The Statistical Mechanics of Sliced Graphene Ribbons

Geometry, elasticity, fluctuations, and order in 2D soft matter (sheets)

KITP Feb 22, 2016

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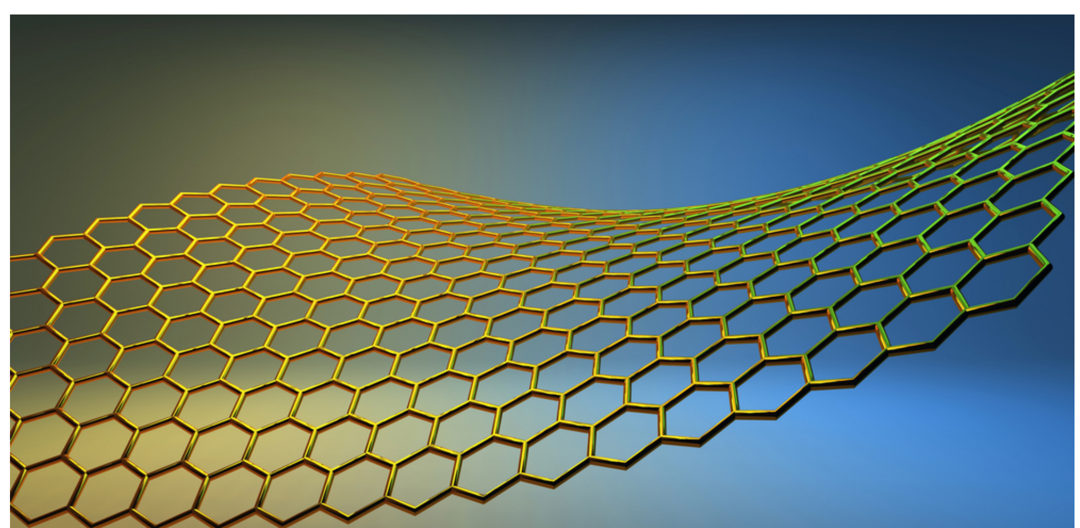
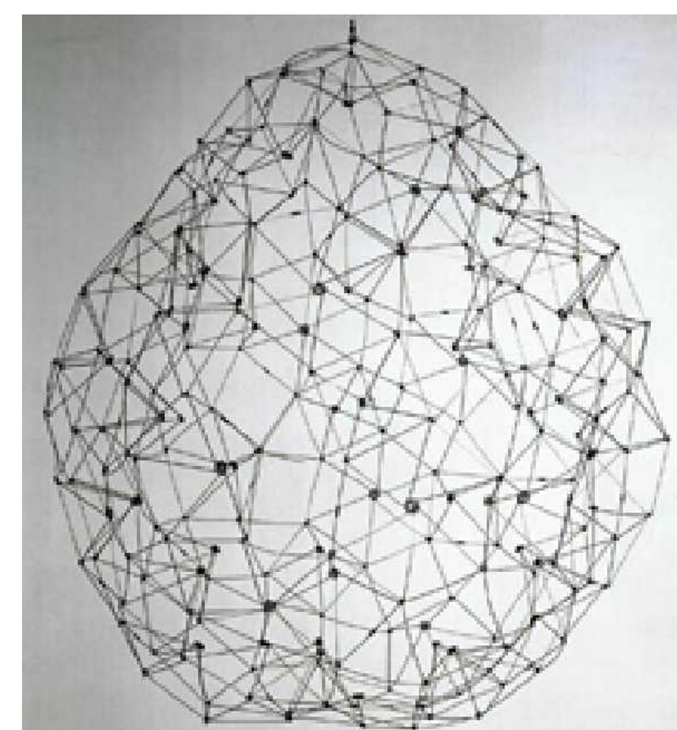




Elastic (polymerized) membranes

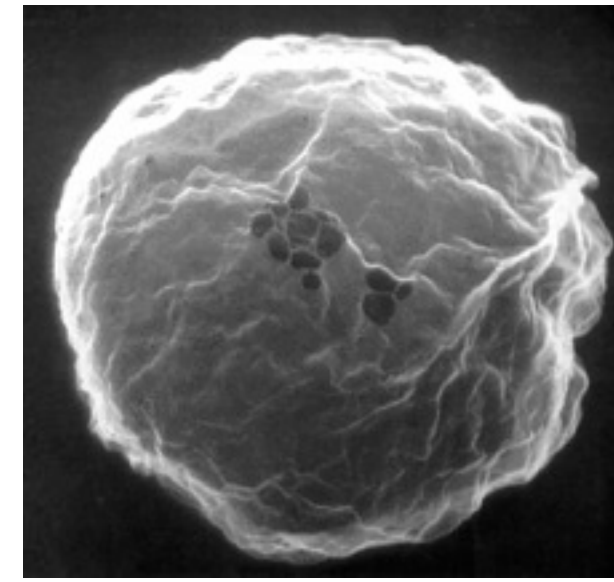
Entropically-stabilized phases

Bowick et al. (1996)

$$\mathrm{E} = \mathrm{E}_{el} + E_{bend}$$

↑

shear (μ) + compression (K)



RBC Ghost: Steck (77)

$$d^2r = d^2r_0 + 2u_{ij}dx_idx_j$$ displacement

$$\mathrm{E}_{el} = \frac{1}{2}\int d^2x[2\mu u_{ij}^2 + \lambda u_{kk}^2]$$

where $$\mathrm{u}_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i h \partial_j h)$$ strain tensor

$$\mathrm{E}_{bend} = \frac{\kappa}{2}\int d^2x(\nabla^2 h)^2$$

$$A_{ij}(\vec{x}) = \partial_i h \partial_j h$$

Nelson-Peliti (1987)

$$A_{ij} = \partial_i h \partial_j h \equiv \frac{1}{2}\left[\partial_i \phi_j(\vec{x}) + \partial_j \phi(\vec{x})\right] + P_{ij}^T \Phi(\vec{x})$$

$$P_{ij}^T = \delta_{ij} - \frac{\partial_i \partial_j}{\nabla^2}$$

$\int$ out the phonons

$$\int \mathcal{D}u(\vec{x}) \mathrm{e}^{-\beta E} = \mathrm{e}^{-\beta F_{eff}}$$

$$F_{eff} = \frac{1}{2}\kappa \int d^2x (\nabla^2 h)^2 + \frac{1}{2} Y \int d^2x \left(\frac{1}{2} P_{ij}^T (\partial_i h)(\partial_j h) \right)^2$$

Nonlinear stretching energy

$$Y = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda} = \frac{4\mu K}{\mu+K}$$

2D Young's modulus

Gaussian curvature suppression of height fluctuations

$$\nabla^2 \left(\frac{1}{2} P^T_{ij} \partial_i h \partial_j h \right) = -\det(\partial_i \partial_j h) = -S(\vec{x})$$

$$F_{eff} = \frac{1}{2}\kappa \int d^2x (\nabla^2 h)^2 + \frac{1}{2} Y \iint d^2x d^2y S(\vec{x}) G(\vec{x},\vec{y}) S(\vec{y})$$

IR suppression via Gaussian curvature

$$\Delta^2 G(\vec{x},\vec{y}) = \nabla^4 G(\vec{x},\vec{y}) = \delta(\vec{x},\vec{y})$$

$$G(\vec{x},\vec{y}) \sim |\vec{x}-\vec{y}|^2 \ln(|\vec{x}-\vec{y}|)$$

Running bending rigidity

$$k_B T \kappa_R^{-1}(q) \equiv q^4 < |\tilde{h}(\vec{q})|^2 >$$

Calculate perturbatively in Y

$$\kappa_R(q) = \kappa + \frac{(k_B T)Y}{\kappa_R} \mathcal{I}(\vec{q})$$

$$\mathcal{I}(\vec{q}) = \int \frac{d^2k}{(2\pi)^2} \frac{[\hat{q}_i P_{ij}^T(\vec{k})\hat{q}_j]^2}{|\vec{q}+\vec{k}|^4}$$

Power counting

As $|\vec{q}| \to 0$, $\mathcal{I}(\vec{q})$ diverges like $1/|\vec{q}|^2$

IR Stiffening!

$$\kappa \to \kappa_R(\vec{q}+\vec{k}) \text{ in } \mathcal{I}(\vec{q})$$

$$\kappa_R(q) = \frac{k_B T Y}{\kappa_R(q) q^2}$$

$$\kappa_R(q) \sim \sqrt{k_B T Y}\,\frac{1}{q}$$

Fluctuations of surface normals

$$\langle \Theta^2(\vec{x}) \rangle = \langle (\partial h)^2(\vec{x}) \rangle = k_B T \int \frac{d^2q}{(2\pi)^2} \frac{1}{\kappa_R(q) q^2} \approx \sqrt{\frac{k_B T}{Y}} \int \frac{d^2q}{(2\pi)^2} \frac{1}{q} < \infty$$

Order from Disorder!

Aronovitz, Golubovic & Lubensky (1989)
LeDoussal & Radzihovsky (1992) (SCSA)

$$< h^2 > \sim L^{2\zeta} = \int \frac{d^2q}{(2\pi)^2} \frac{1}{\kappa_R(q) q^4} \sim L^{2-\eta} \quad (\zeta = 1 - \eta/2)$$

$$\kappa_R(q) \sim q^{-\eta} \qquad \mu(q) \sim q^{\eta_u} \, ; \lambda(q) \sim q^{\eta_u}$$

$\eta_u = 2(1-\eta)$ Ward identities (remnant rotational symmetry)

$\eta = 1 \, (\text{Nelson\&Peliti})$ $\quad \eta \approx 0.8$ SCSA

$\eta = 0.72(4)$ MJB et al. Monte Carlo (1996)

Poisson Ratio

$$\nu = \frac{\text{Transverse contractile strain}}{\text{Longitudinal Tensile Strain}} = -\frac{\delta y/y}{\delta x/x}$$

$$\nu \equiv \lim_{q \to 0} \frac{K(q) - \mu(q)}{K(q) + \mu(q)}$$

Flat phase fixed point

$$K(0) = \frac{1}{2}\mu(0) \quad \text{(anti-rubber)}$$

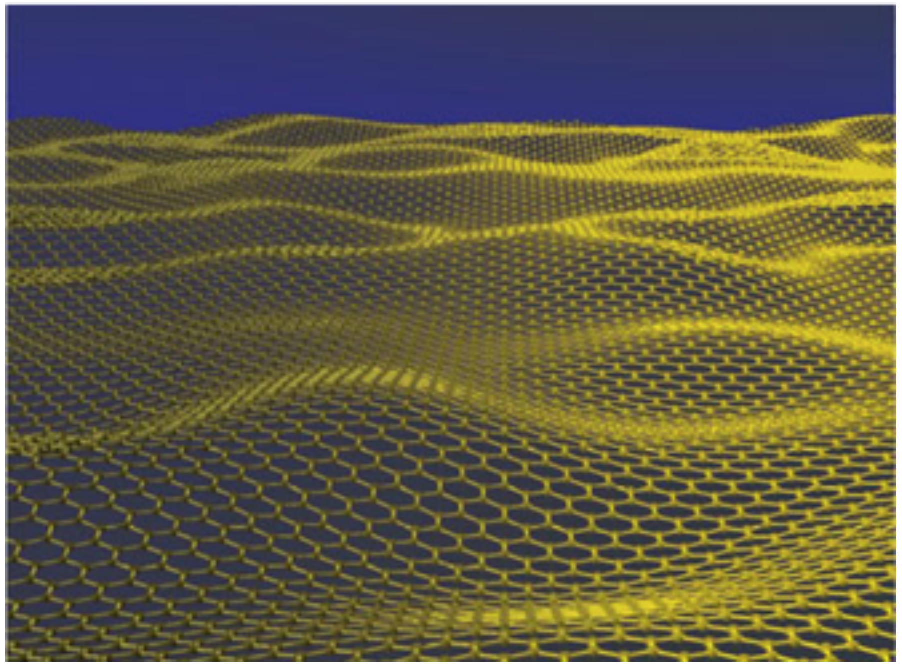
$$\implies \nu = -1/3$$

Auxetic

MJB, Falcioni, Guitter and Thorleifsson (1997)

Graphene as Atomic Paper

$Y \approx 20\mathrm{eV}\text{Å}^{-2}$ $\kappa_0 \approx 1.2\mathrm{eV}$ $k_B T \approx 1/40\,\mathrm{eV}$



$$\kappa_R(l) = \kappa_0 + \frac{(k_B T)Y}{\kappa_0} l^2$$

$$\kappa_R(l)/(k_B T) = \kappa_0/(k_B T) + \mathrm{vK}(l)$$

vK = Foppl-von Karman # = Yl^2/κ_0

$$200\mu\mathrm{m\,sheet\,of\,graphene\,vK} \approx (\mathrm{L/h})^2 = 10^{12}\ \mathrm{cf.\,paper\,vK} \approx 10^6$$

$$\kappa_R(l_{th}) = 2\kappa_0 \text{ for } l_{th} = \frac{\kappa_0}{\sqrt{Y k_B T}} \approx 1.5\mathring{A}!$$

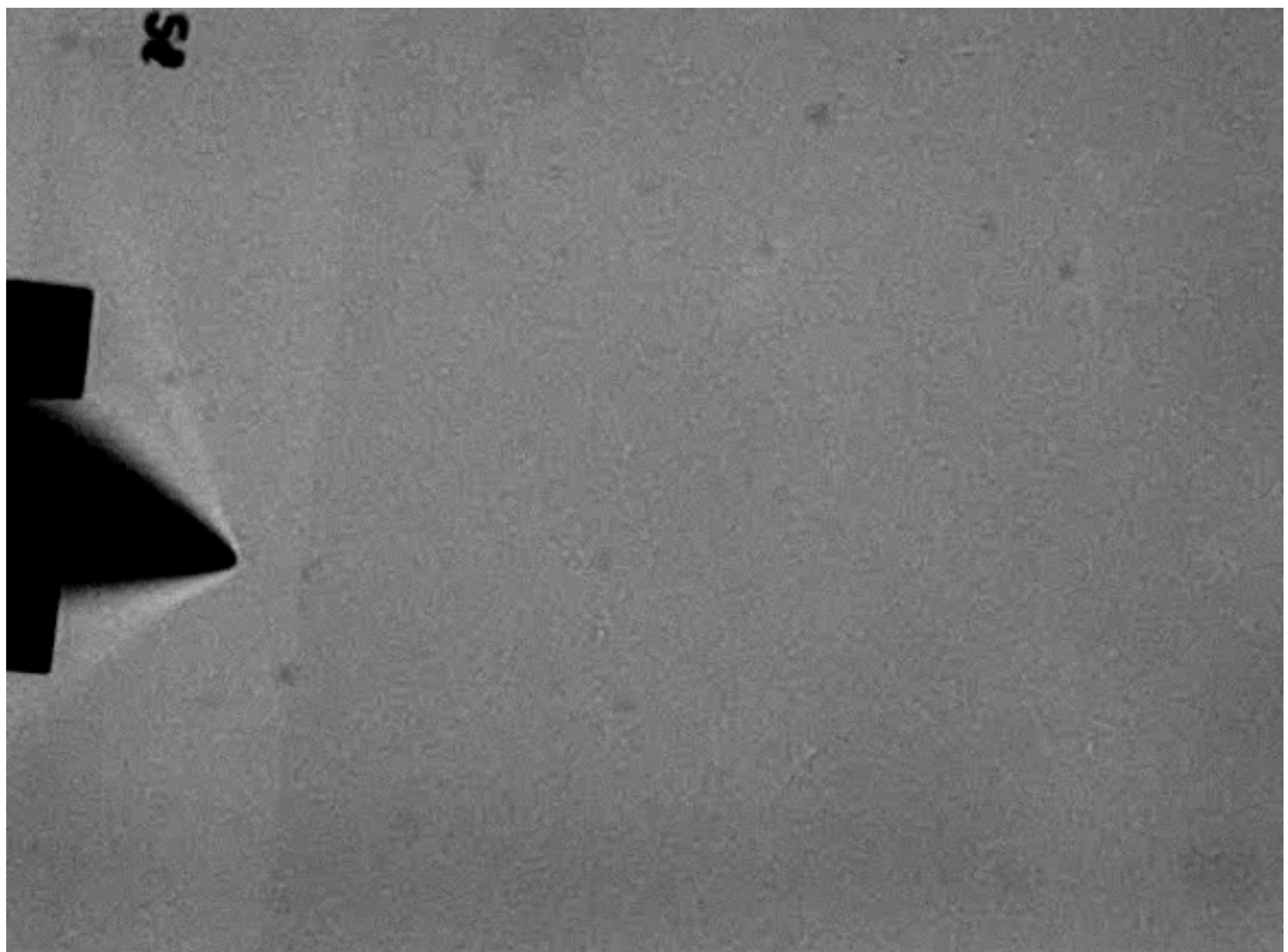
Fopply graphene is self-stiffening to bend via ***soft*** thermal fluctuations of a ***hard*** material

$$\frac{\kappa_R(l)}{\kappa_0} \approx \Big(\frac{l}{l_{th}}\Big)^{\eta}$$

For $l = 10\mu m \approx 10^8 l_{th} \quad \kappa_R/\kappa_0 \approx 10^6$

Makes vK (micron scale graphene) like vK of paper!

Experiments: Blees et al. (McEuen group, Cornell) Nature (2015)



