Kirigami and Origami Simulations of 2D Materials

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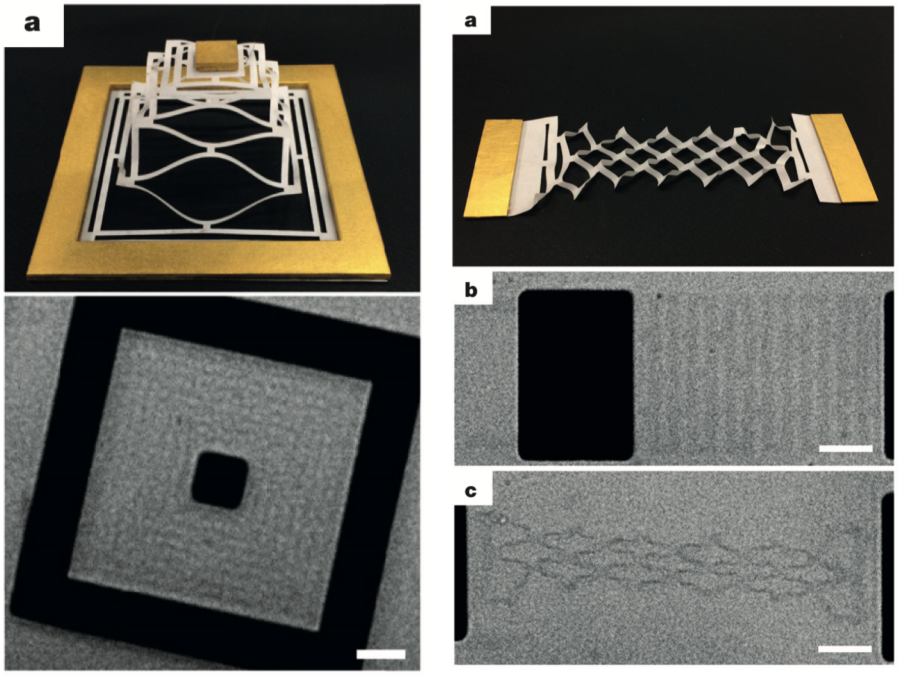
Introduction

- **Origami:** a creative art of paper folding, making 3D structures out of 2D sheets.
- **Kirigami:** a creative art of paper cutting and folding.
- **Two simulations:**
  - Nanoindentation on kirigami MoS_2
  - Origami of graphene under water flow
- **Our goal is to:** showcase mechanical properties of kirigami MoS_2, and demonstrate a new technique to fold graphene.



Blees, M. K. *et al*. Graphene kirigami. *Nature* **524,** 204 – 207 (2015)

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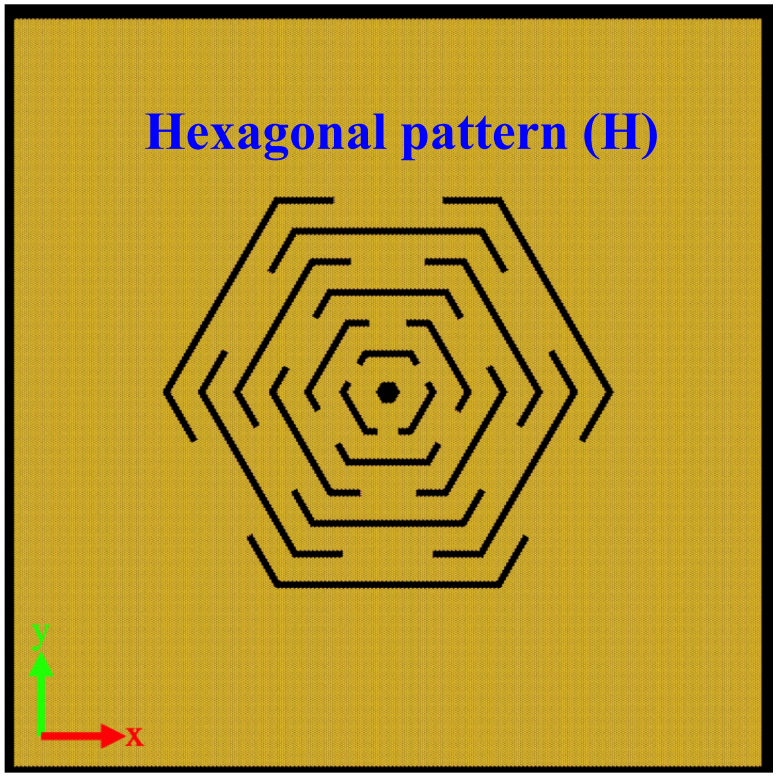
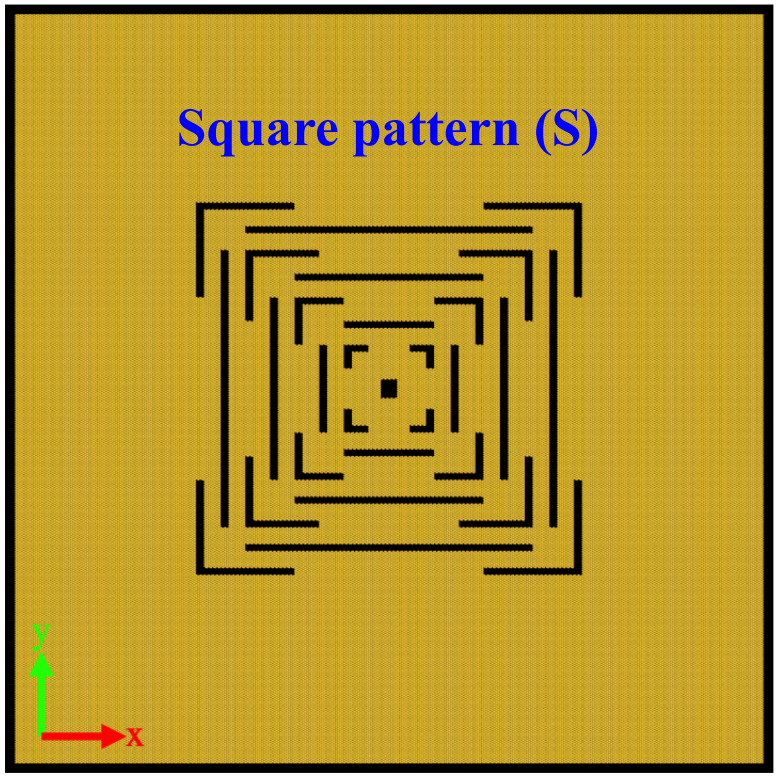
Kirigami Simulation Setup





