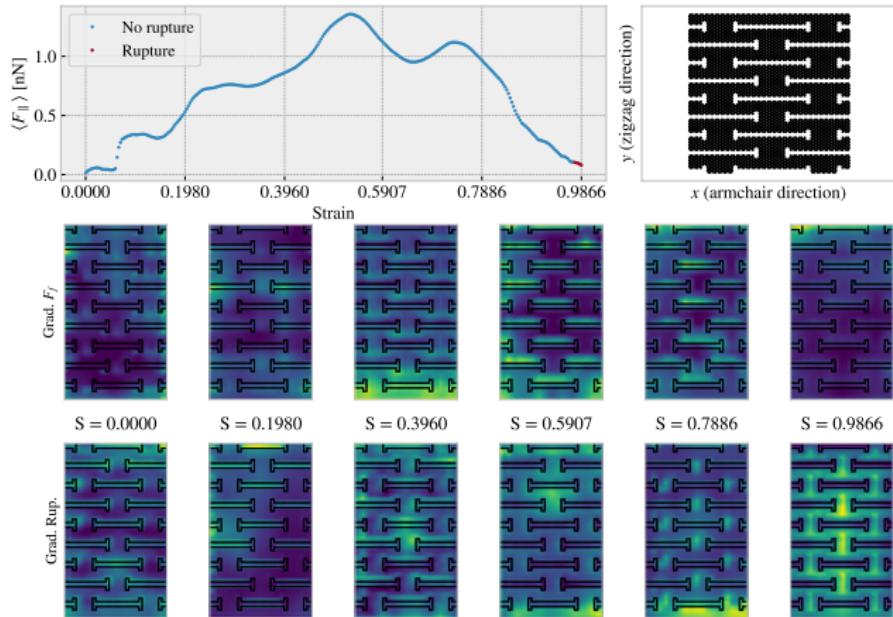


Figure: Honeycomb (3, 3, 5, 3). Top: Friction-strain curve and configuration. Bottom: Grad-CAM analysis.

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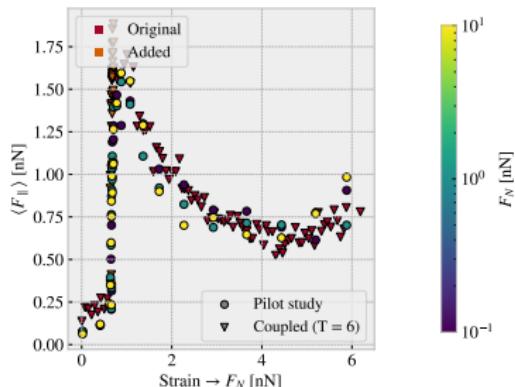
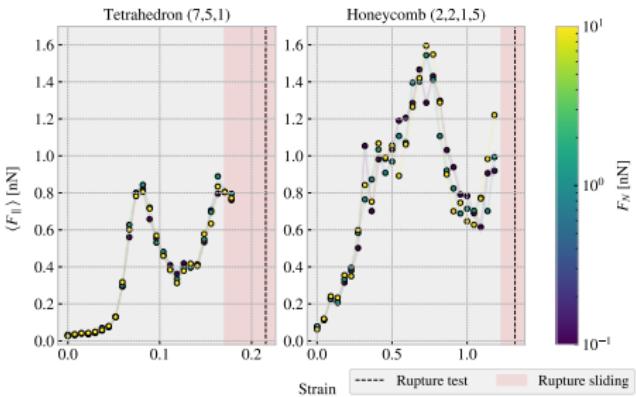
Summary and outlook

Key findings

- Non-monotonous friction-strain
- Coupled system → 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)
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- [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).