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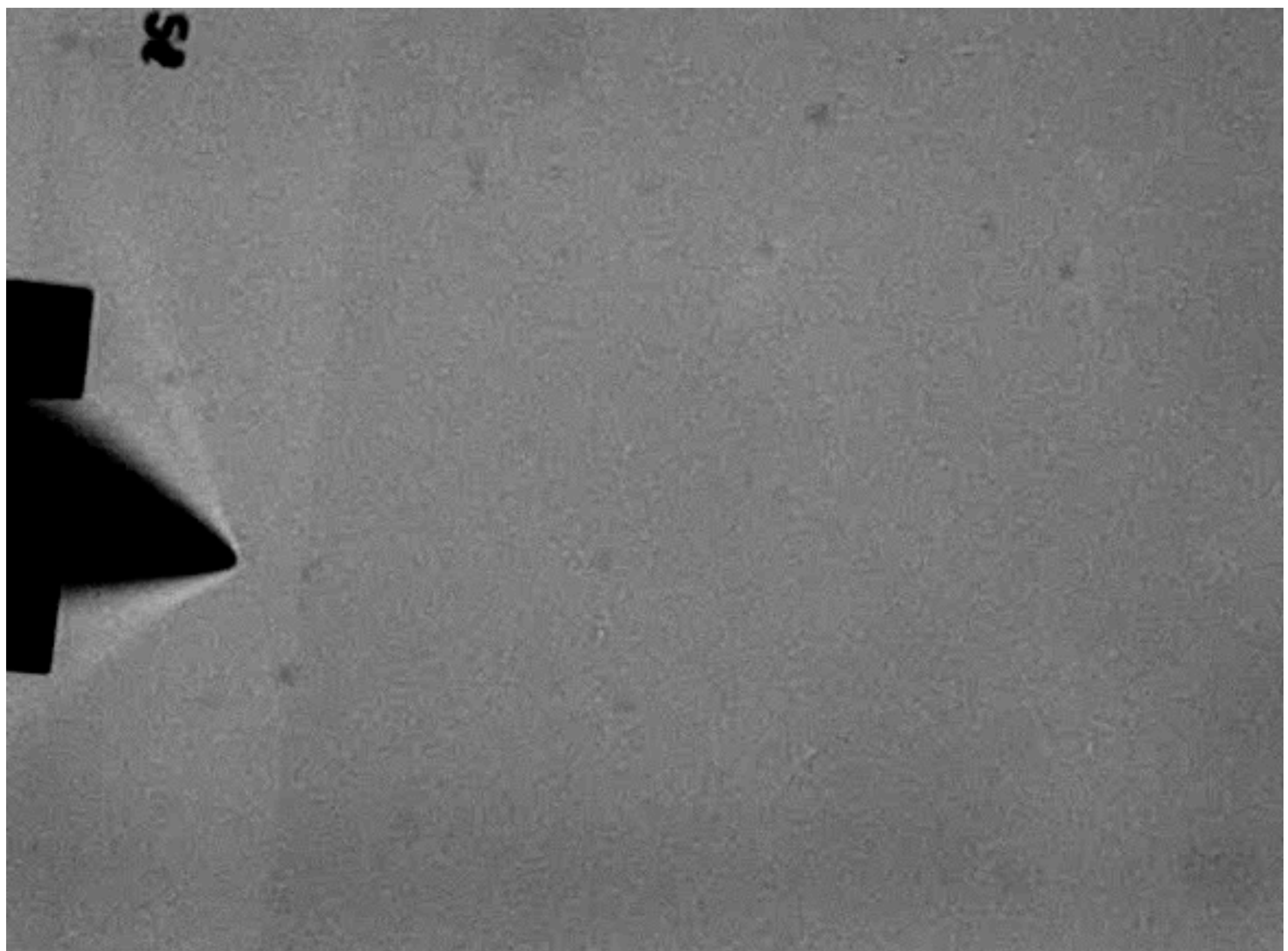
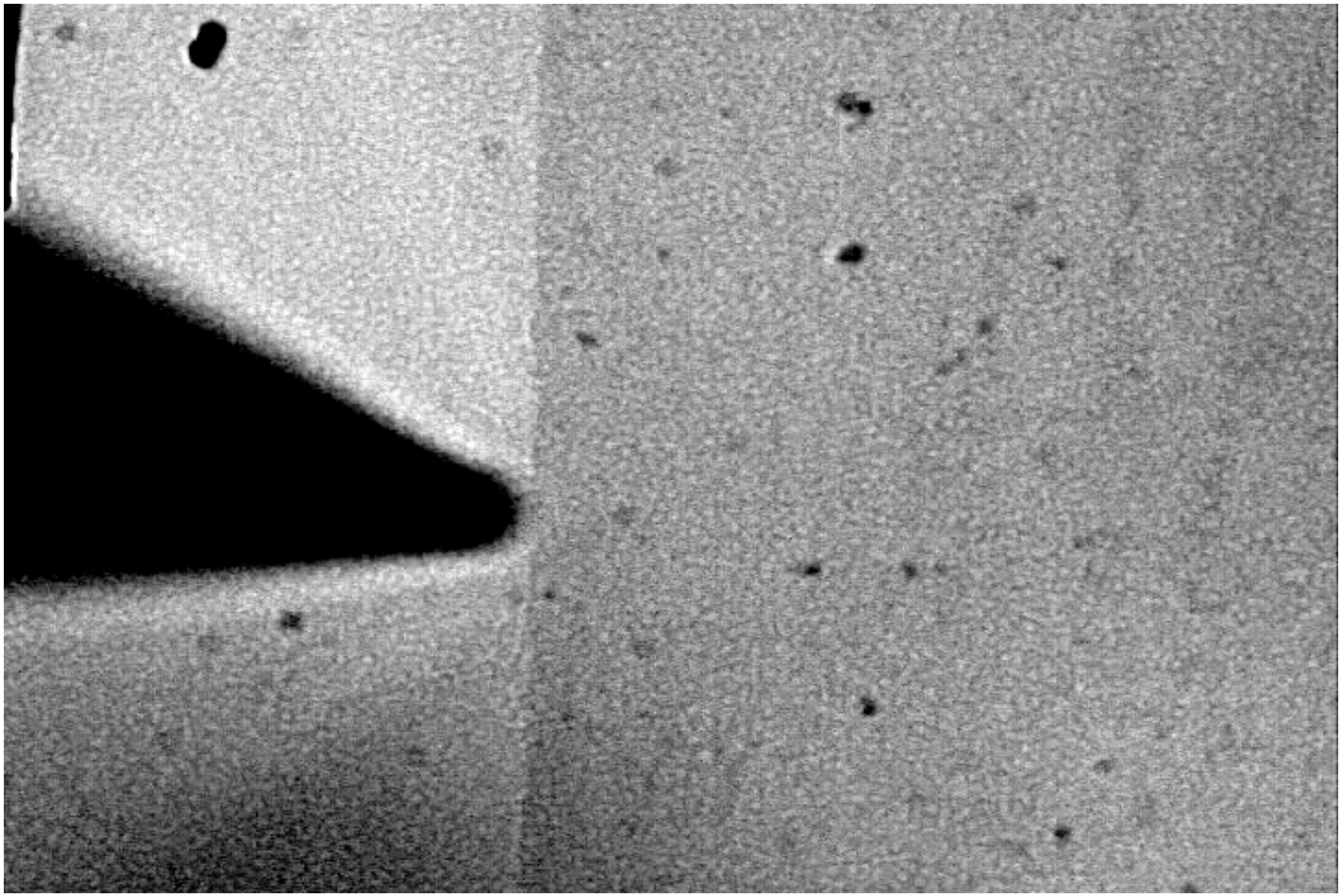
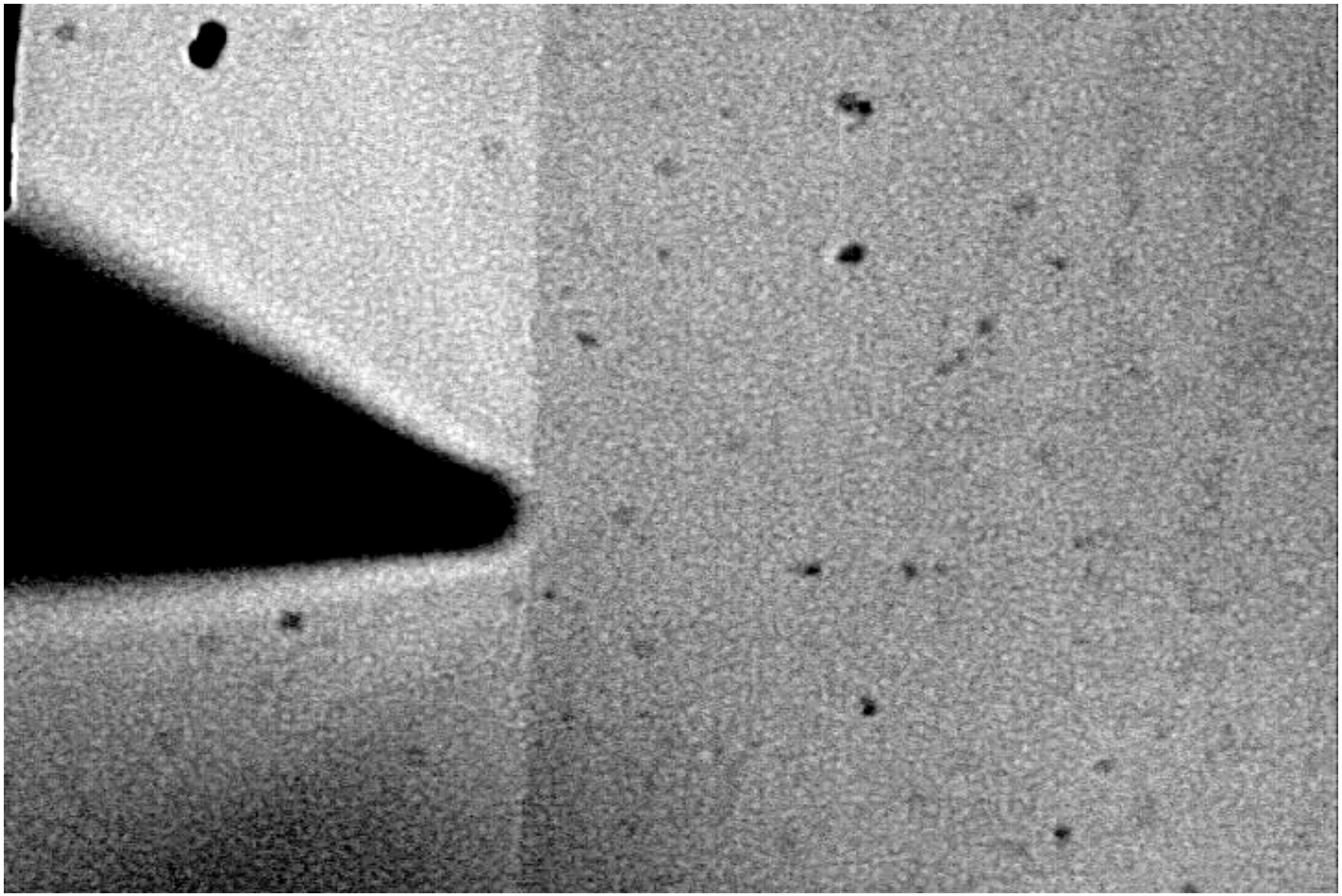




Melina Blees (McEuen group, Cornell)



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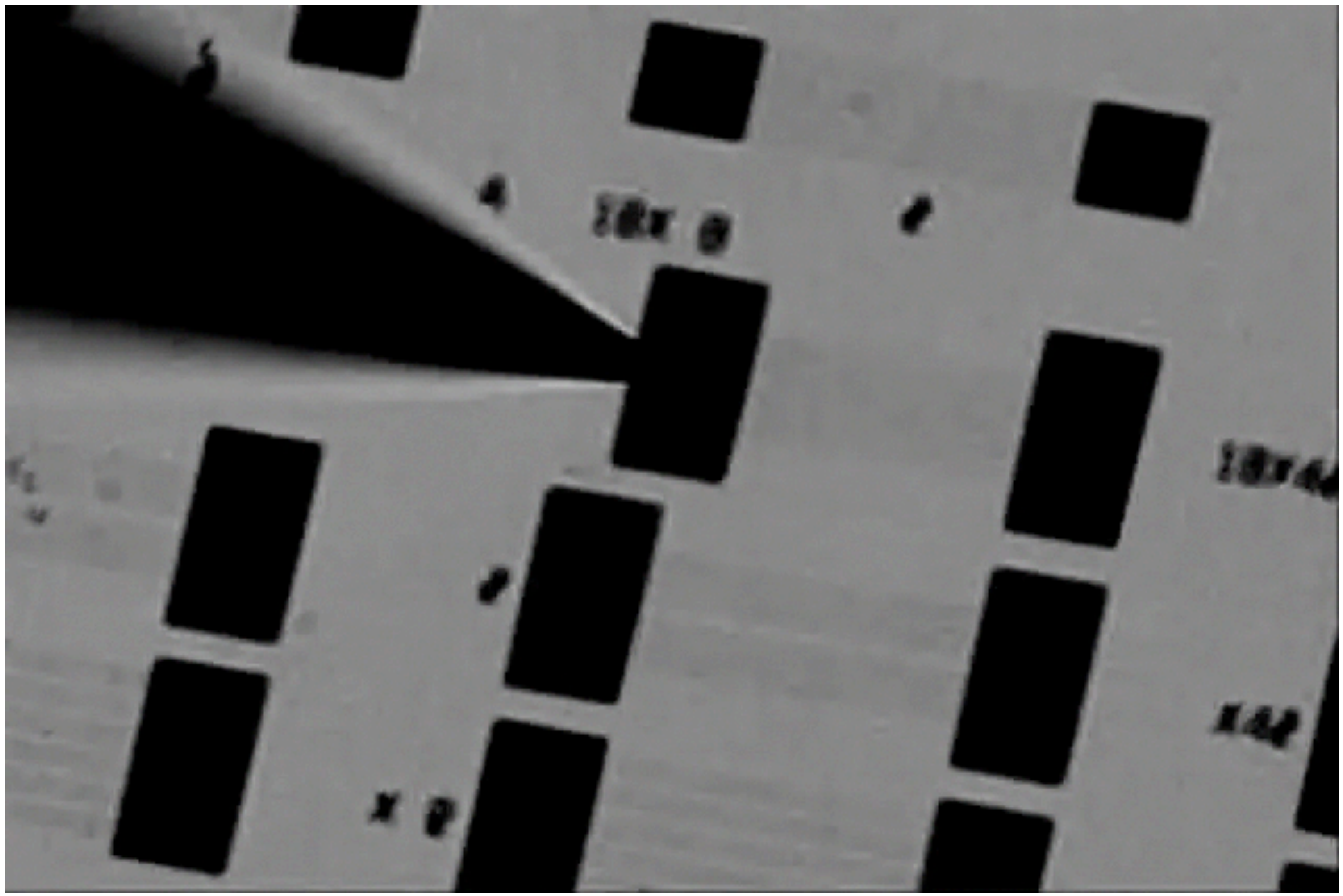
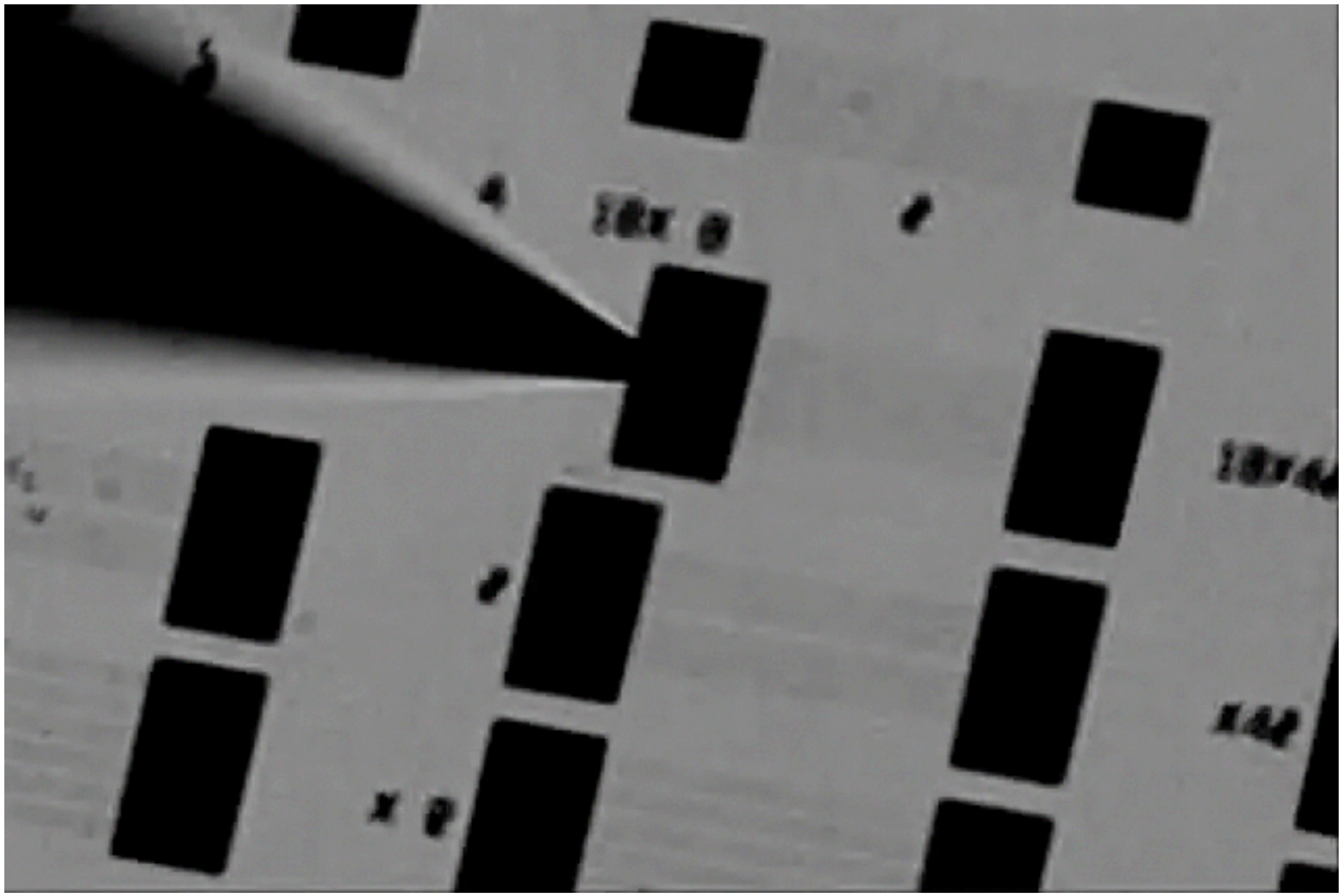
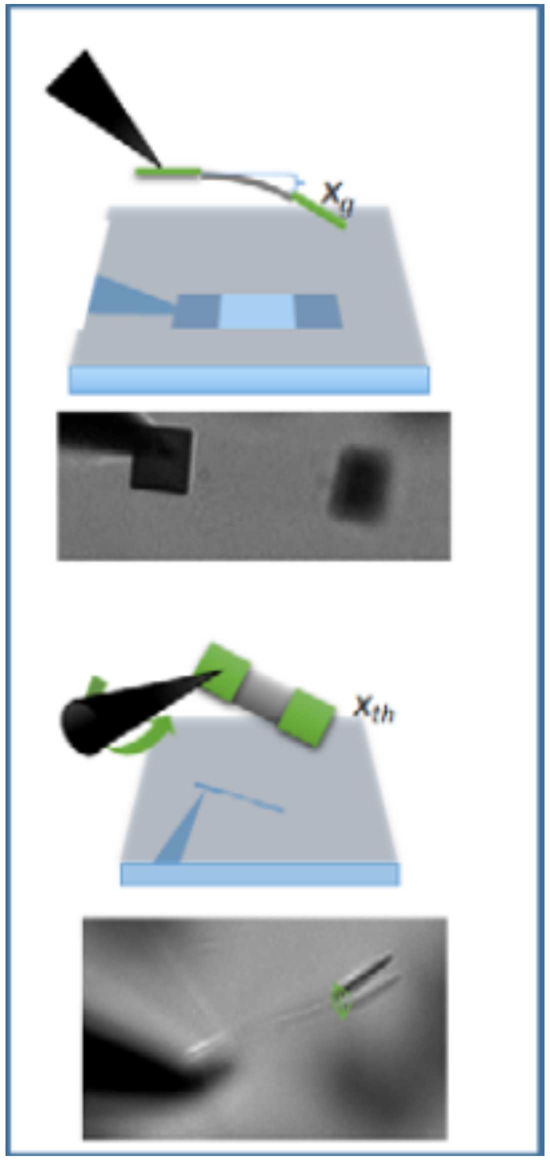