- 100 × 100 nm^2 MoS_2 monolayer
- Black region: removed Mo and S atoms
- Conical indenter is applied in the middle from above (see video in next slides)

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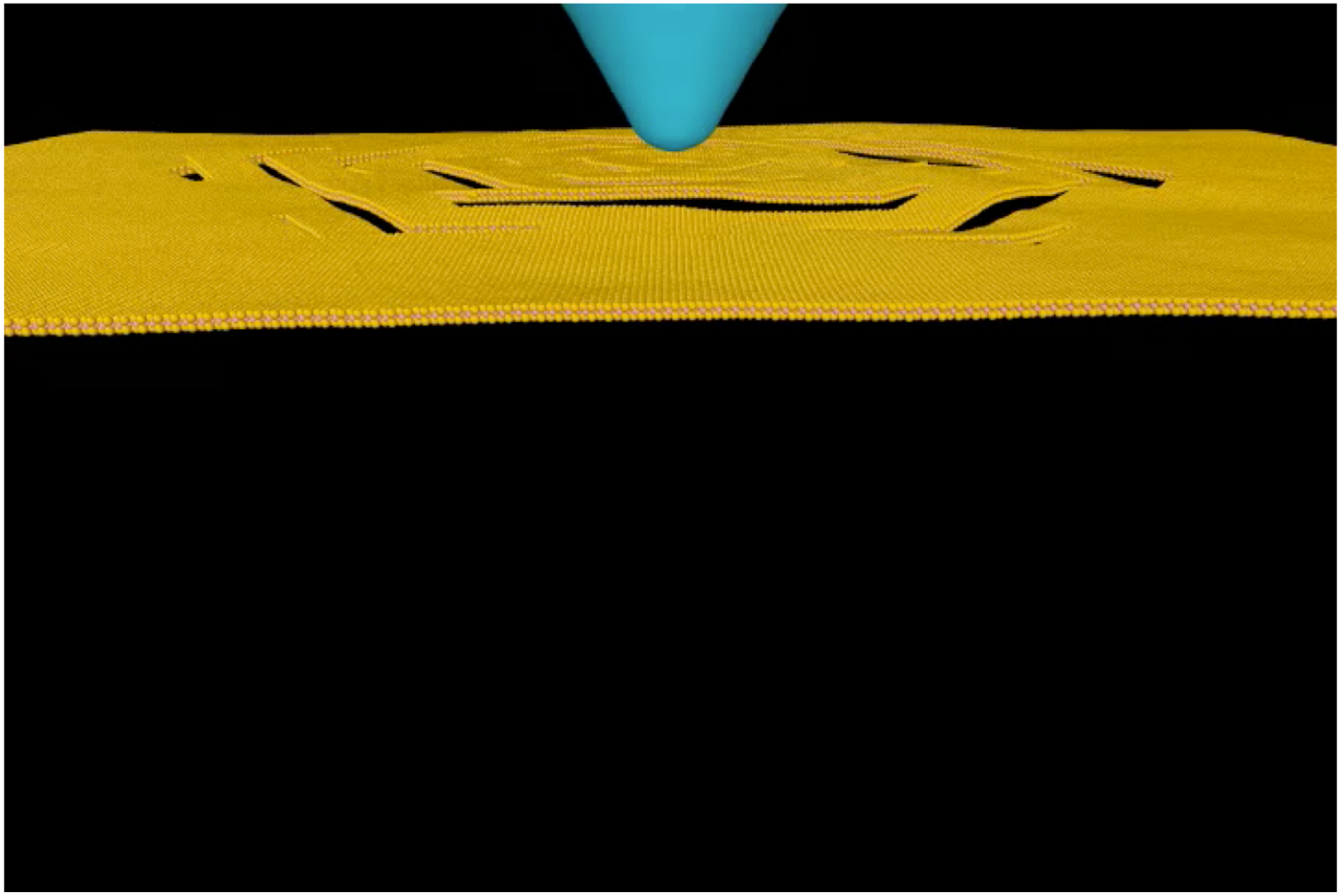
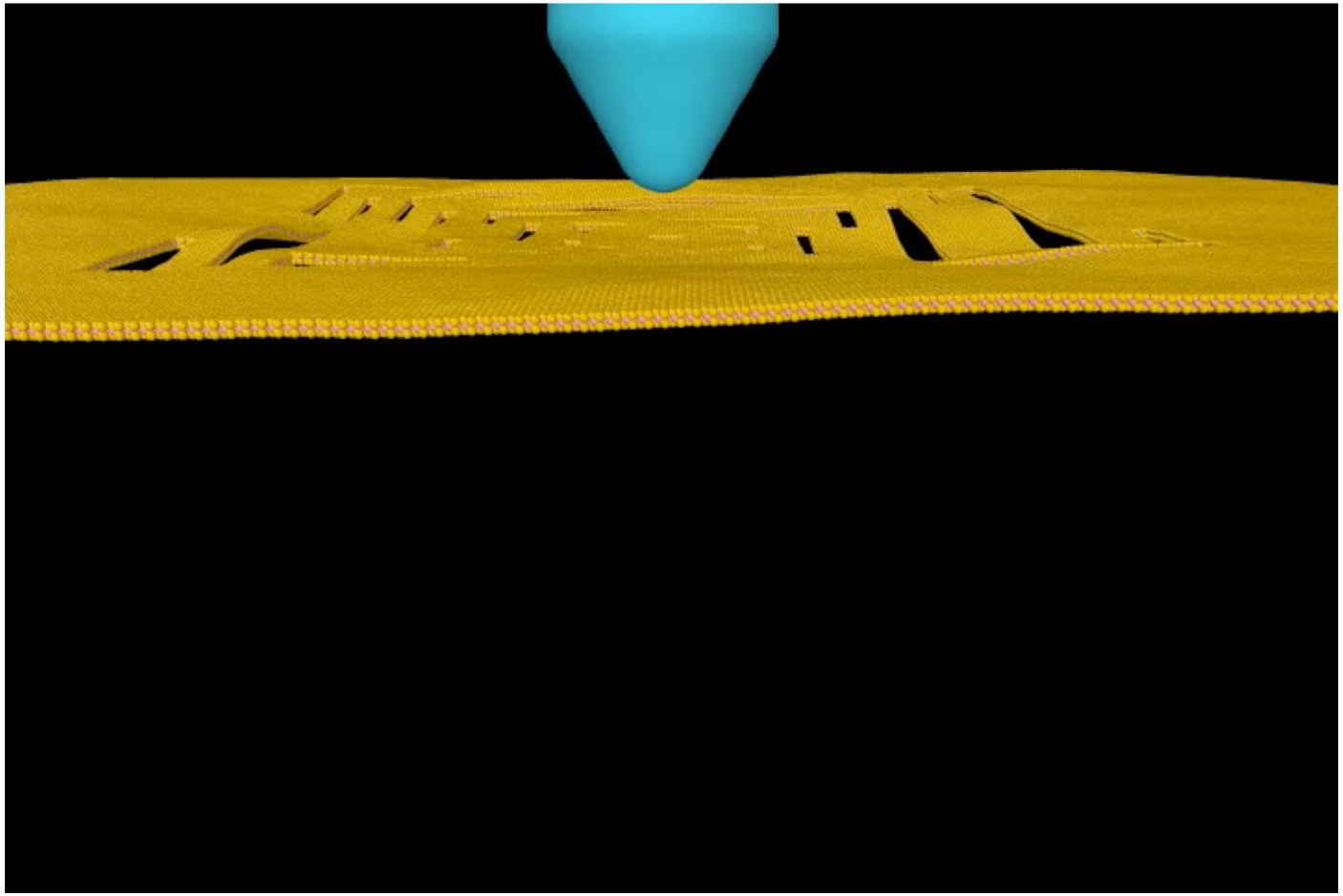
Visualization

Visualization of nanoindentation: part 1

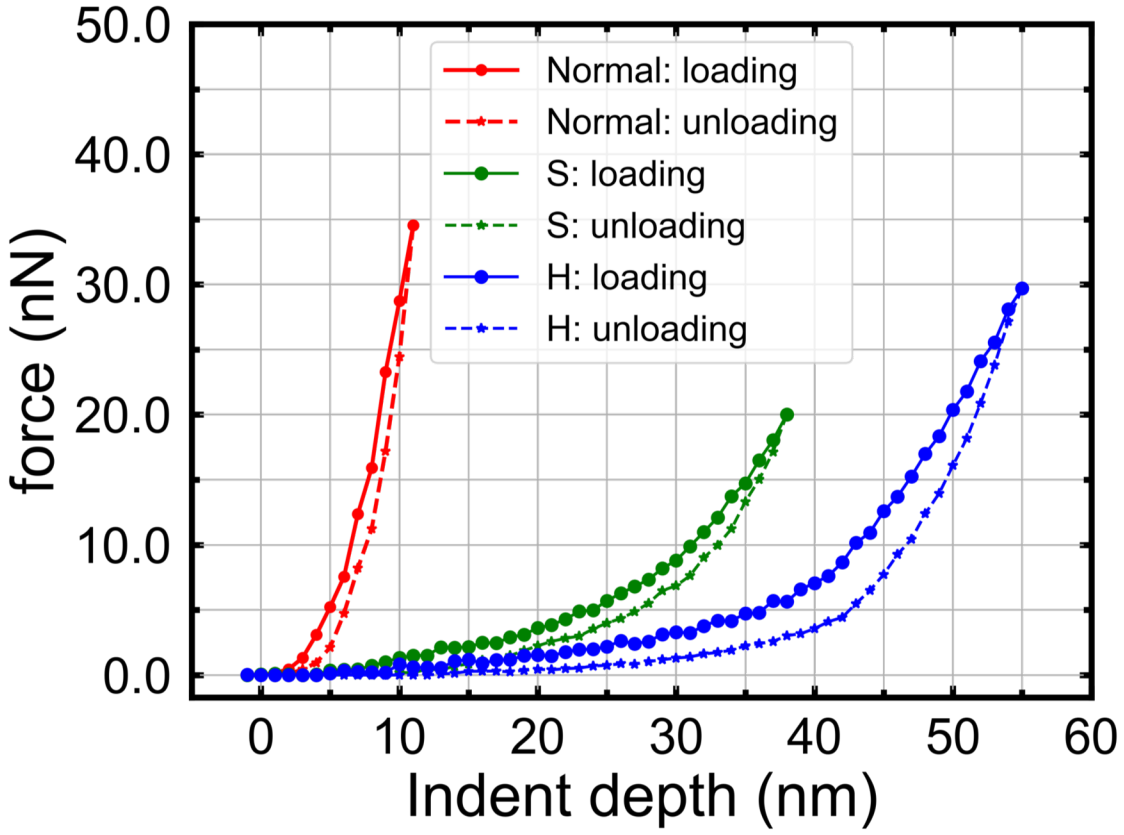


Visualization

Visualization of nanoindentation: part 2



Results



- **Spring constant:**
  - **Hexagonal pattern: 0.2 N/m**
  - **Square pattern: 0.1 N/m**
  - **Normal: 5.0 N/m**
- **Kirigami pattern makes materials more "elastic"**
- **"out-of-plane rigidity" is reduced 20~50 times by introducing kirigami pattern**