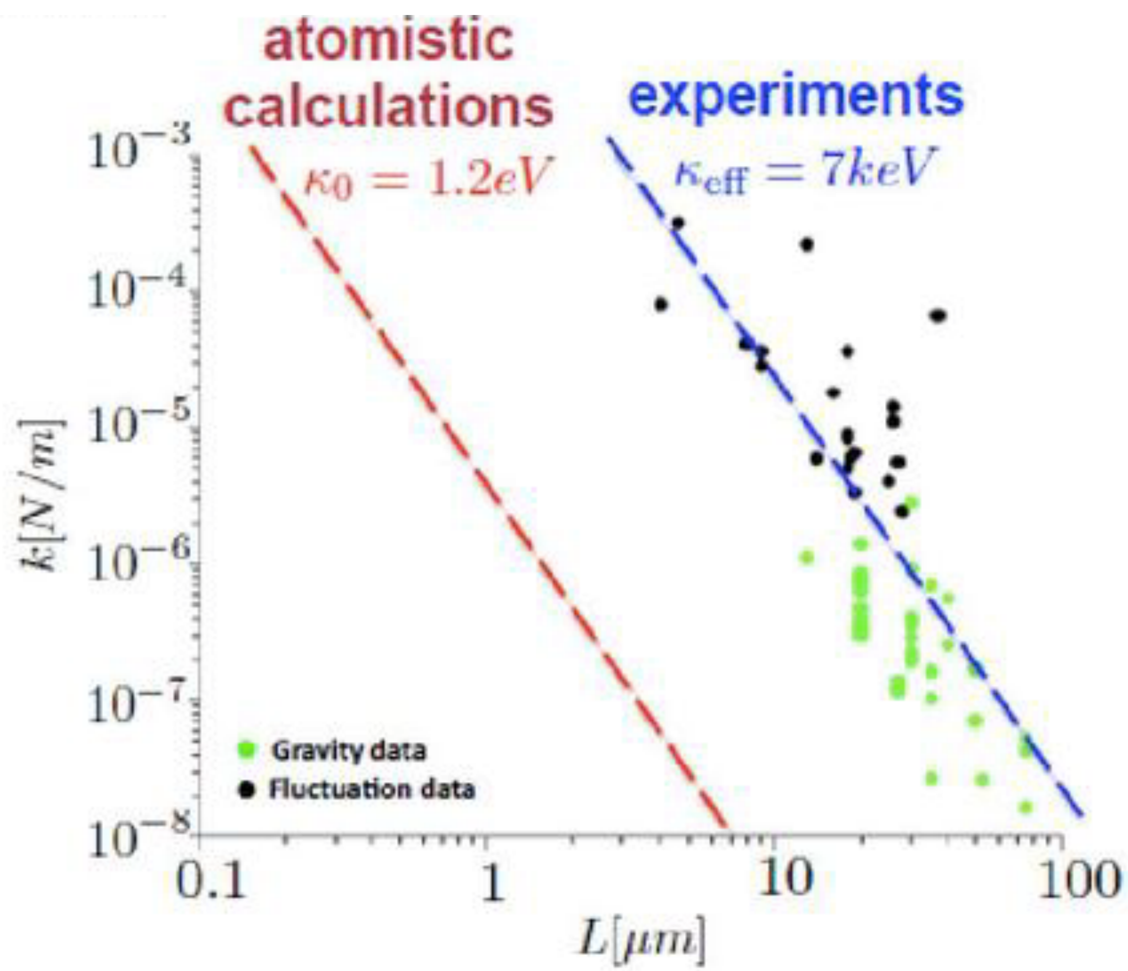
McEuen group



McEuen group

Bending Rigidity Measurements





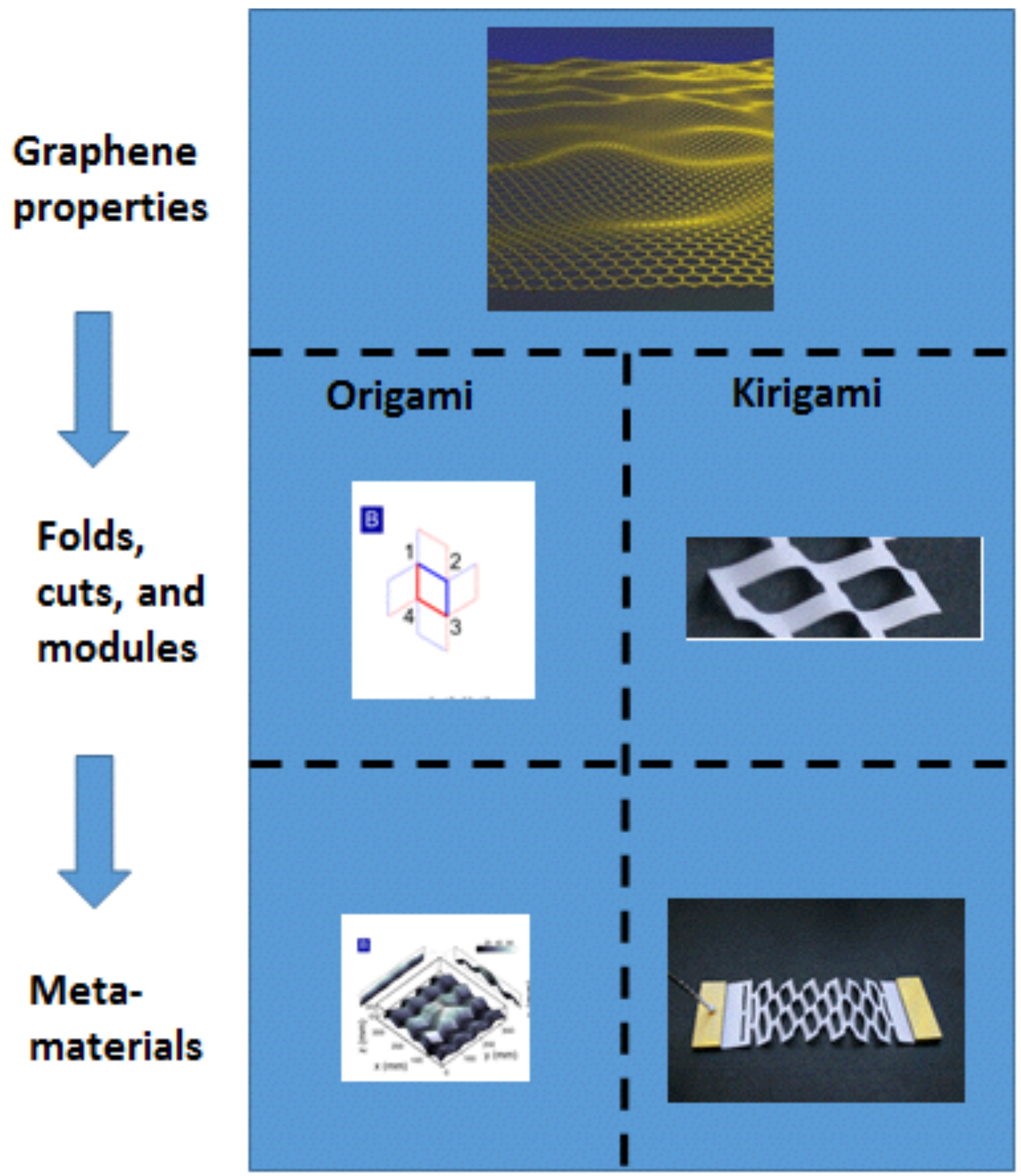
McEuen group

Graphene Kirigami

w/ Itai Cohen, Paul McEuen and David Nelson

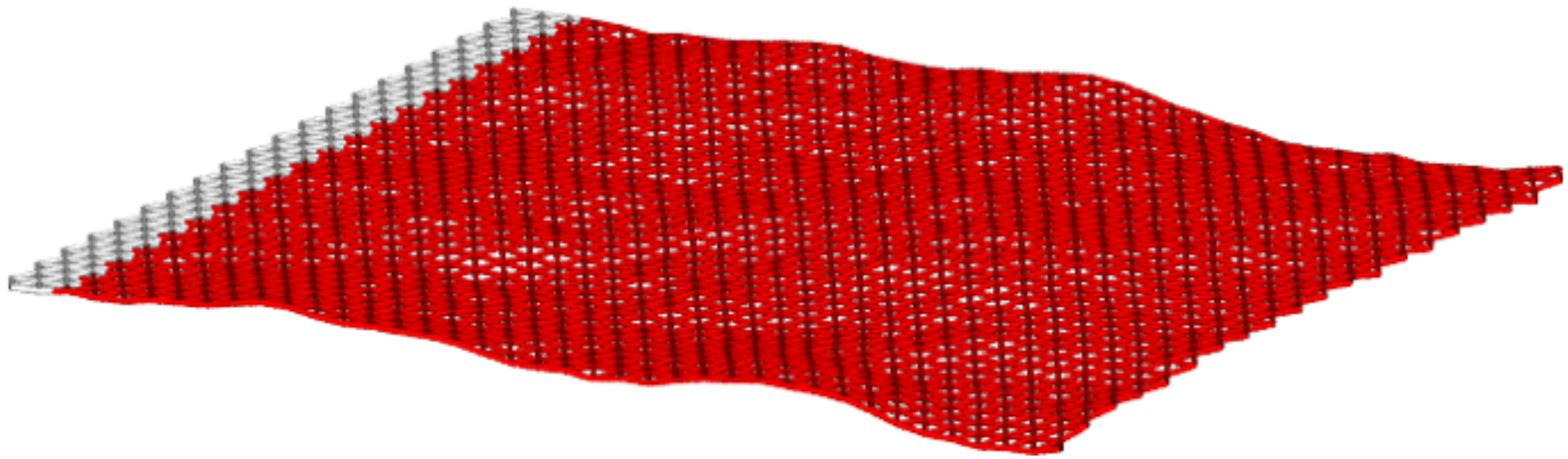
Graphene material properties depend on the geometry through thermal fluctuations

Slice and dice pure graphene to produce metamaterials with distinct elastic moduli and mechanical response



Simple scaling: Ribbons

w/ Andrej Kosmrlj, David Nelson and Rastko Sknepnek



Two system size scales to play with: length L and width W

1. short ribbon L < W: L controls the scaling $\kappa_R(L, W) \approx \kappa_0(L/l_{\rm th})^\eta$

2. long ribbon L >> W: W controls the scaling $\kappa_R(L, W) \approx \kappa_0(W/l_{\rm th})^\eta$

MD simulations

W=10, L=100

W=10, L=200

MD simulations

W=10, L=100

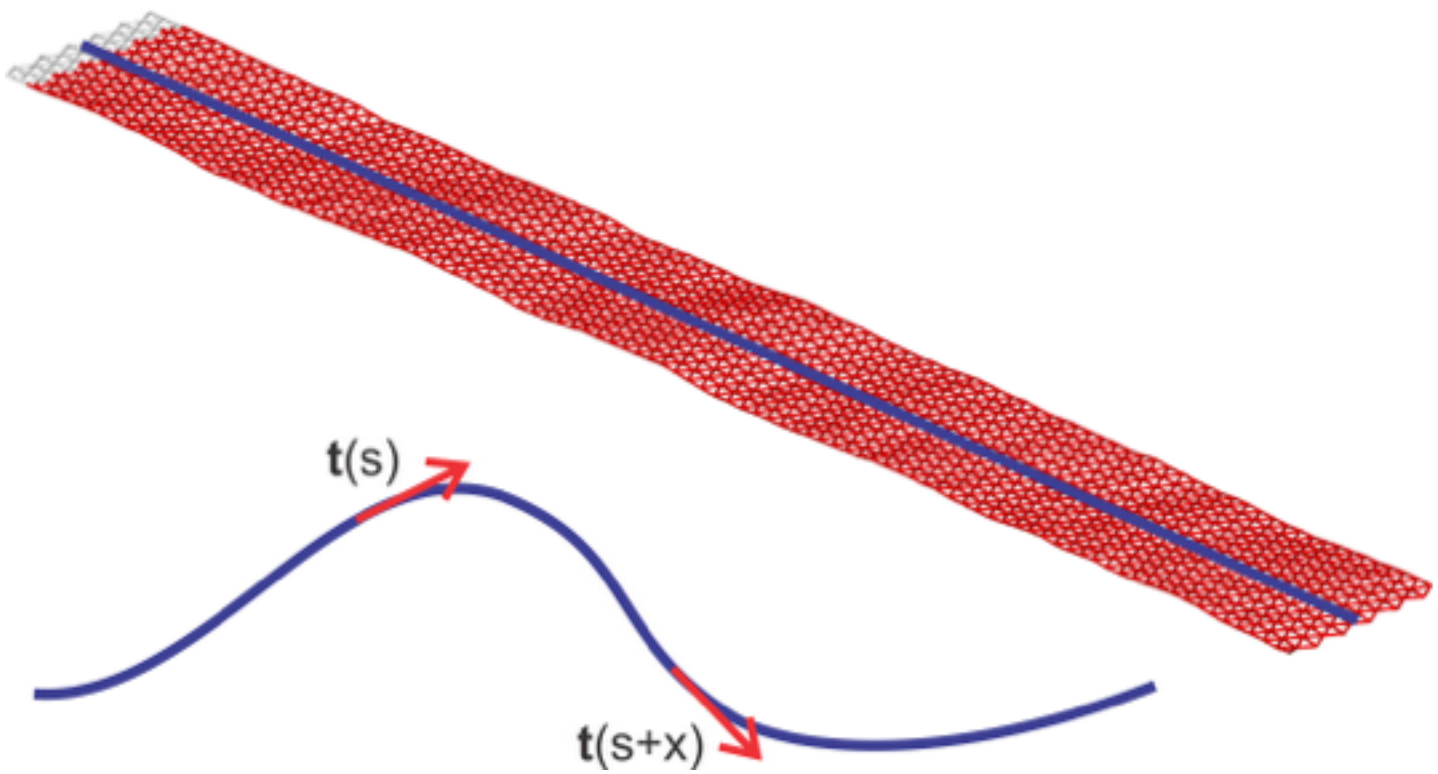
W=10, L=200

MD simulations

W=10, L=100

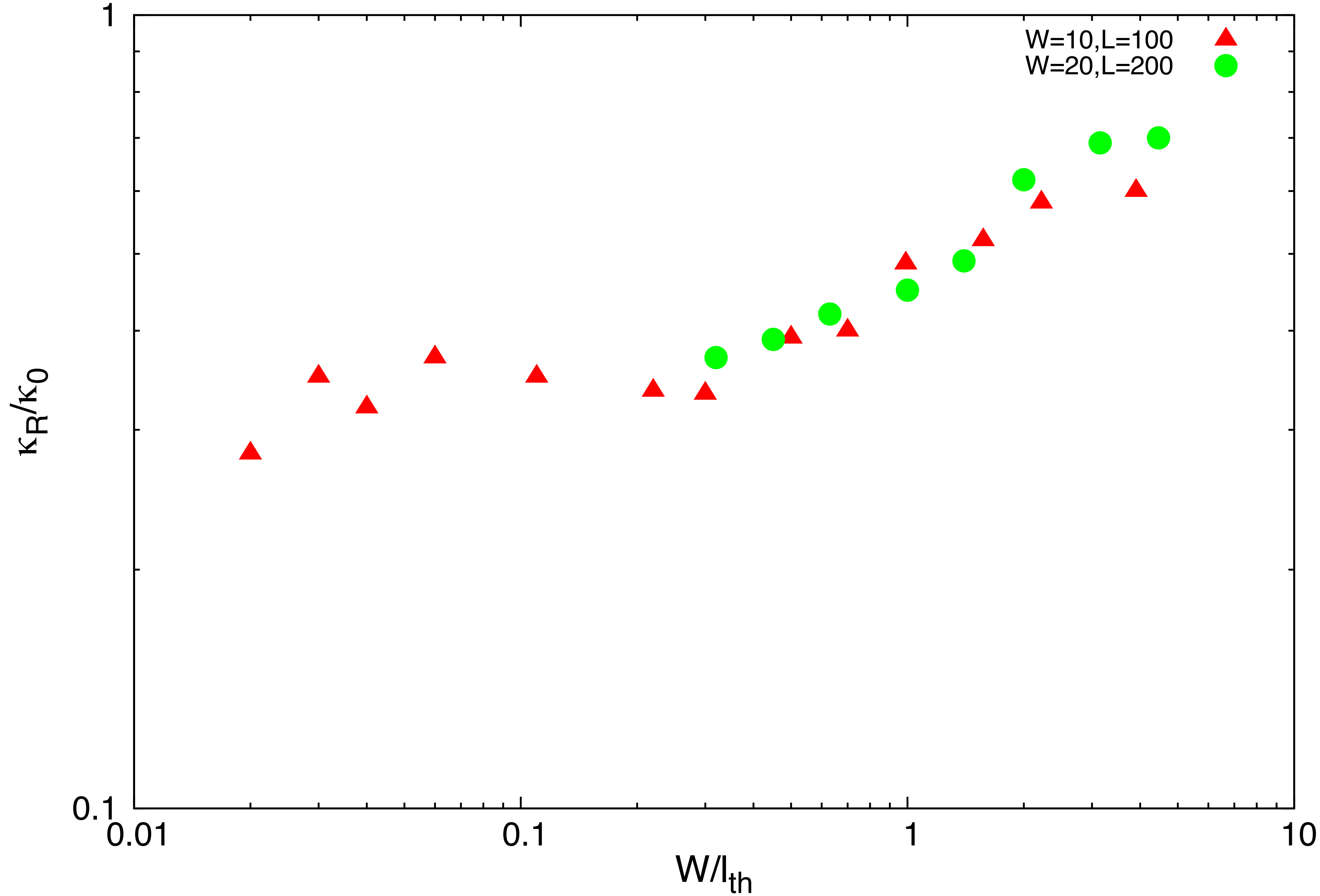
W=10, L=200

We can extract κ_R from the persistence length obtained from the tangent-tangent correlation function



$$\langle \vec{t}(s+x)\vec{t}(s)\rangle \sim \exp(-x/l_p)$$

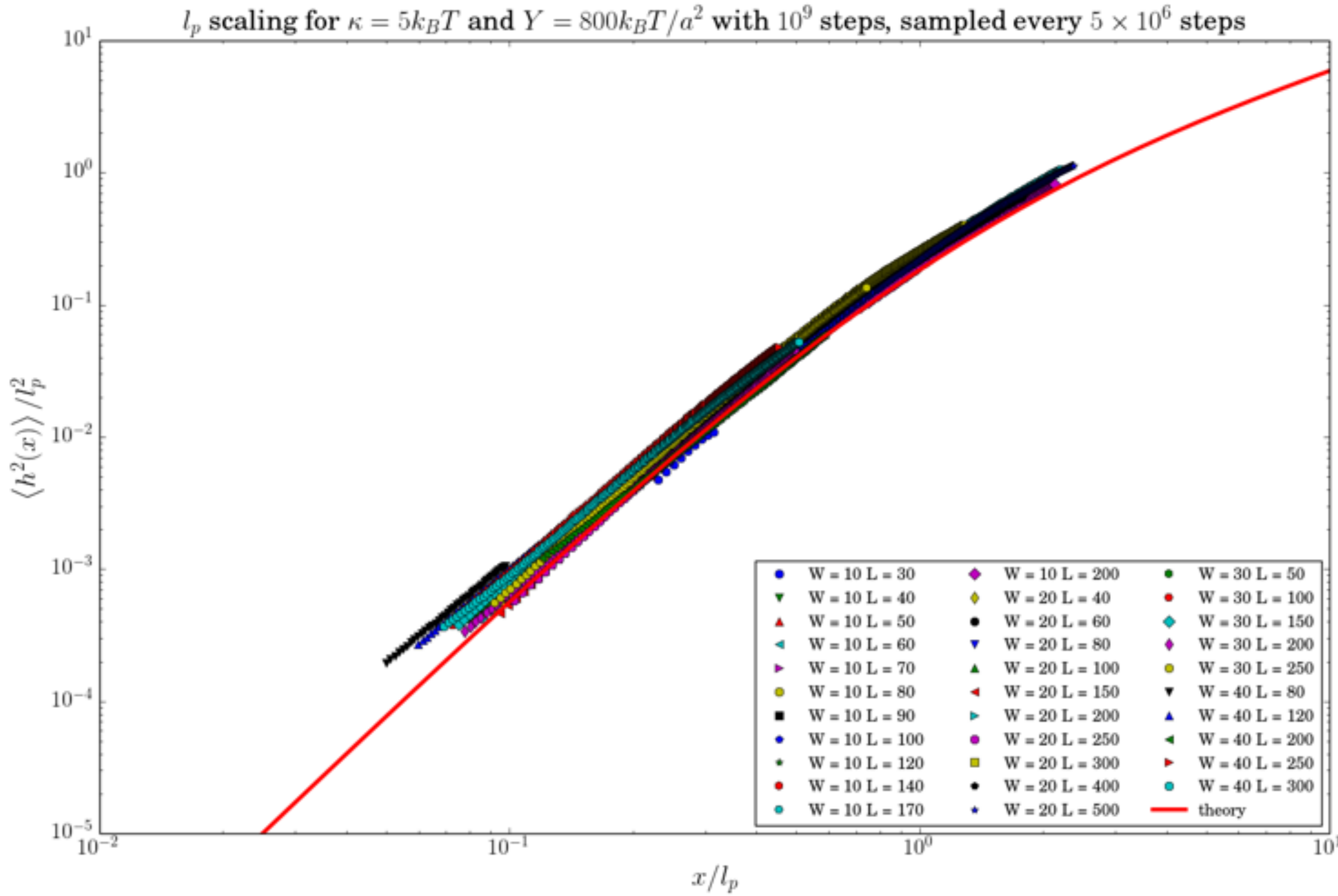
Following Panyukov & Rabin PRE **62** (2000) $l_p \approx 2W\kappa_R/k_BT$



$$\kappa_R/\kappa_0 \sim \left(\frac{W}{l_{th}}\right)^{\eta}$$

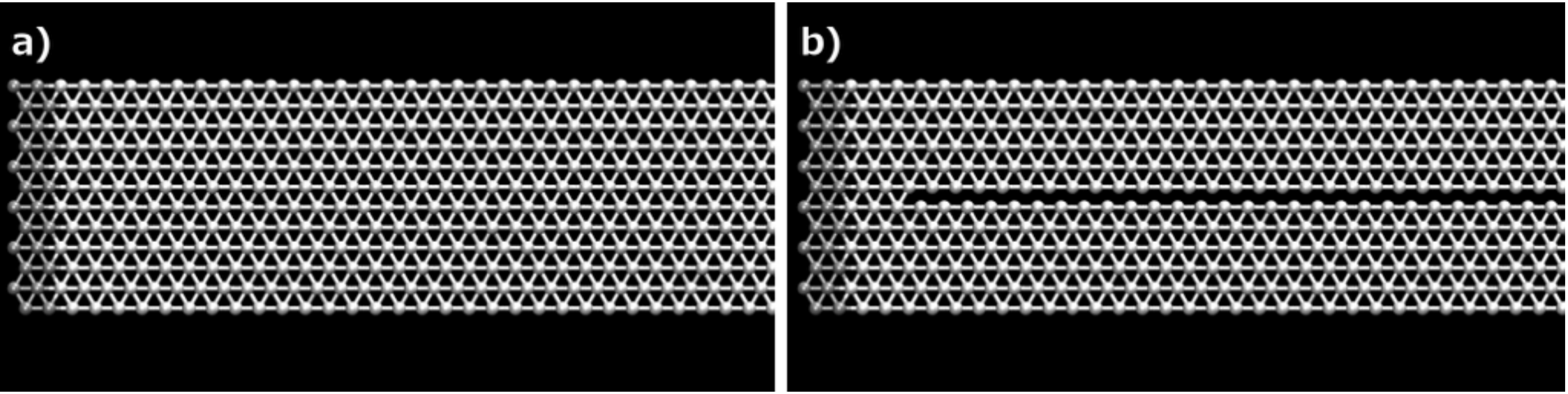
Height Fluctuations

$$\Phi(x) = \frac{1}{W}\int dy \langle h^2(x,y)\rangle / l_p^2 \qquad \Phi(x) \sim (x/l_p)^3 \; (x > W)$$