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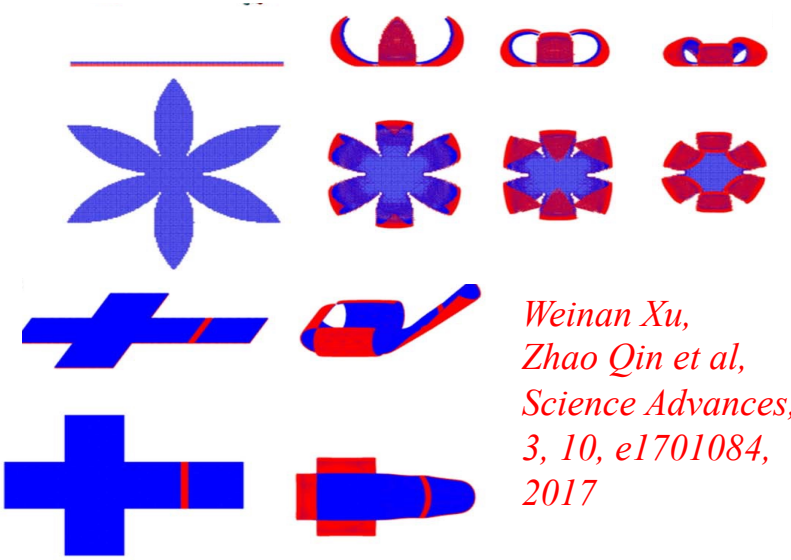
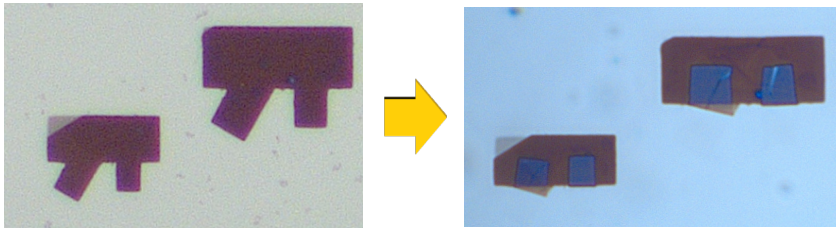
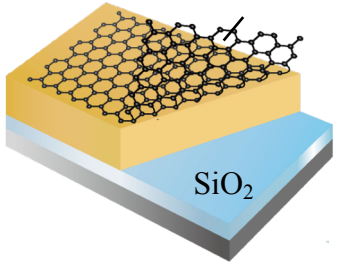
Graphene folding under water flow

- Two dimensional (2D) materials have exceptional mechanical flexibility, can be stretched and folded into origami structures.
- 2 common folding methods:
  - Thermoresponsive folding
  - Mechanical folding
- Our goal is to demonstrate a different technique to fold graphene in water



Weinan Xu, Zhao Qin et al, Science Advances, 3, 10, e1701084, 2017





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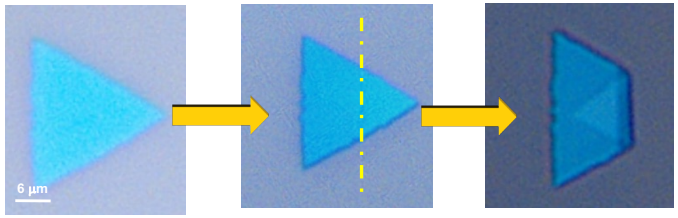

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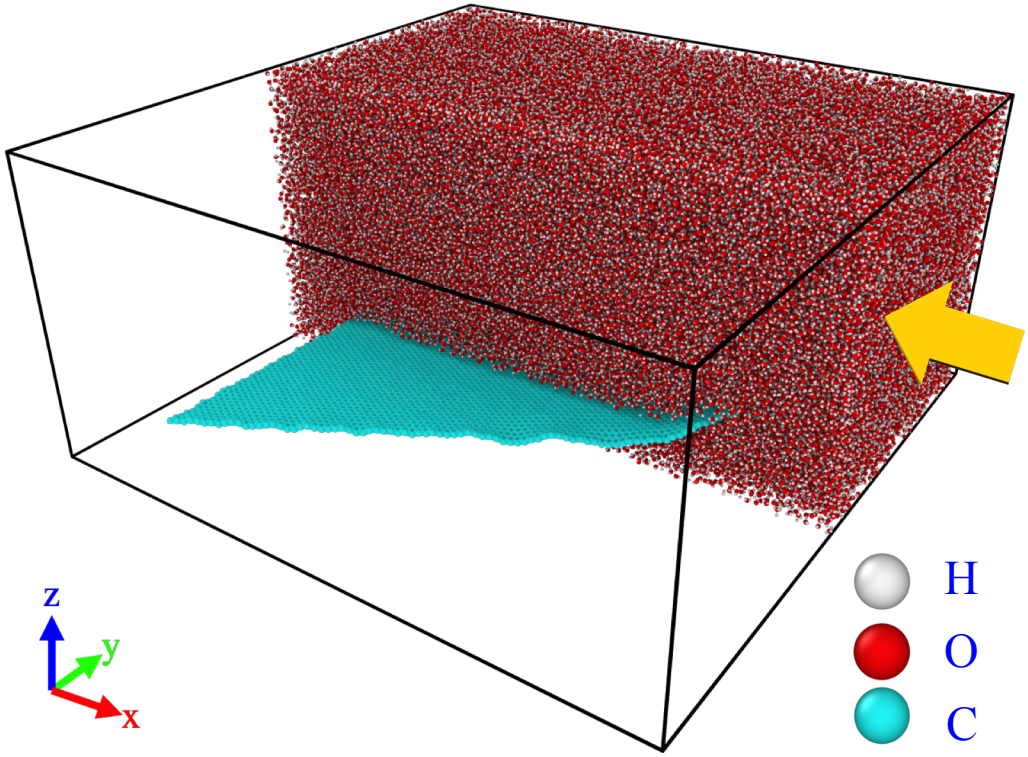
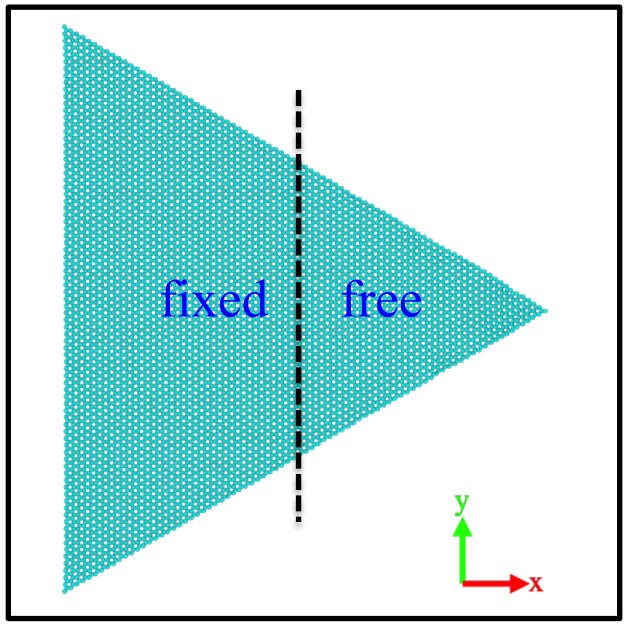
Folding Simulation Setup





- Top view of graphene
- graphene size: 20 nm

- Box size: 24 × 24 × 12 nm^3
- Box is full of H_2O, graphene sheet is in the middle (only half of H_2O is shown)
- As the arrow indicates, we push water with a constant pressure P = 0.16 GPa to simulate water flow

- Left part: we fix it in space with harmonic force to simulate substrate adhesion
- Right part : free to move