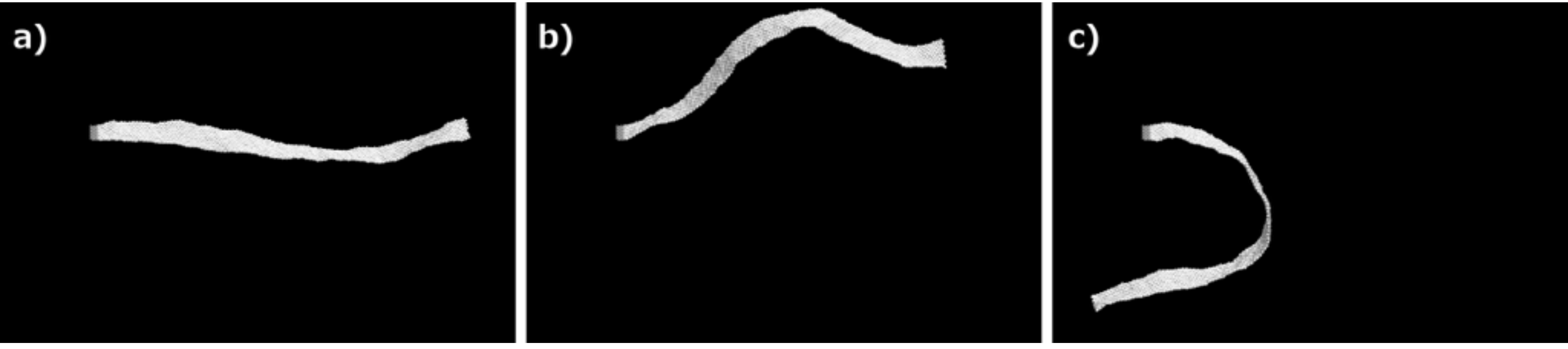
MD simulations of slits

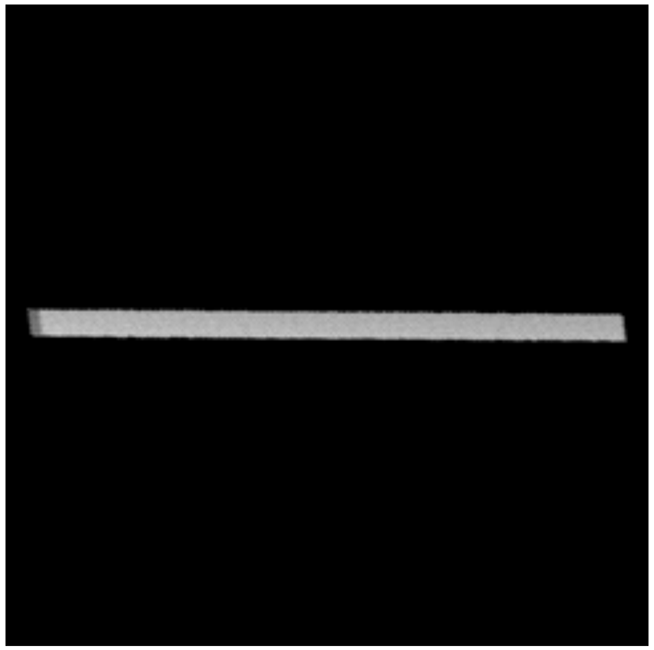
Emily Russell, R. Sknepnek and MJB
arXiv:1512.04670



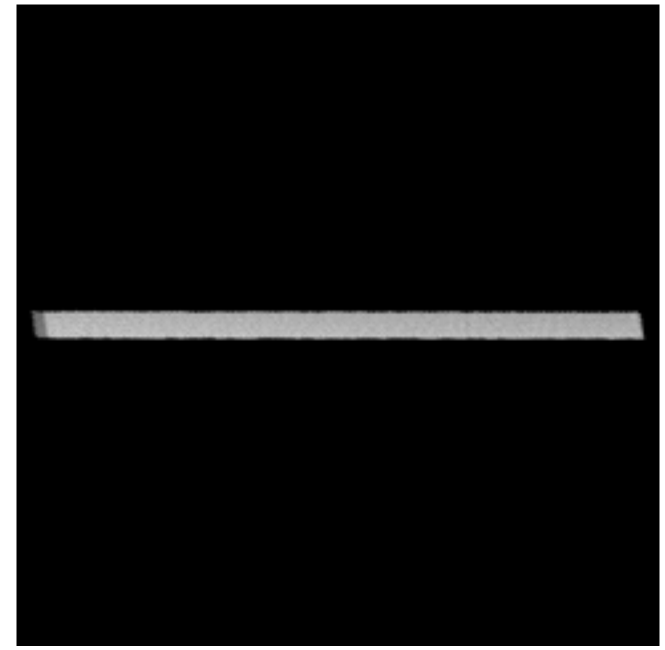
$$L = 100a \quad W = 10a \quad N = 1188 \, \text{vertices}$$

$$k = 3600 k_B T \quad \kappa = 5 k_B T \quad \text{vK} = \frac{YLW}{\kappa} \approx 2 \times 10^6$$

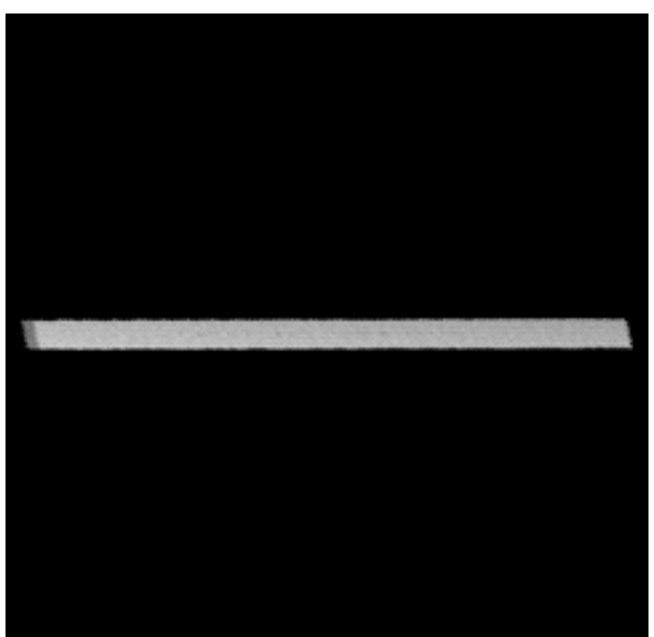




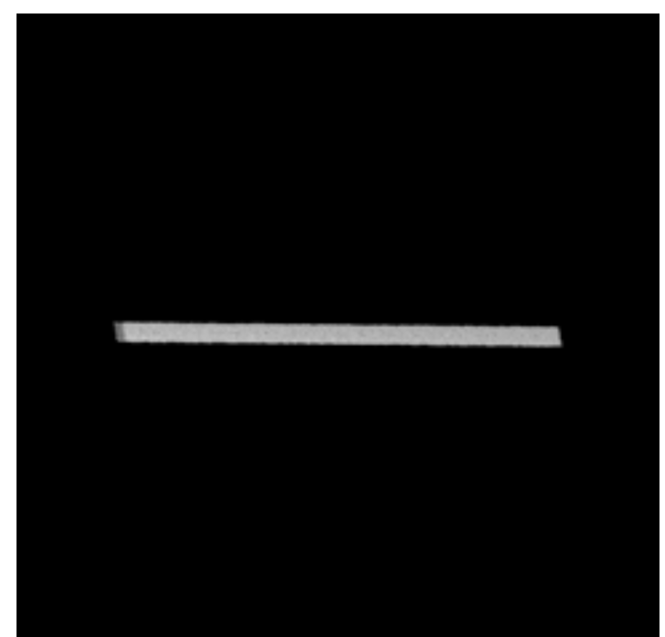
Reference Ribbon



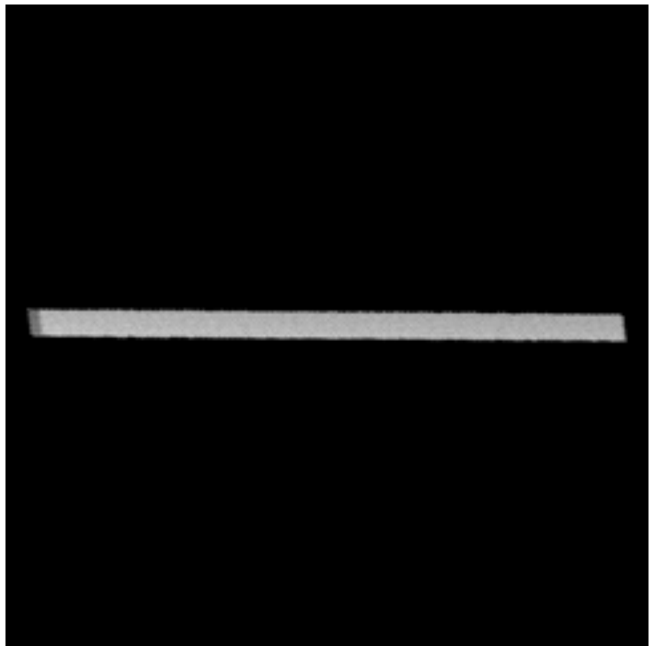
Short slit



Longer slit



End-to-end slit



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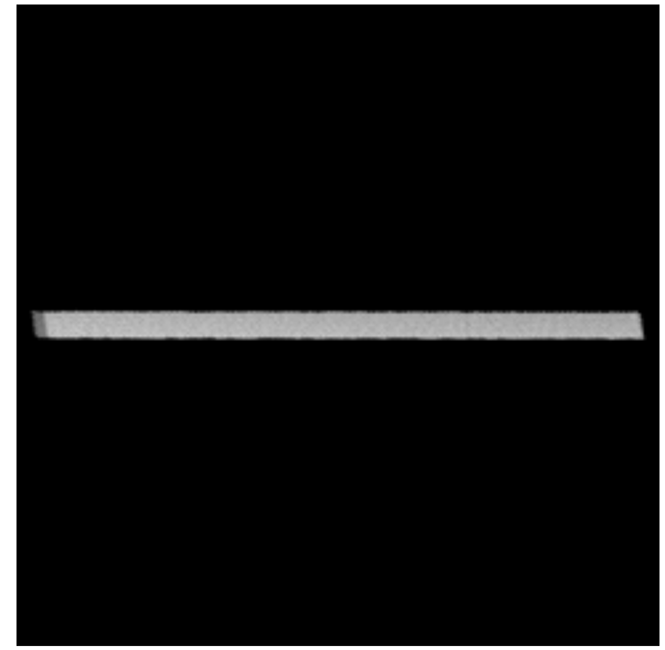

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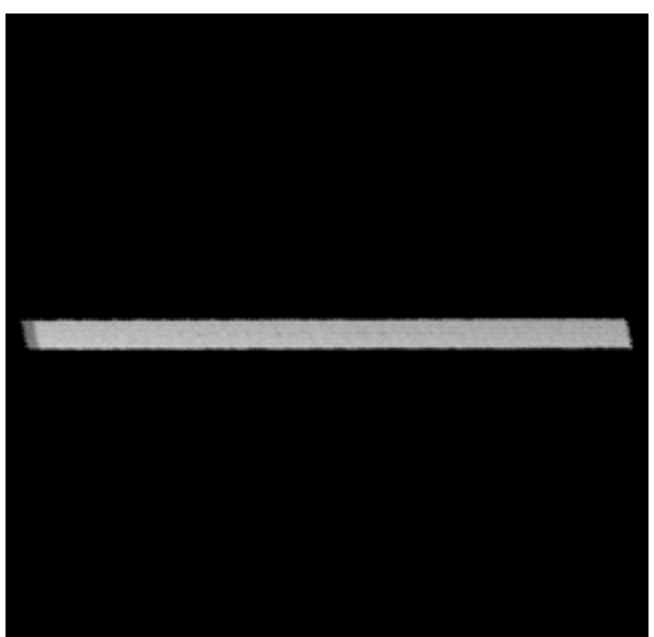

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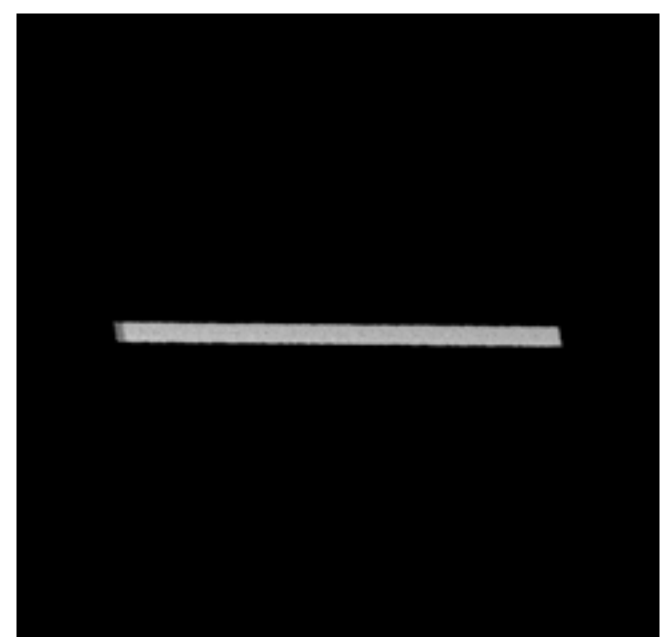

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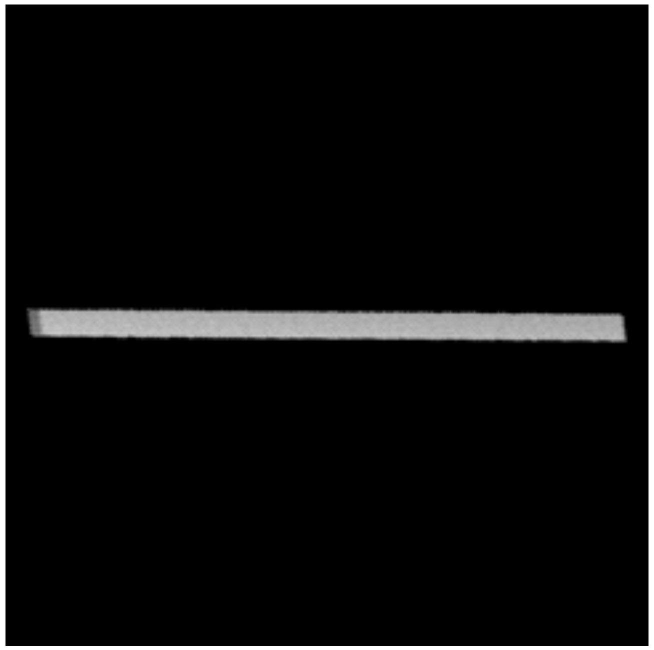

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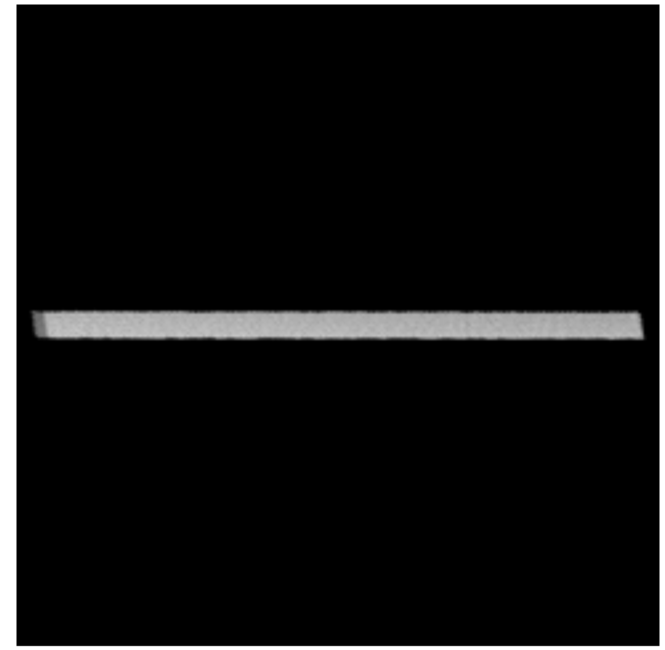

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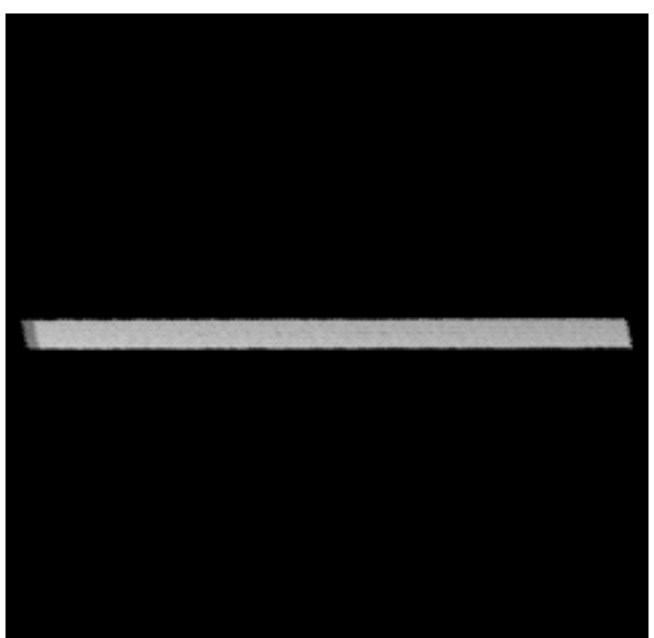

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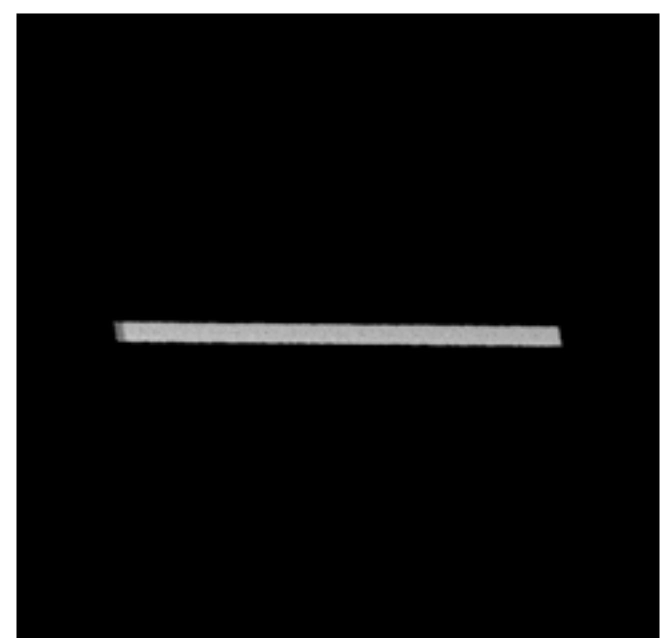

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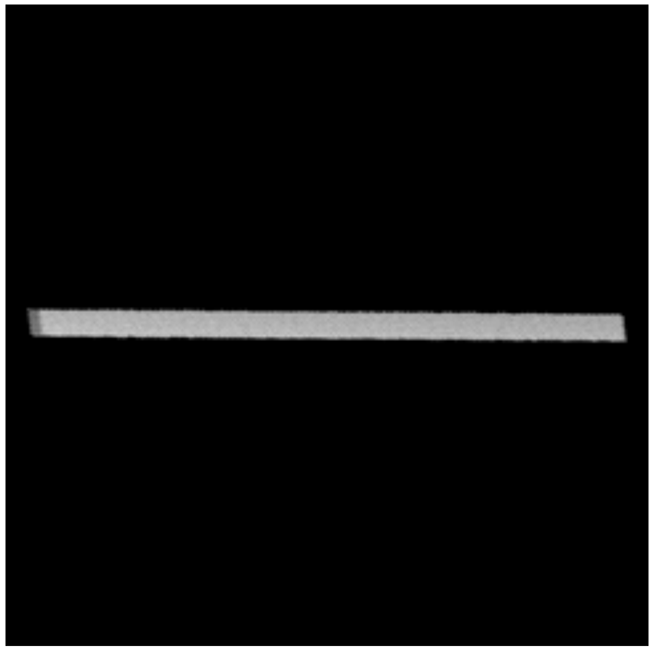

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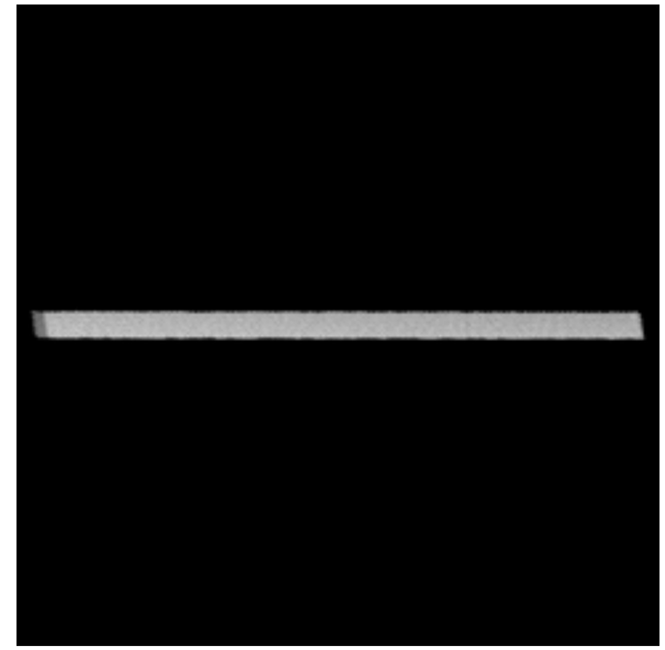