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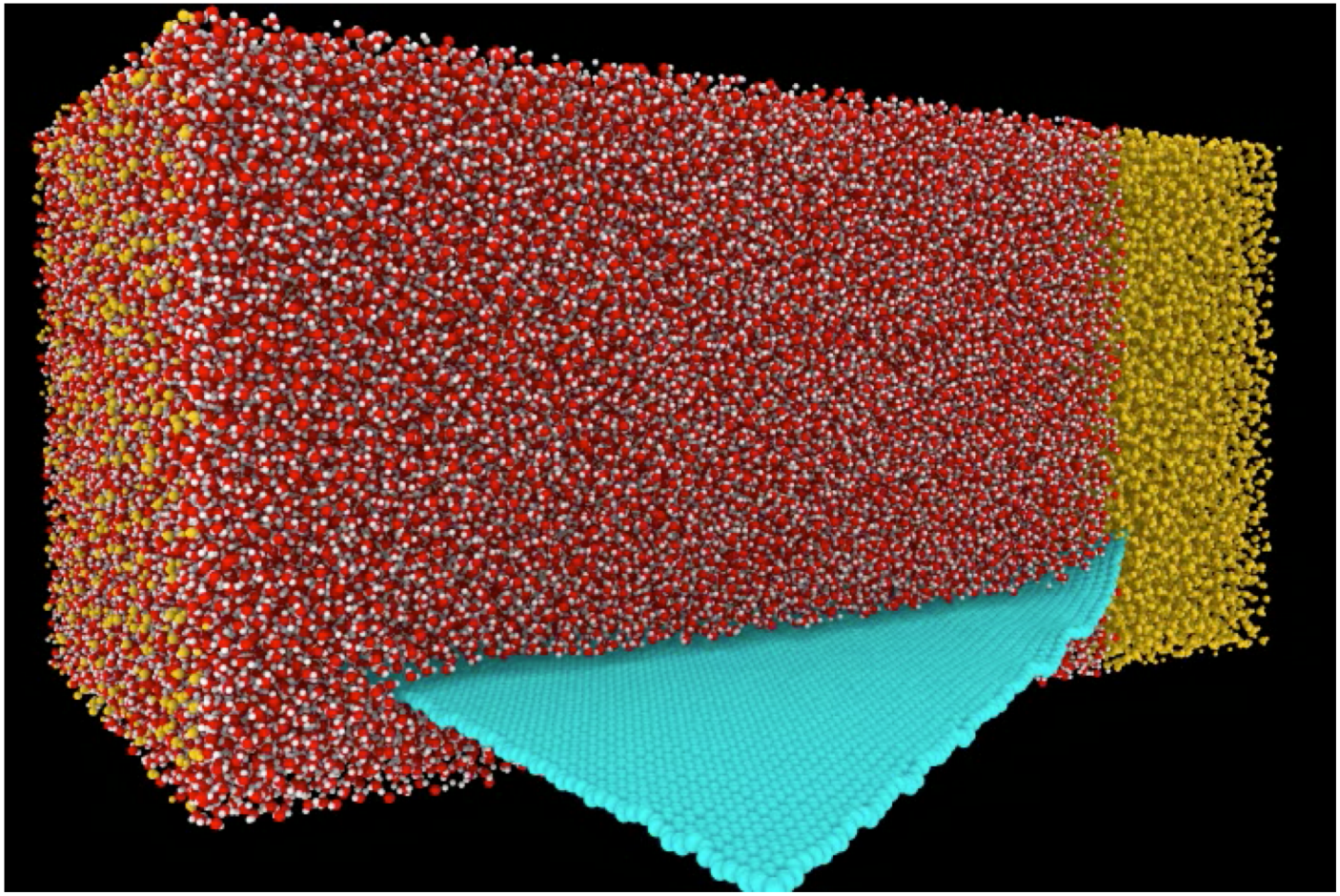
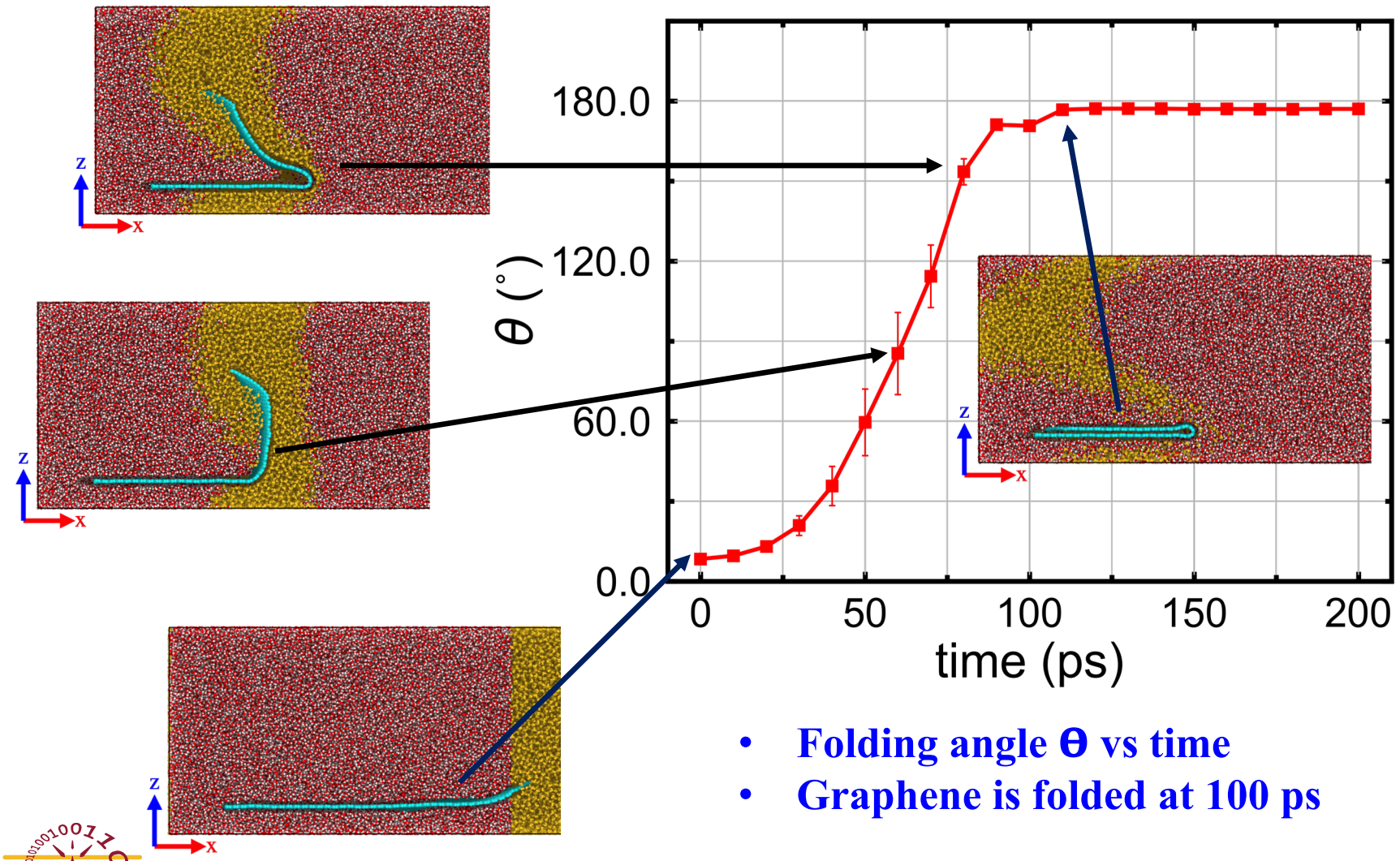
Visualization

- Graphene folding under the flow of water



Results

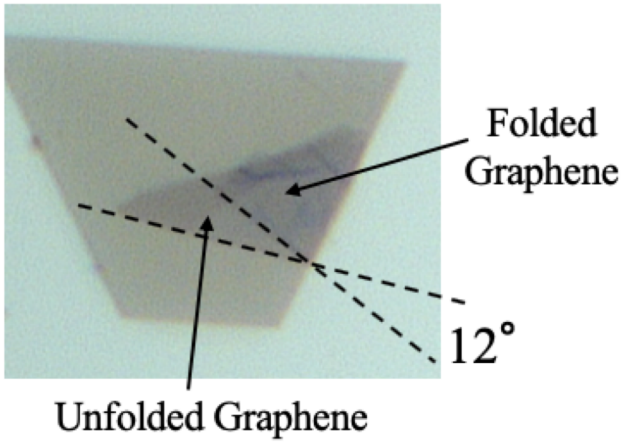


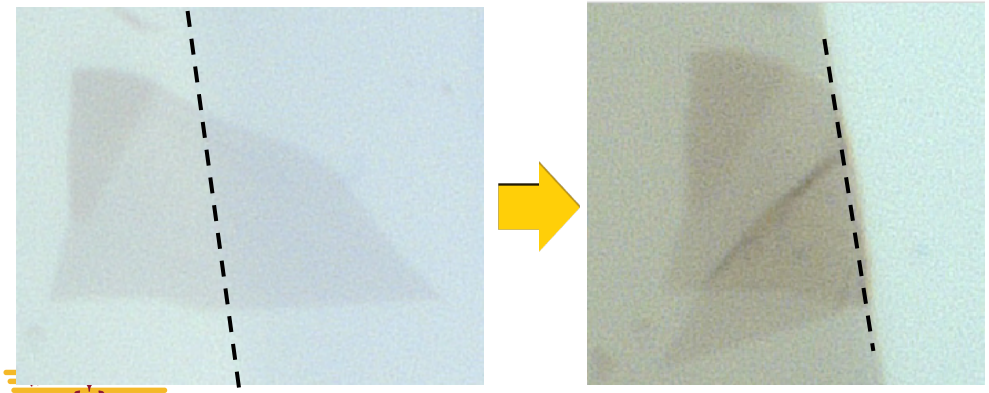
- **Folding angle θ vs time**
- **Graphene is folded at 100 ps**

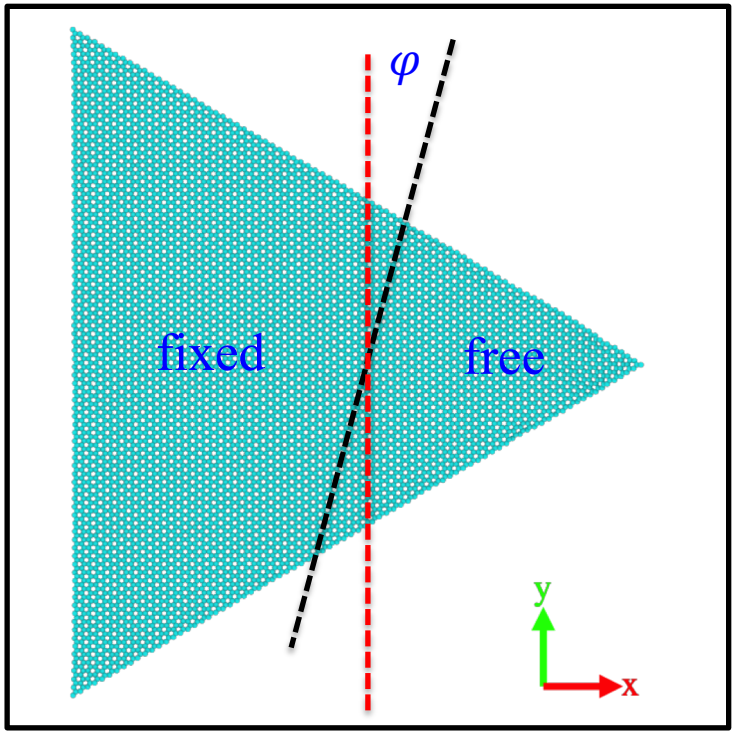
Results

- **Control the orientation of folding crease:**
  - **Make complex origami structures**
  - **Electrical properties, etc.**

Pictures taken from the experimens done by Huan Zhao, Han Wang et al WangLab@USC







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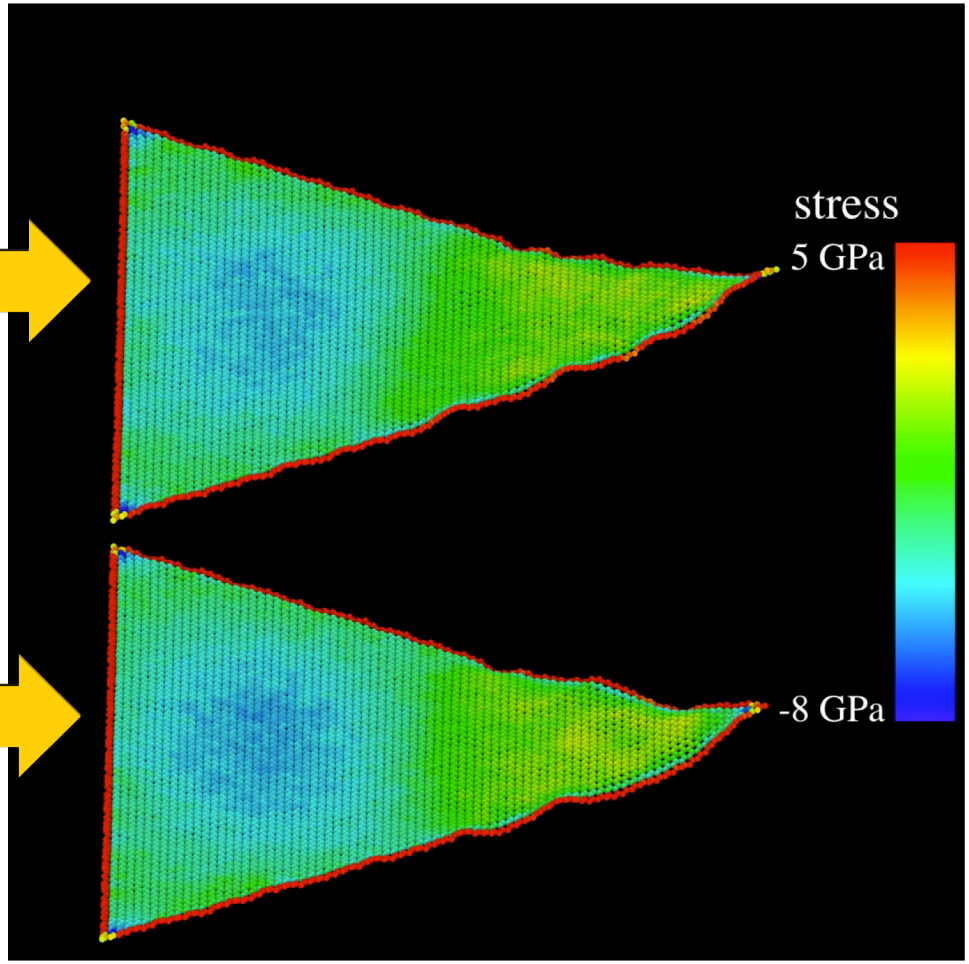
Visualization