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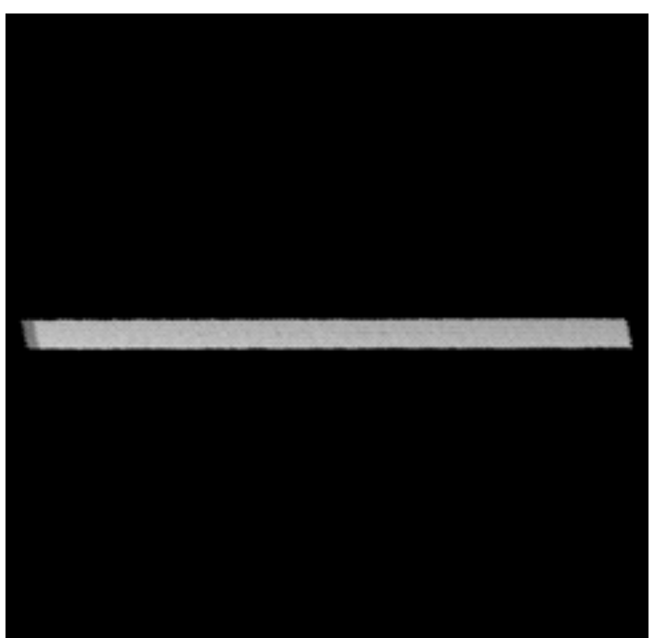

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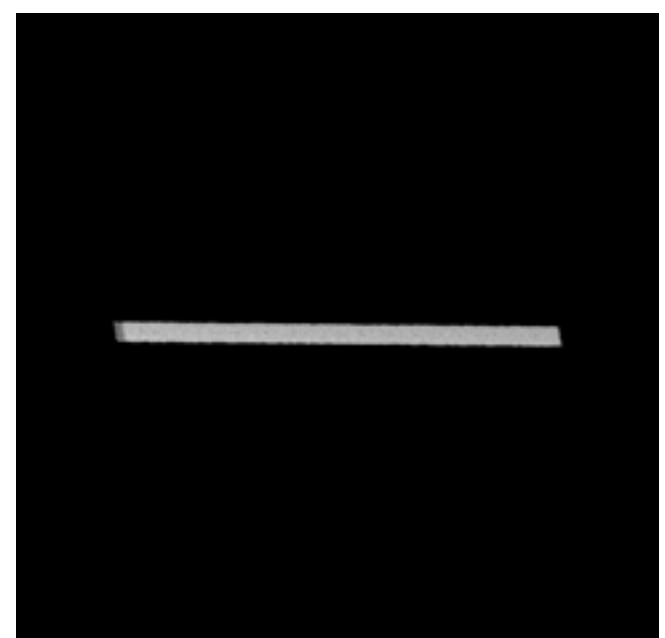

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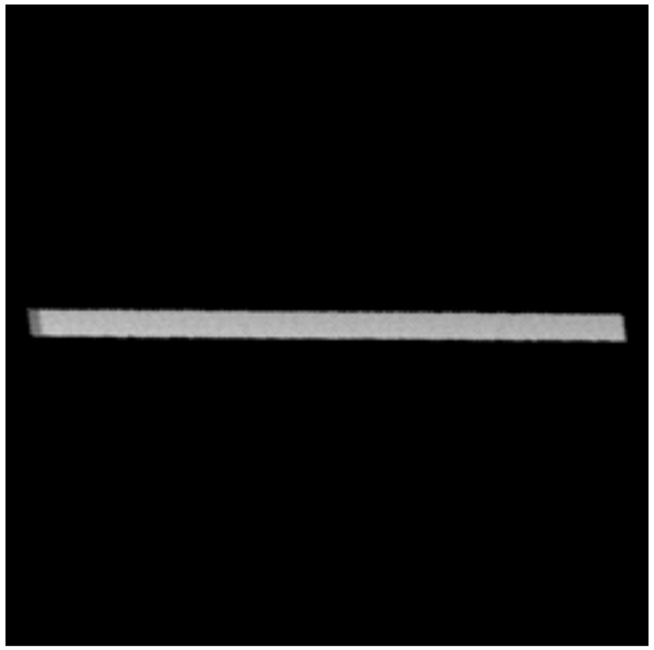

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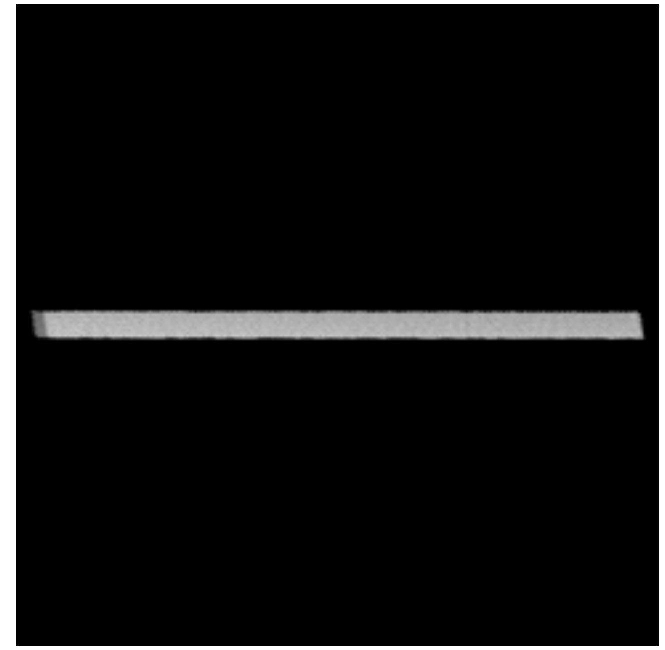

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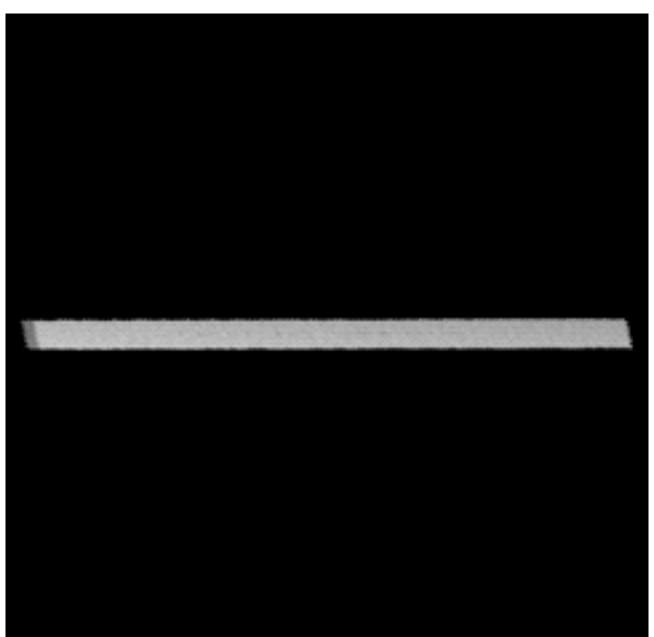

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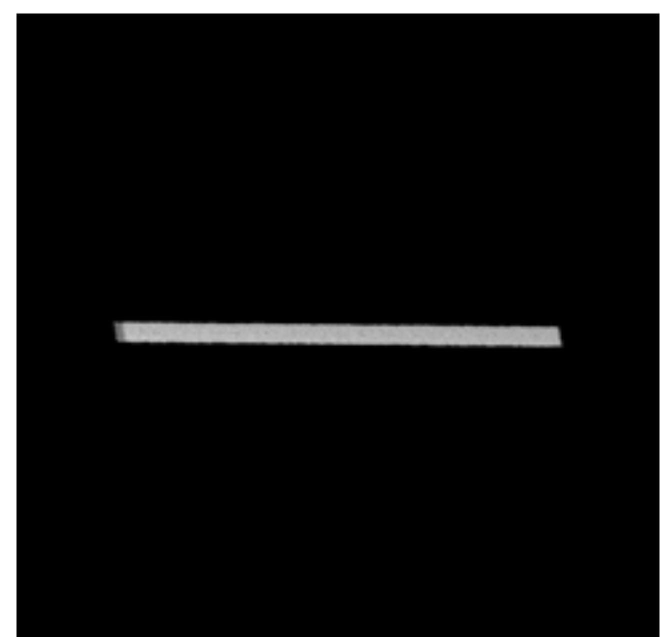

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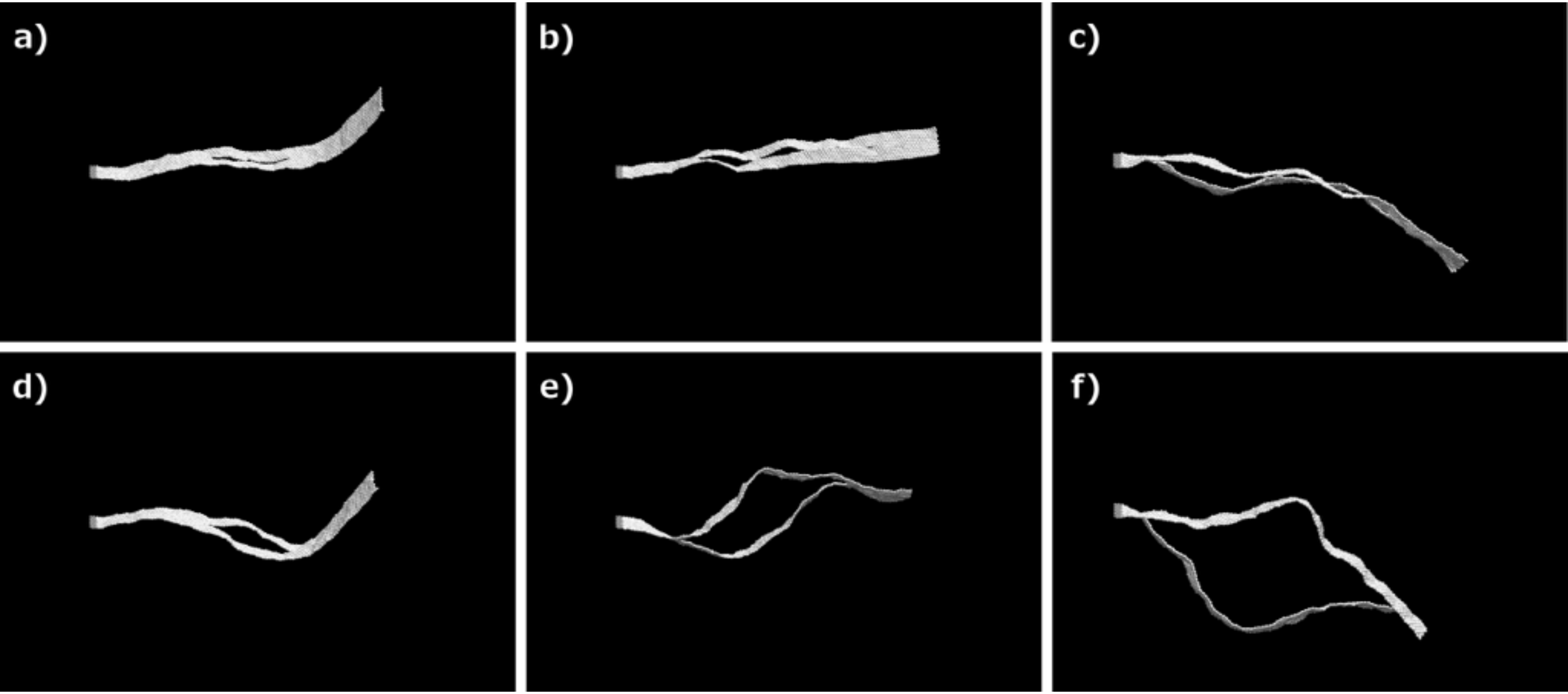
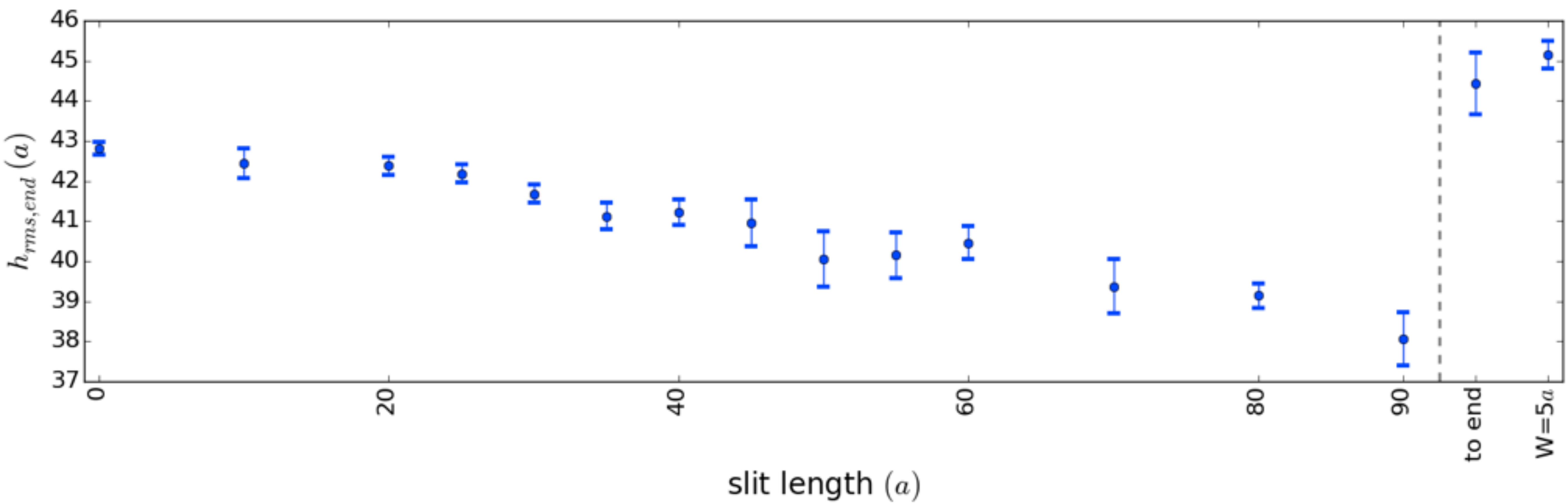
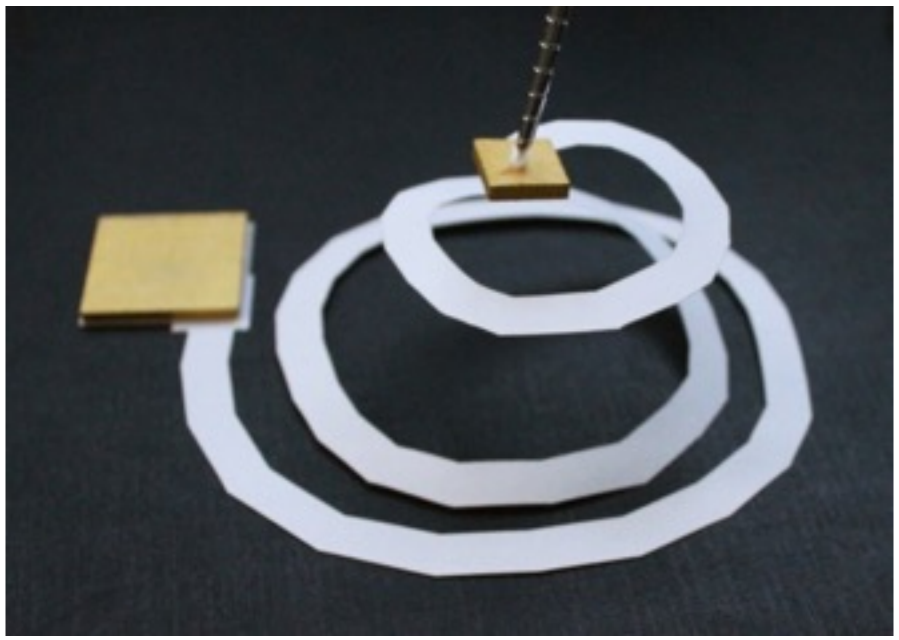

a)
b)
c)
d)
e)
f)

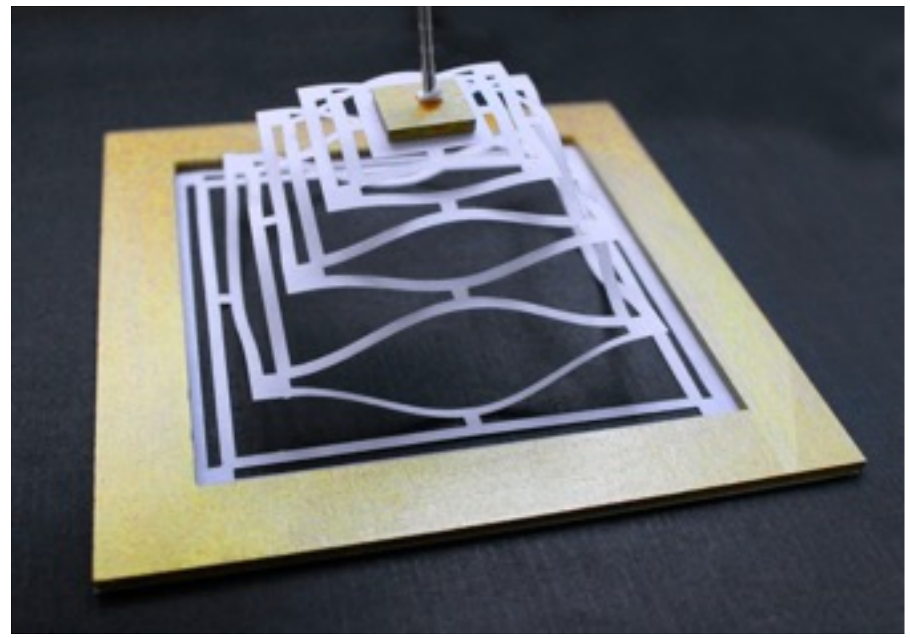
RMS Height Fluctuations vs slit length

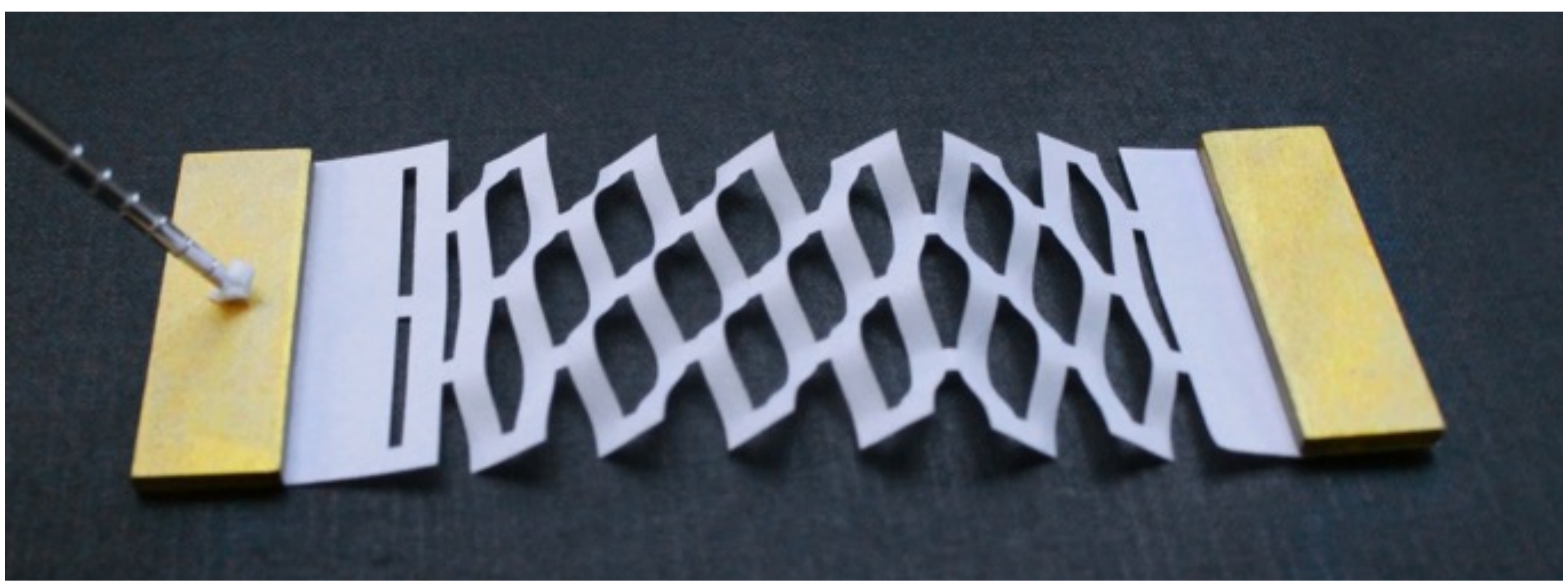


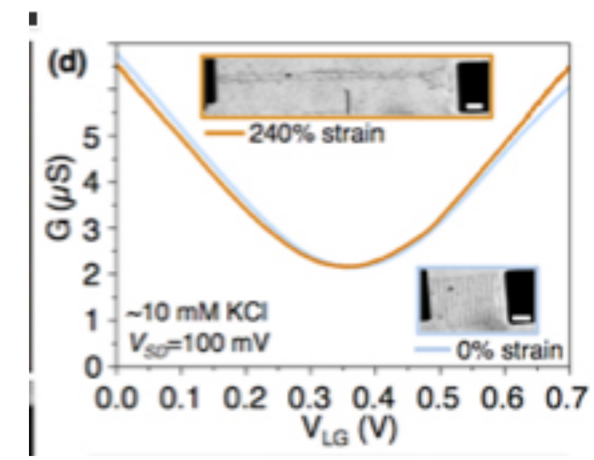
Order from disorder!