- **Control the angle of crease: stress distribution**

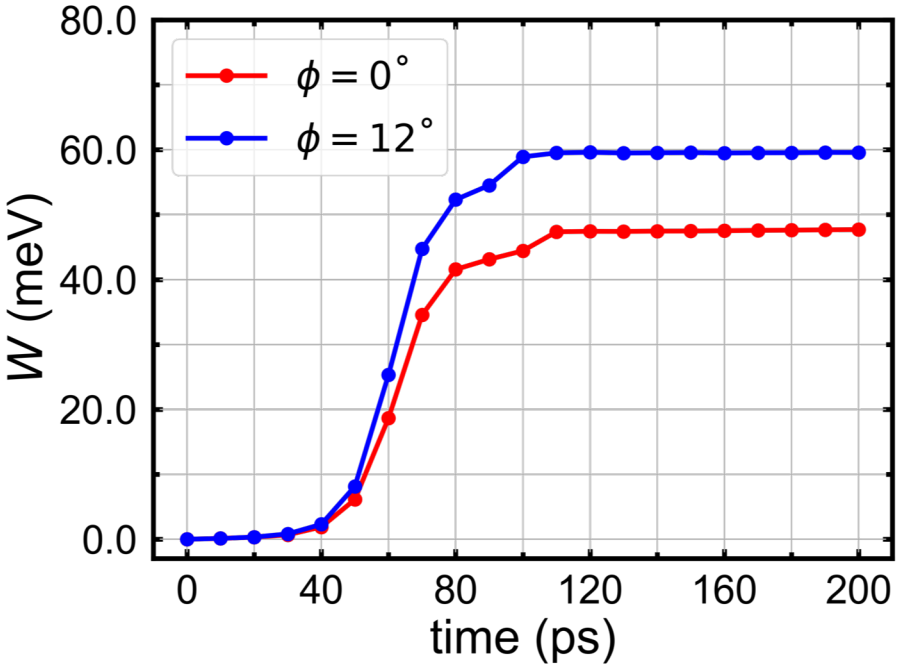
$\varphi = 12^\circ$

$\varphi = 0^\circ$



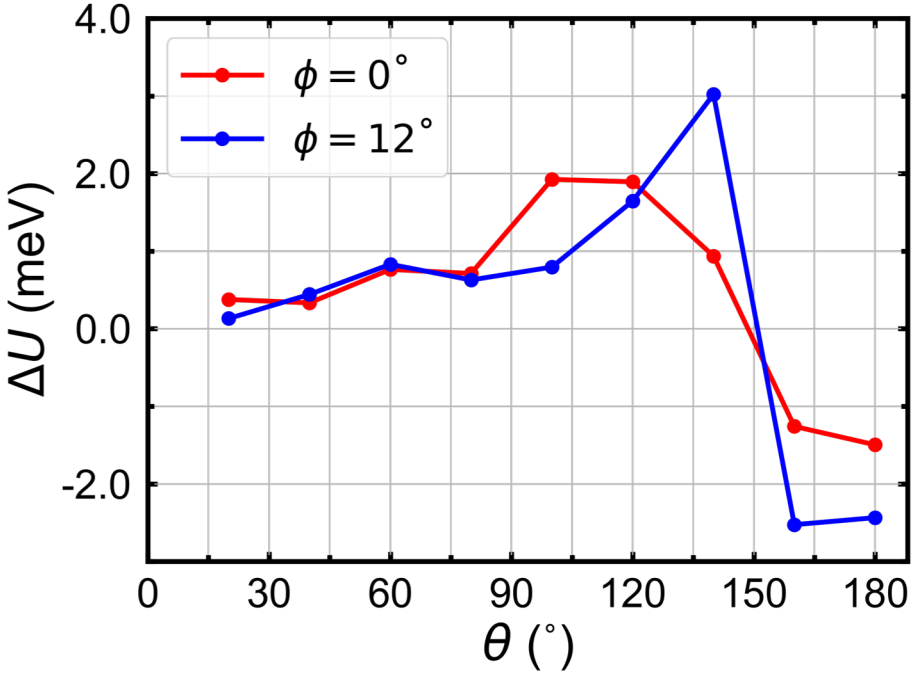
Results

Accumulated work on graphene by water flow



- **Per-atom work done by water flow on graphene:**
  - **47 meV for $\varphi = 0^\circ$**
  - **60 meV for $\varphi = 12^\circ$**

Potential energy vs folding angle



- **Energy Barrier for graphene folding:**
  - **2.0 meV (23 K) for $\varphi = 0^\circ$**
  - **3.0 meV (34 K) for $\varphi = 12^\circ$**

- **Per-atom energy drop after folding:**
  - **-1.5 meV for $\varphi = 0^\circ$**
  - **-2.5 meV for $\varphi = 12^\circ$**

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Summary & Future Work

- **Summary:**
  - Present simulation on kirigami MoS_2
  - Demonstrate a controllable graphene folding method
  - Evaluate the energy barrier and energy decrease between folded & flat graphene with two configurations

Thank you

- **Future work:**
  - Thickness dependence of graphene folding under water flow
  - Various 2D materials

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