Ultimately we want to understand the mechanical/thermal properties of flexible structures such as



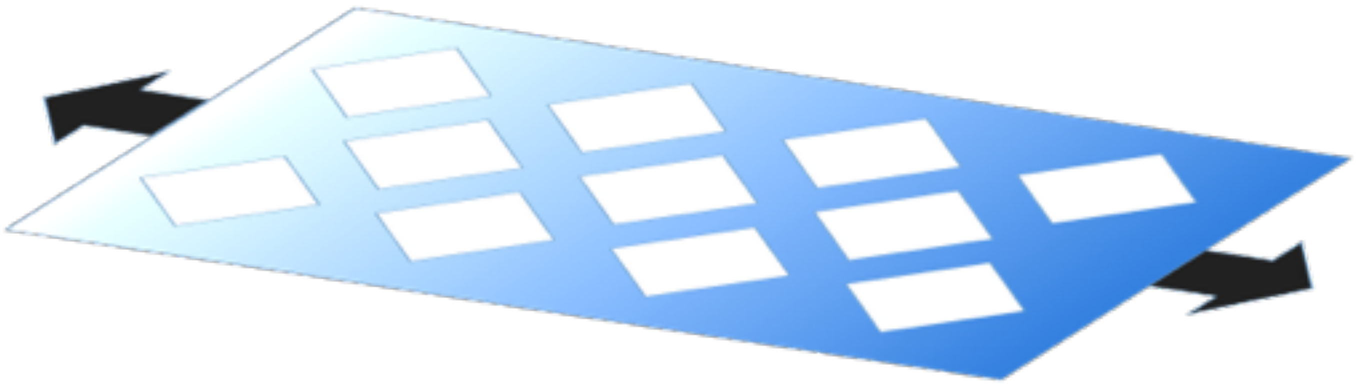


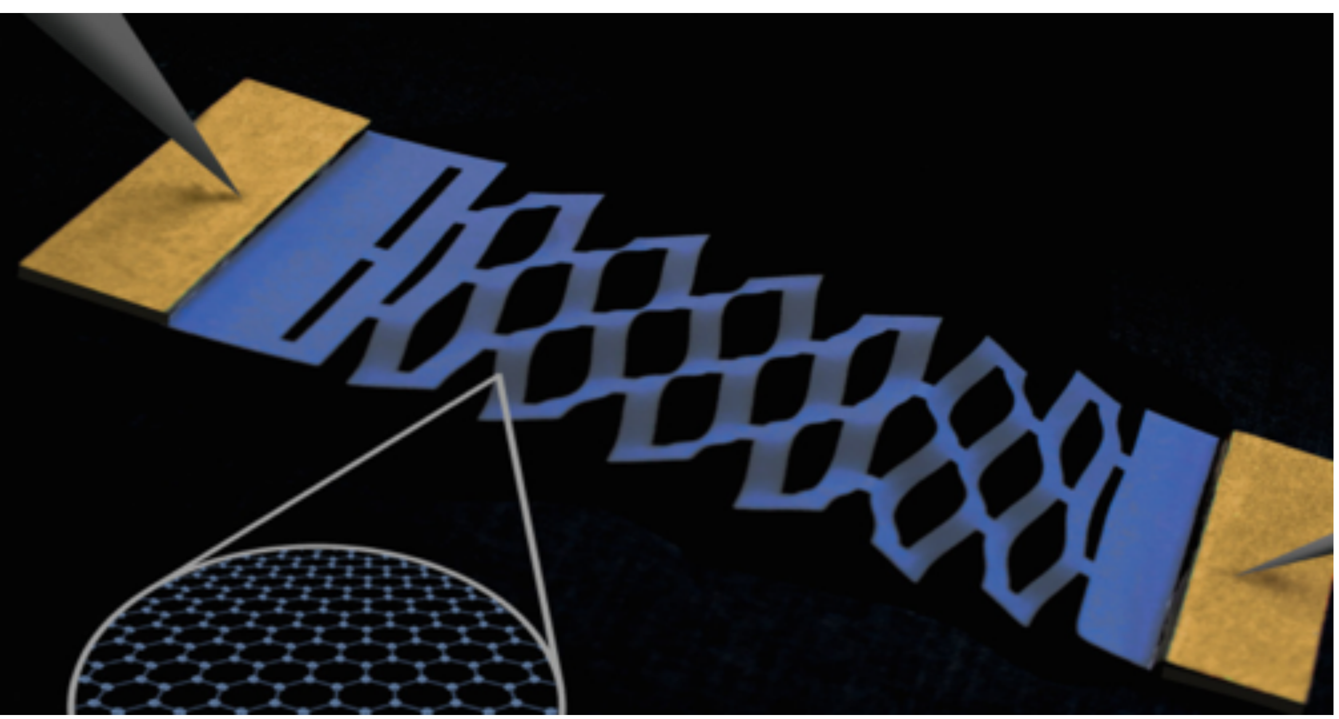


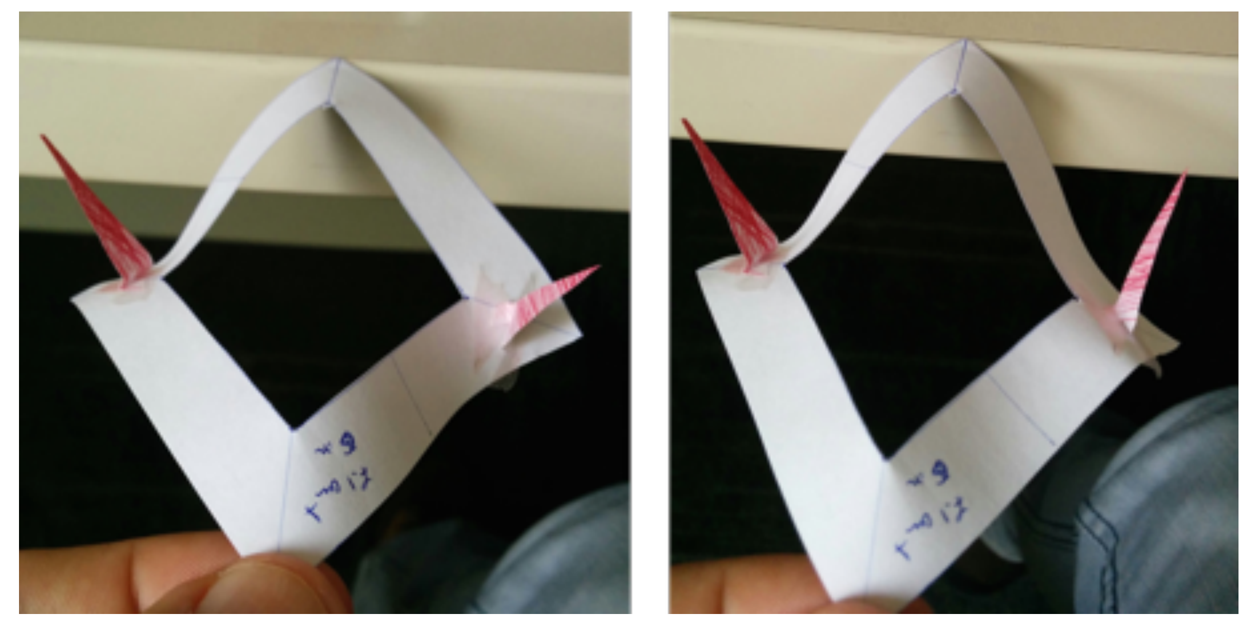


Mechanics of periodic arrays of holes

Michael Moshe and Suraj Shankar



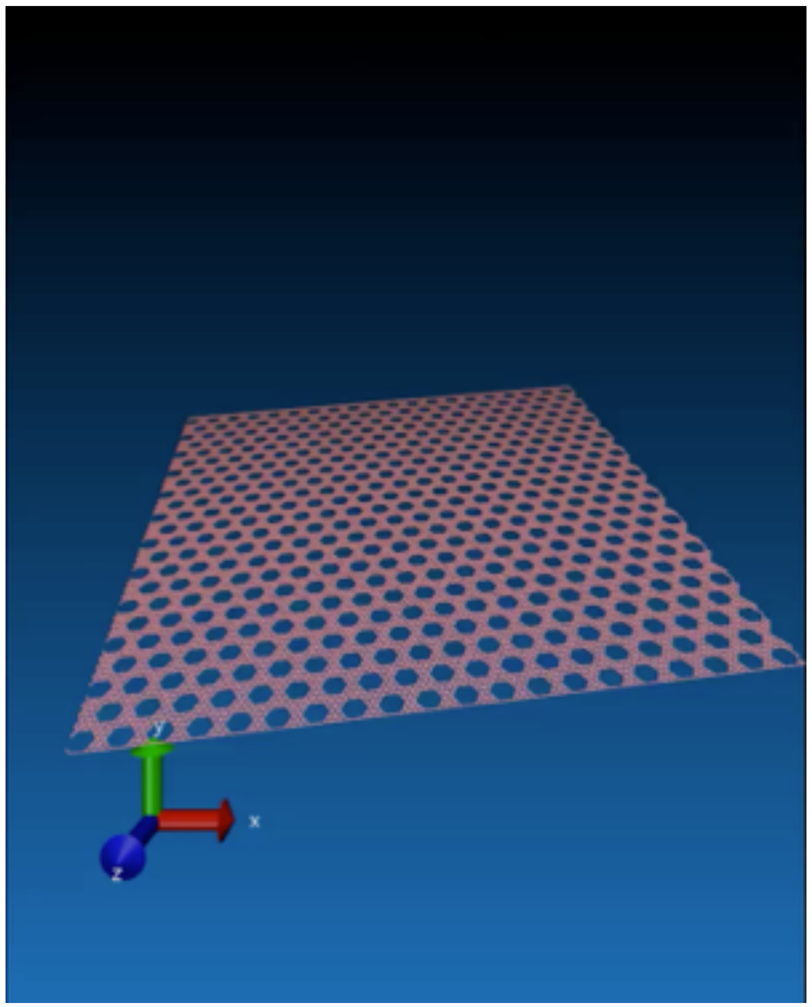


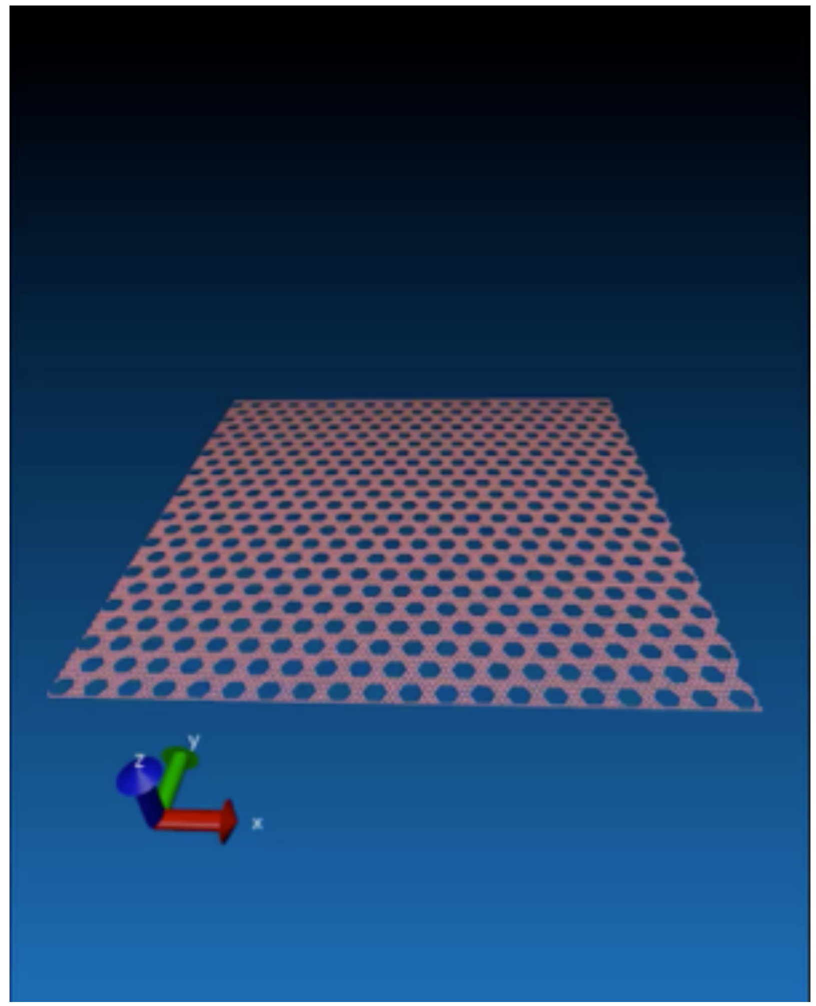


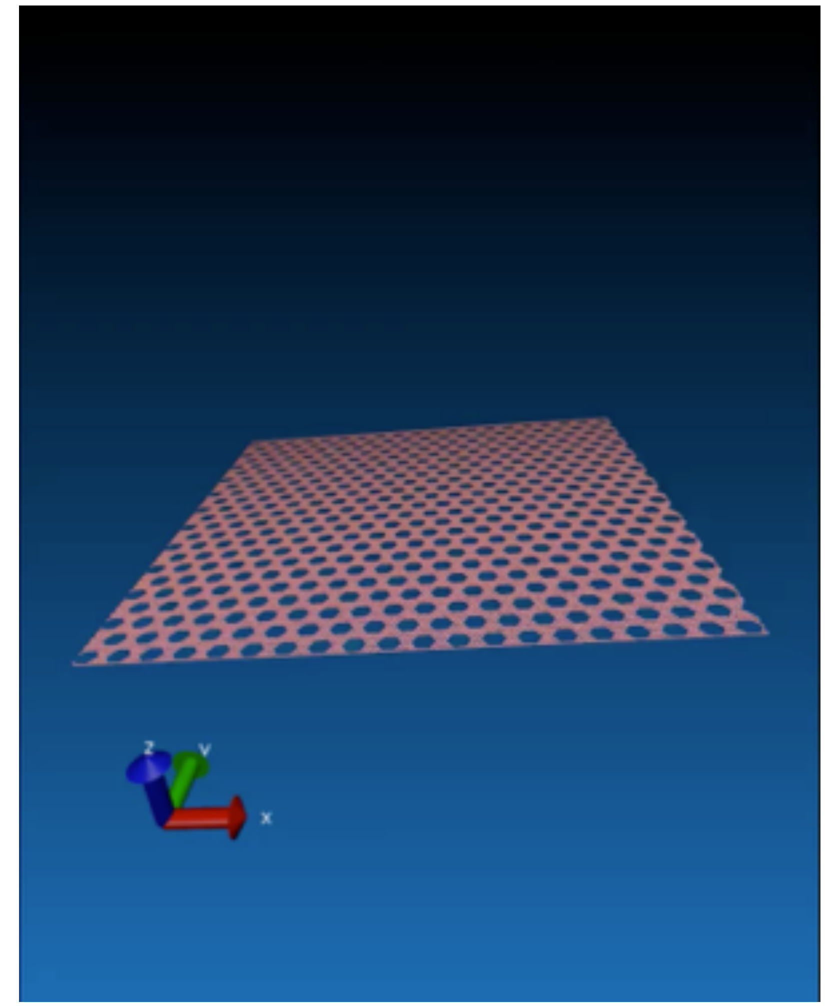
Dramatic change in response to external stress

Perforated (*Holey*) Membranes

David Yllanes and MJB

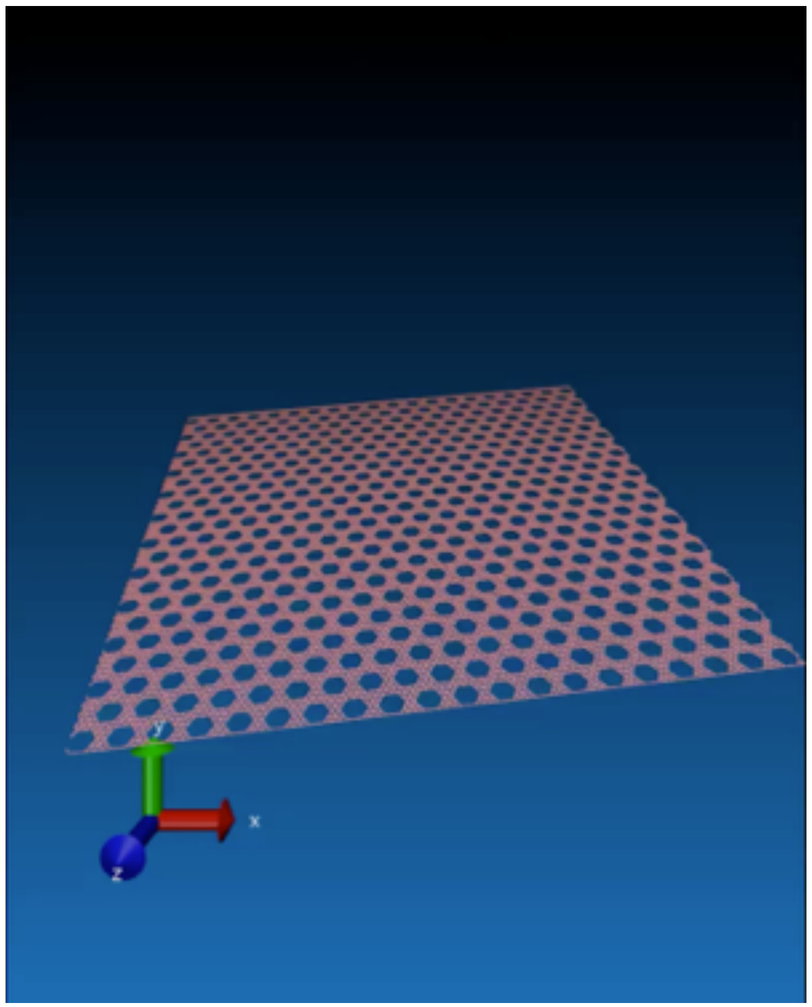


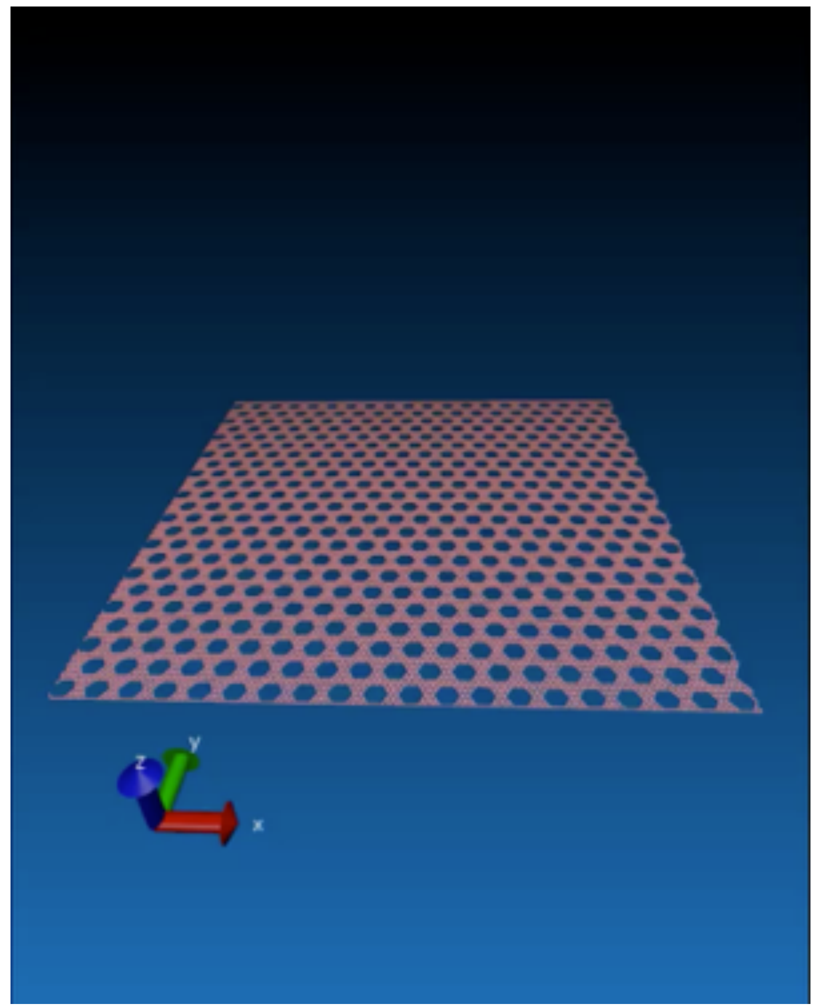


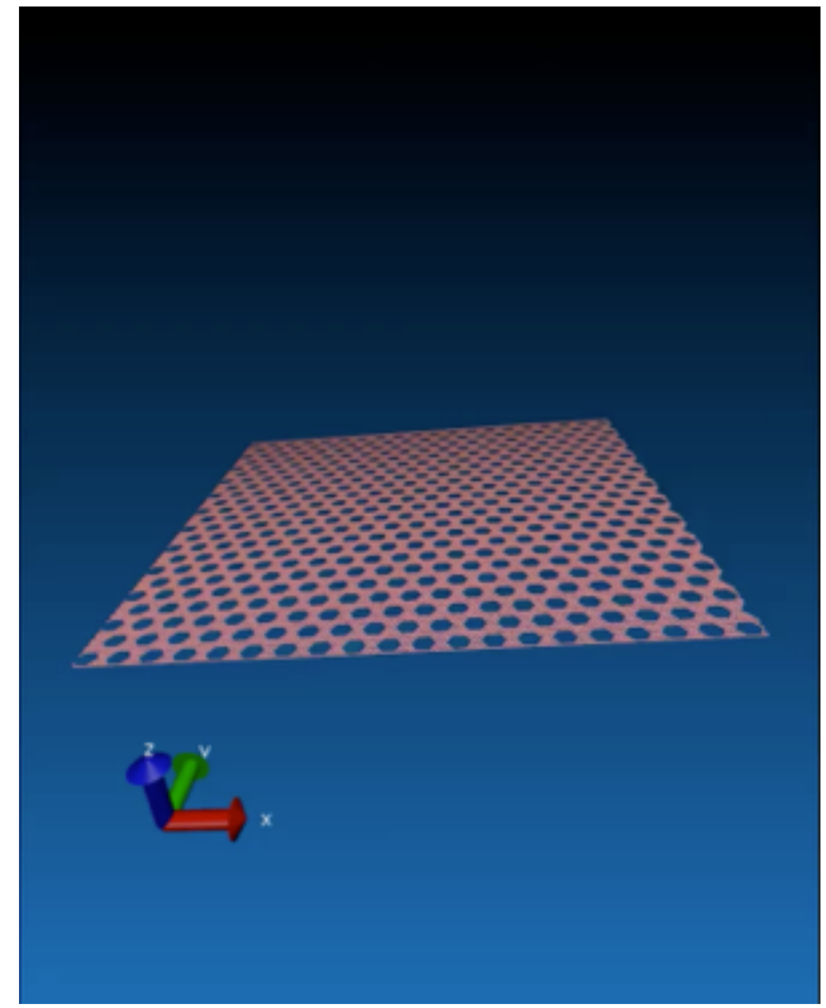


Perforated (*Holey*) Membranes

David Yllanes and MJB

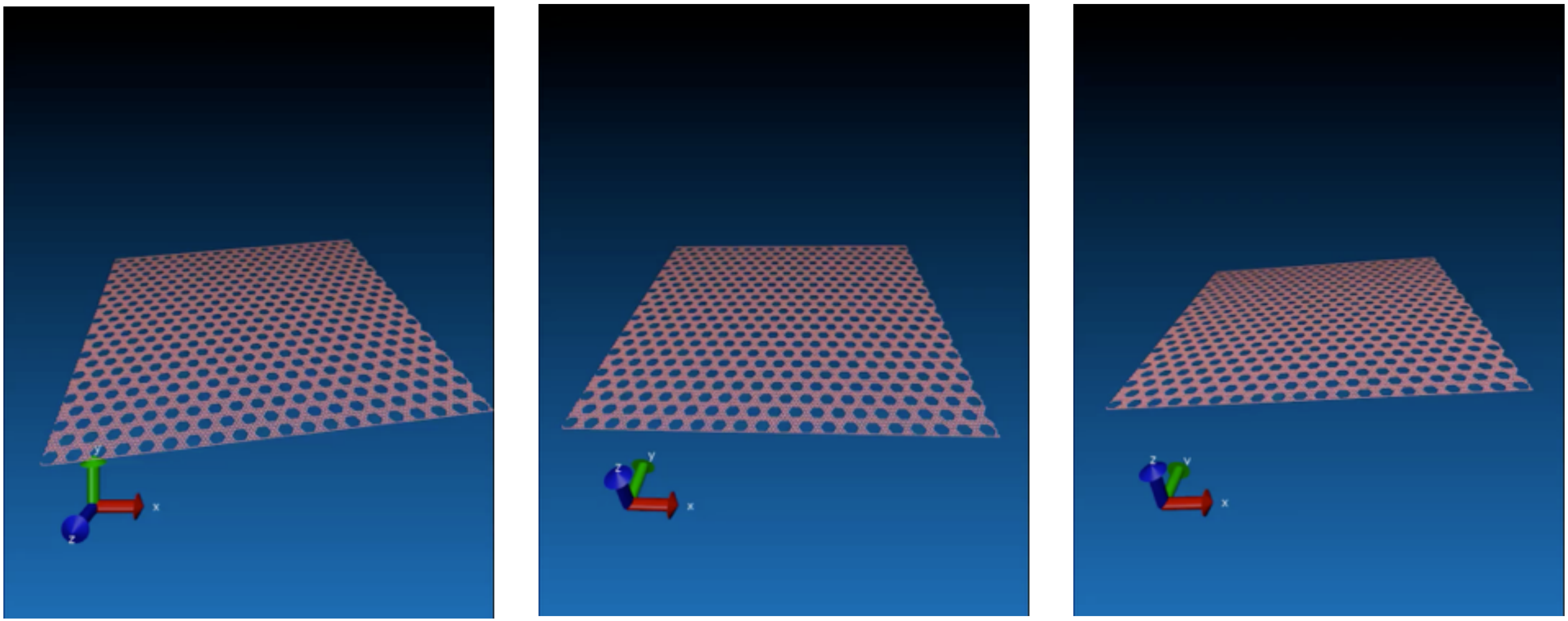






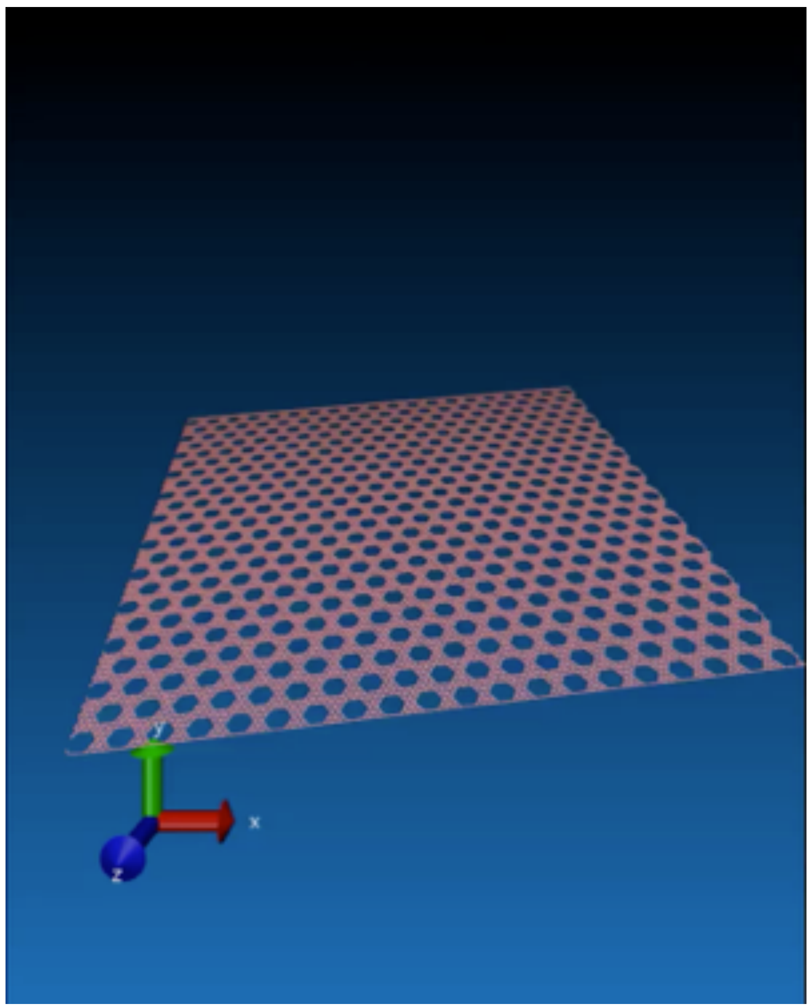
Perforated (*Holey)* Membranes

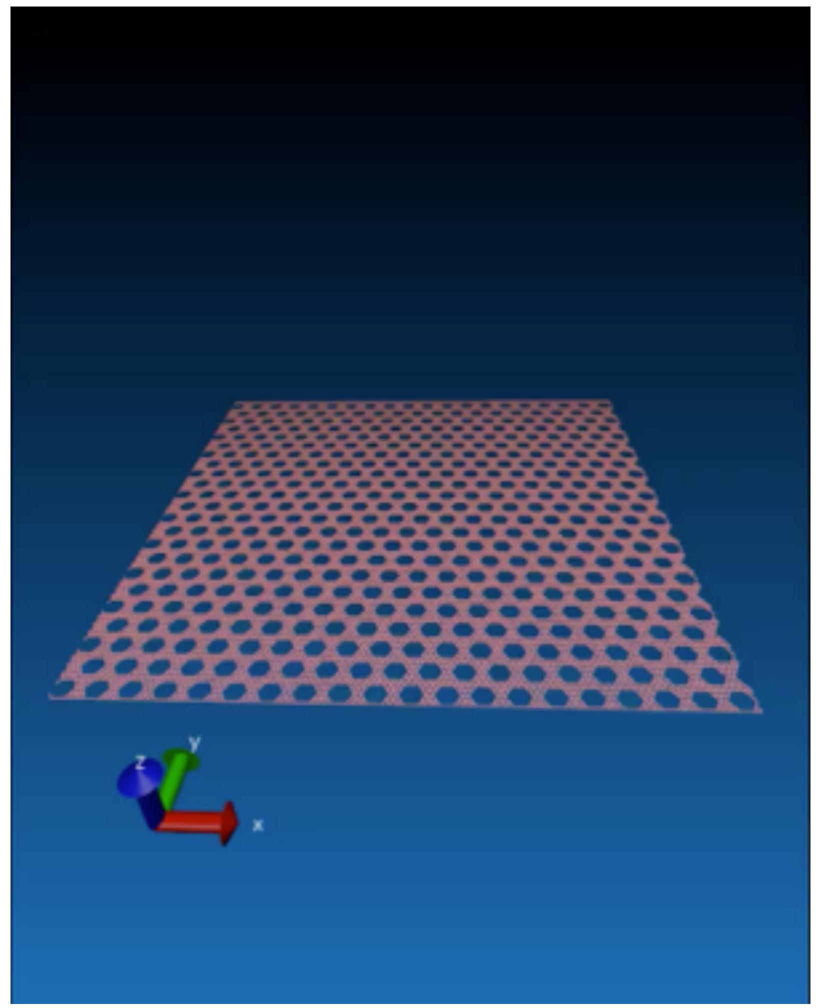
David Yllanes and MJB

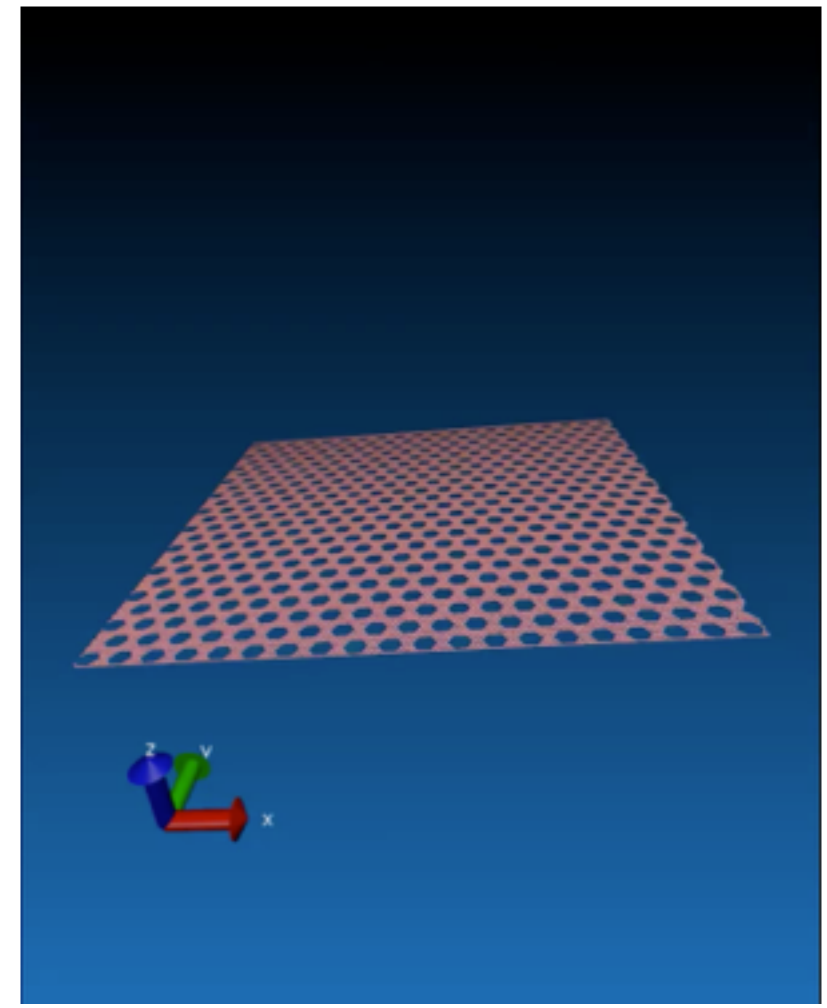


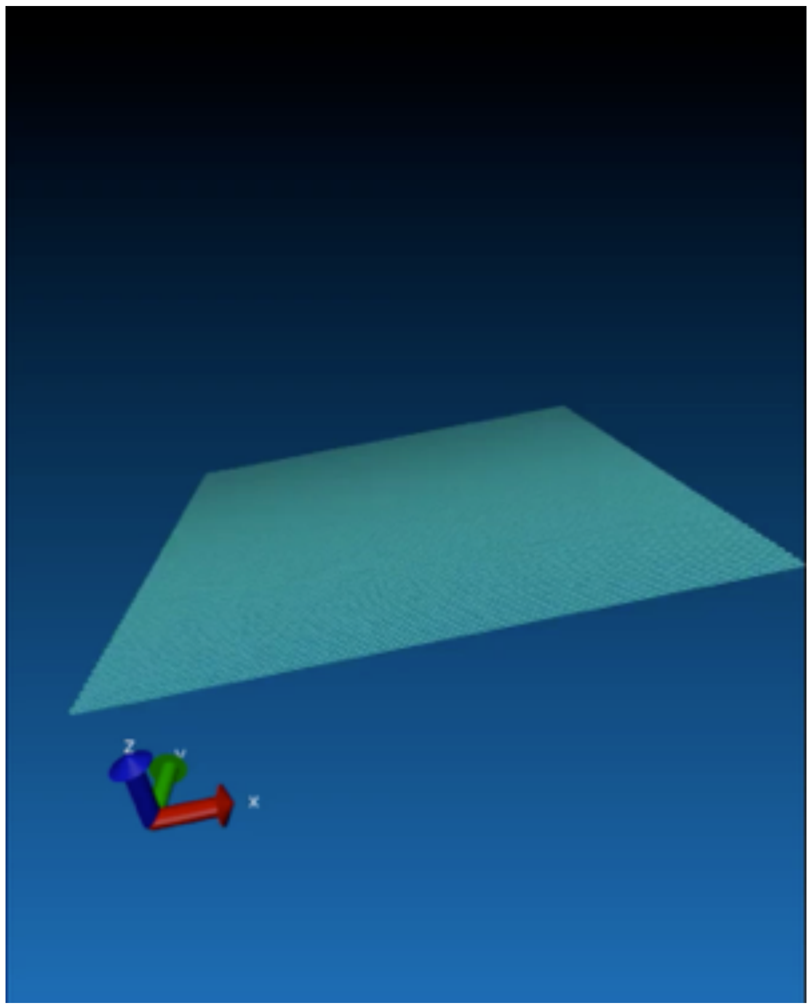
Perforated (*Holey*) Membranes

David Yllanes and MJB





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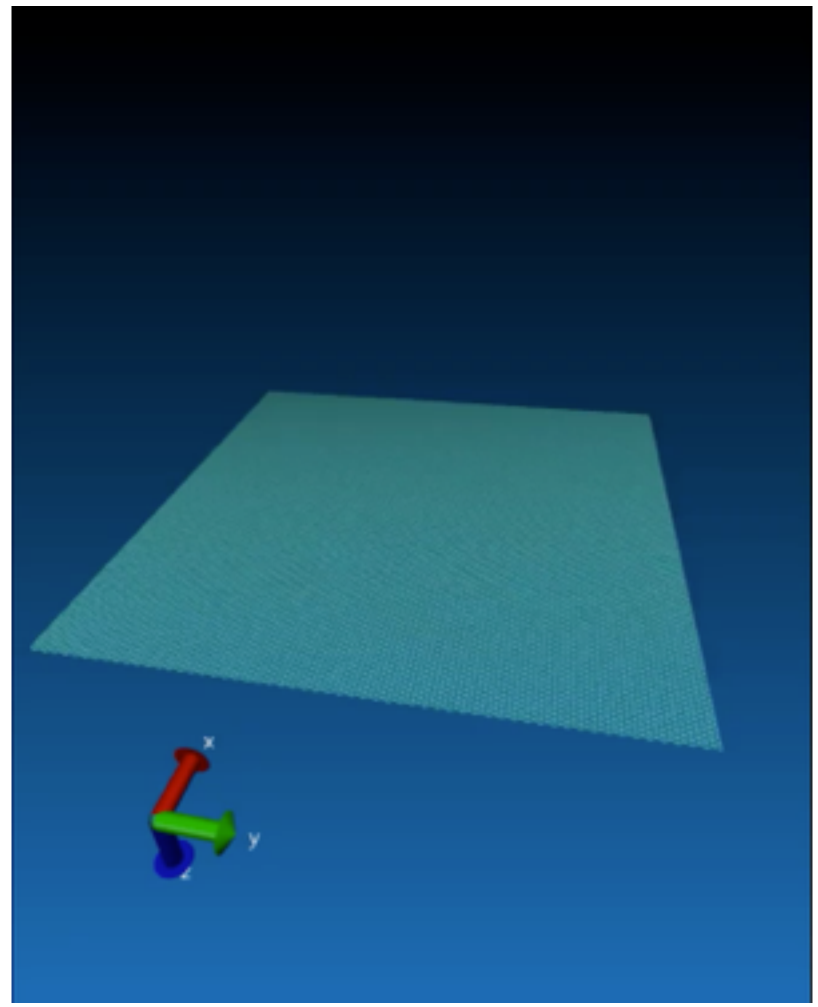
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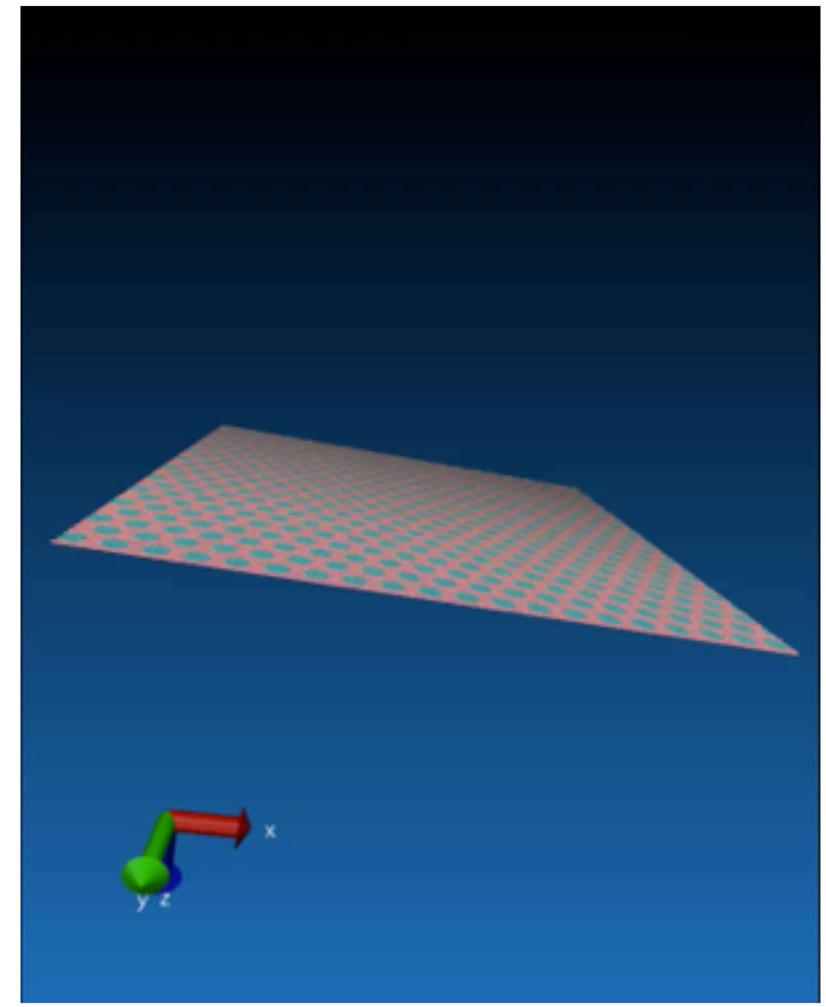
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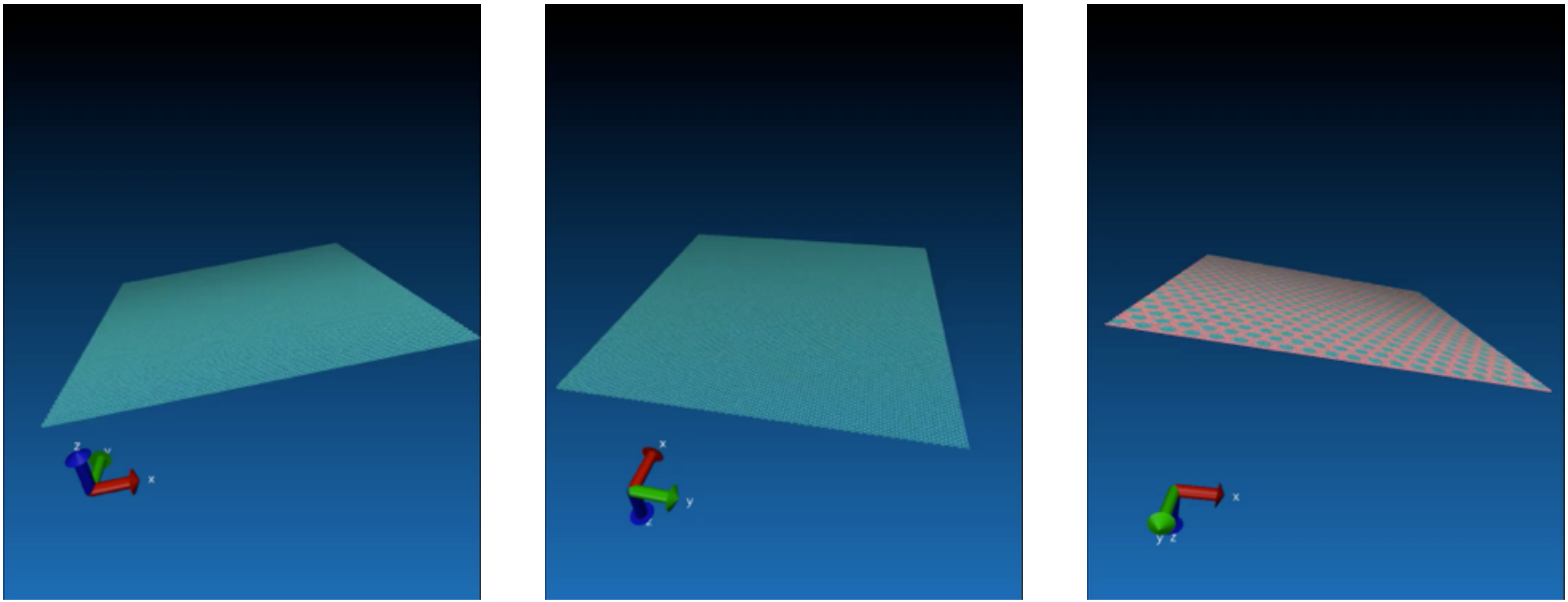

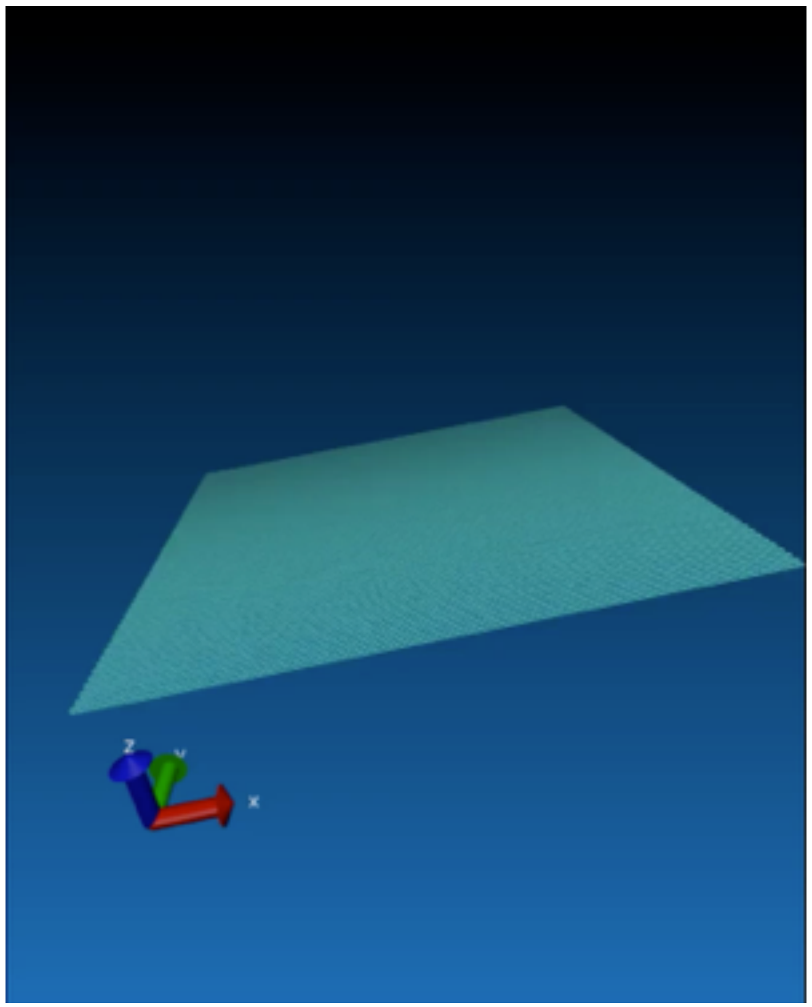
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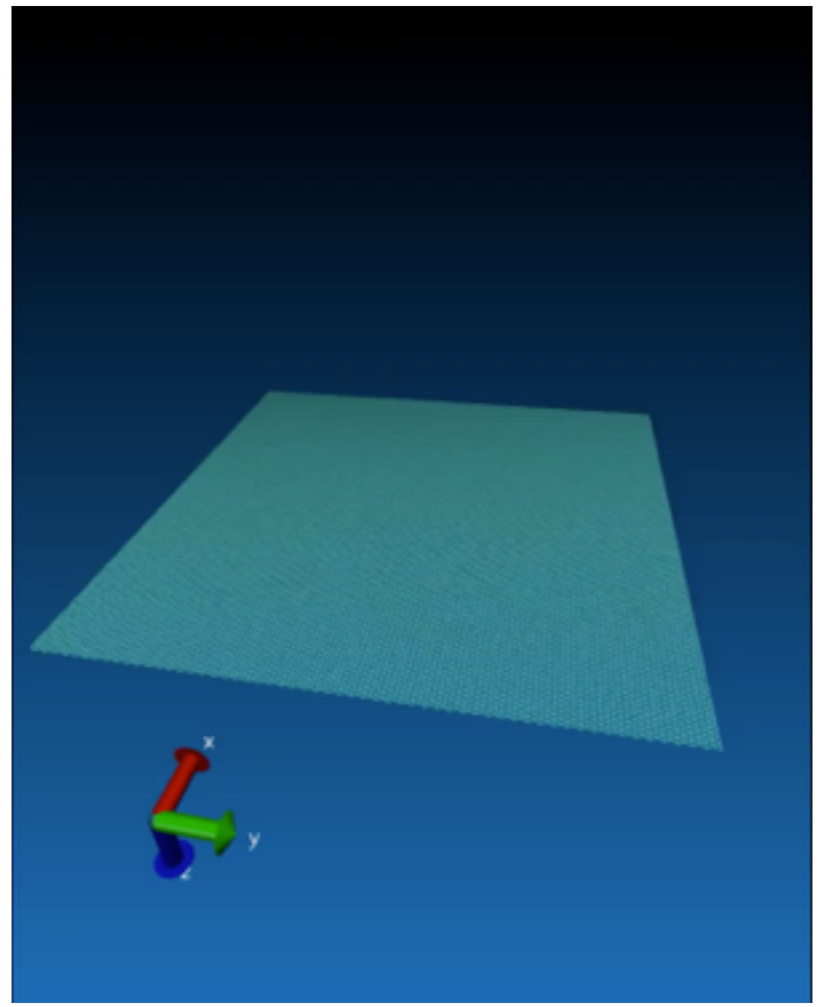
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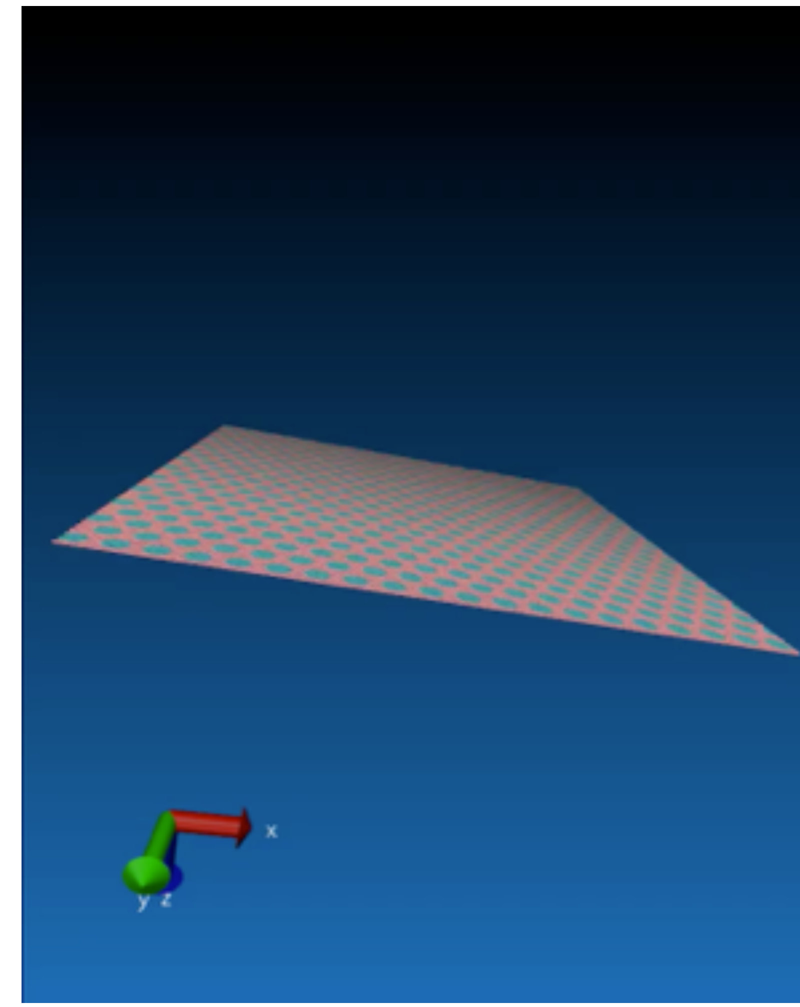
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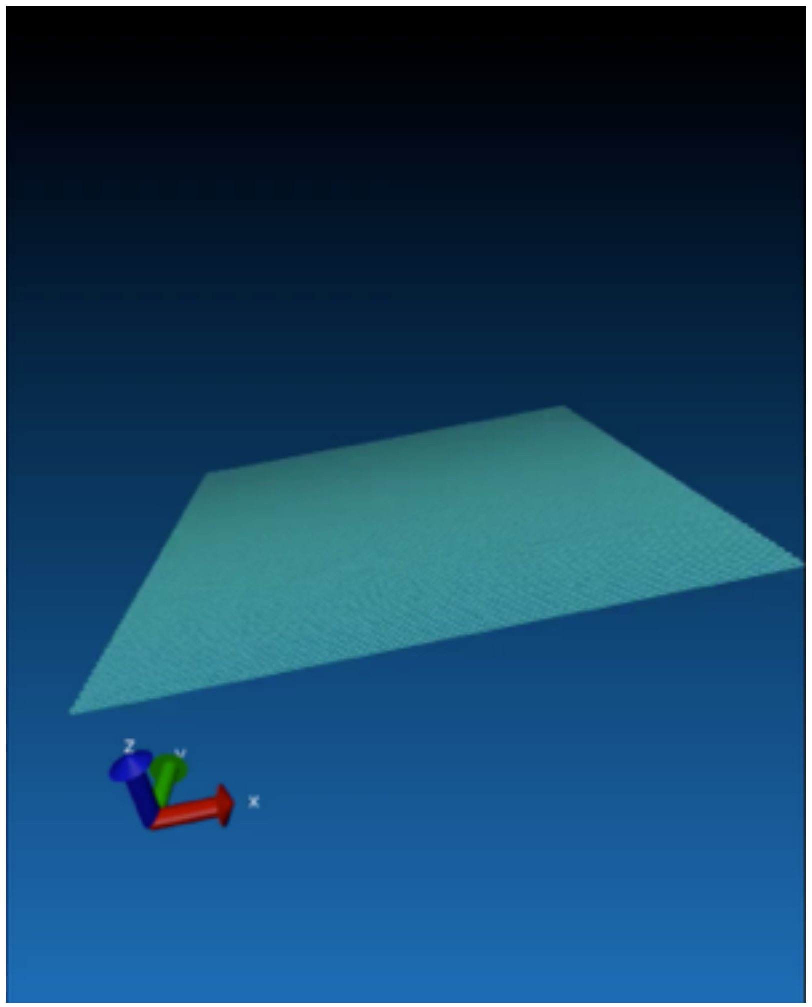
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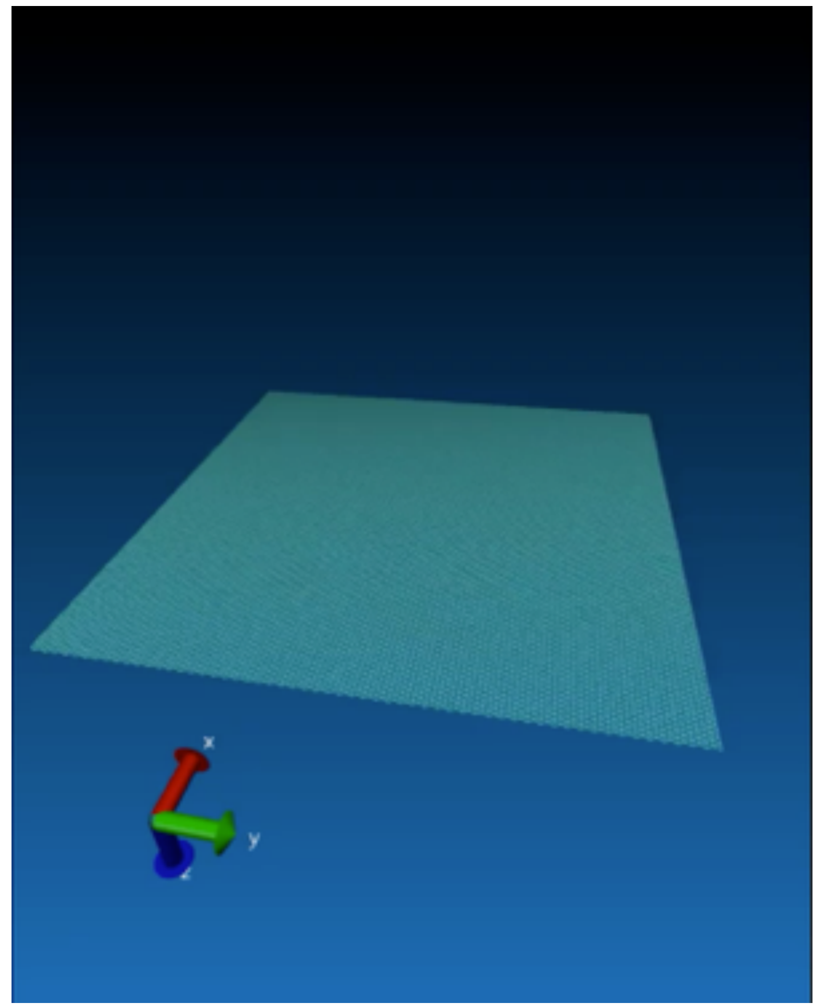
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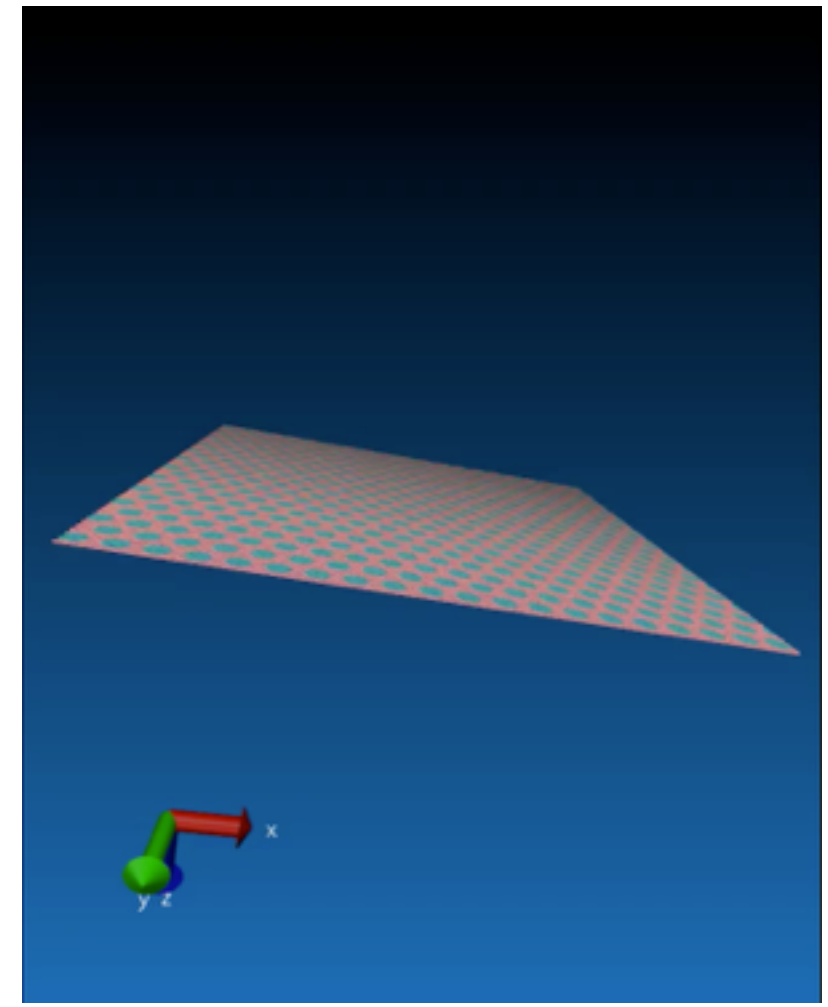
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Conclusions

Remarkable interplay of hard and soft matter in graphene statistical mechanics

Wonderful realization of a 2d elastic membrane

Material properties are strongly geometry dependent

Controlling the geometry may allow us to design distinct metamaterials with a variety of mechanical properties starting from graphene alone