

Graphene Statistical Mechanics

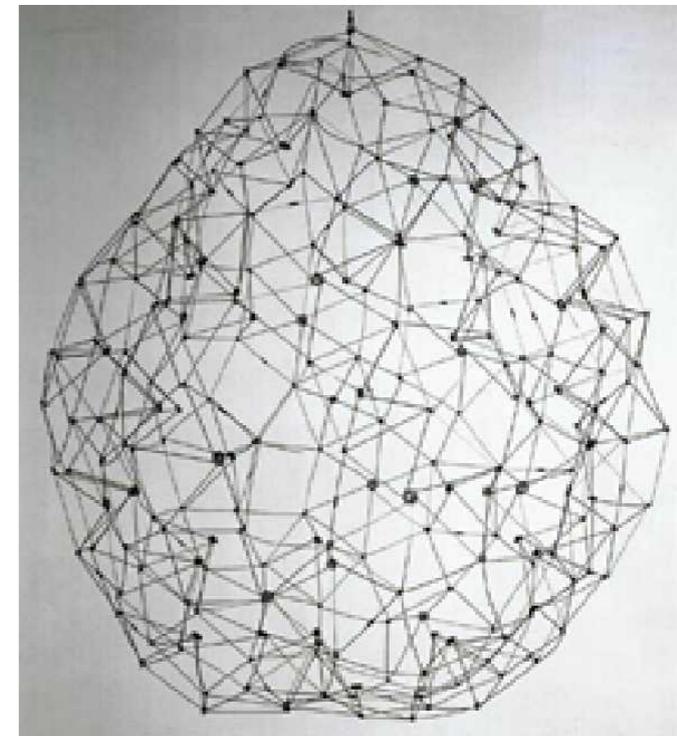
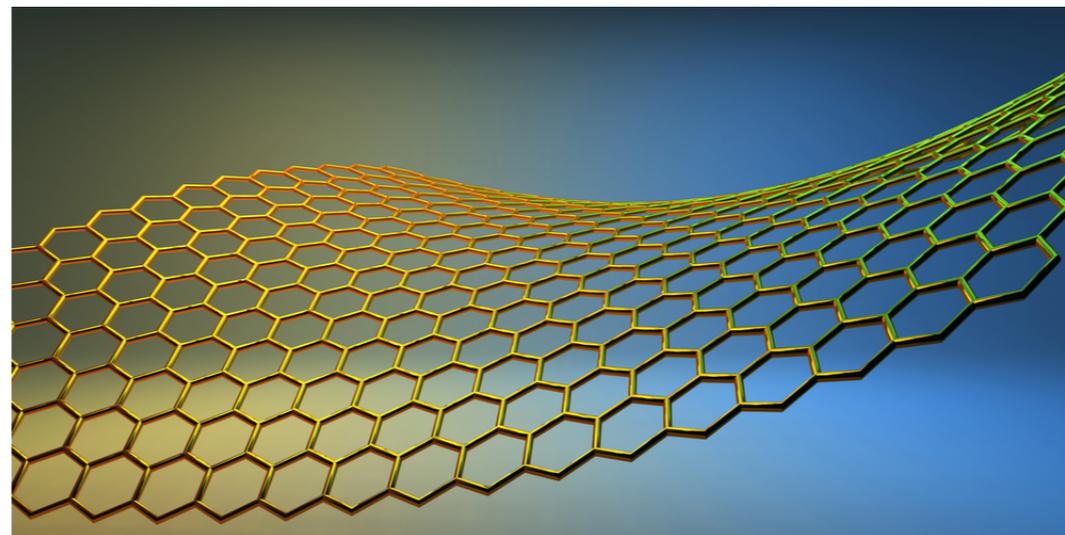
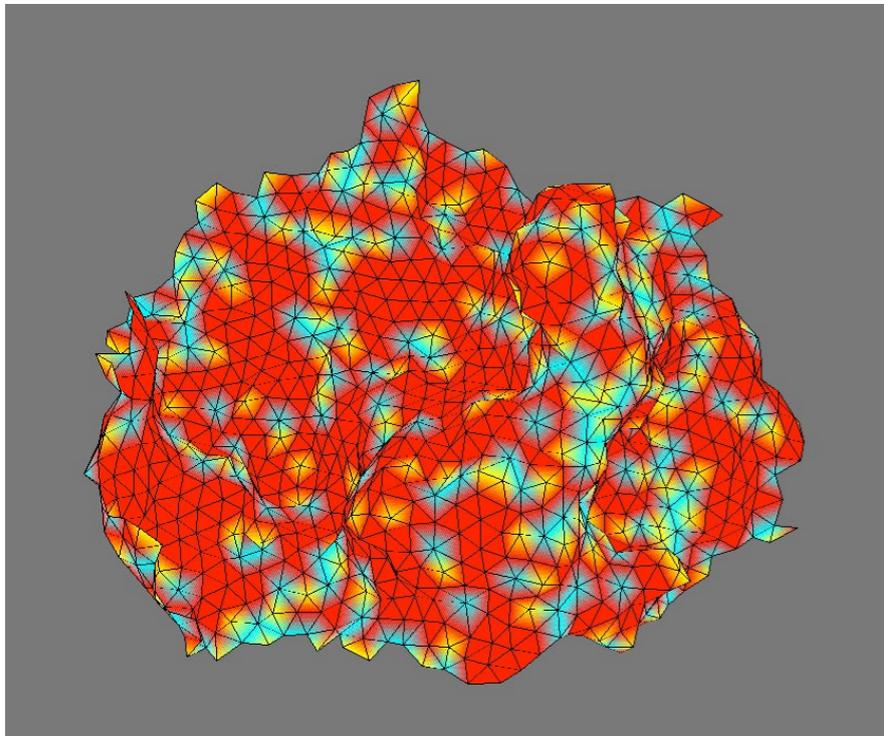
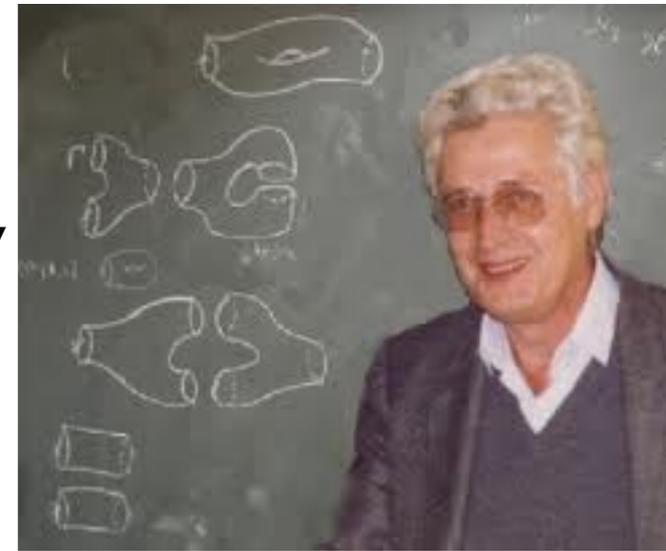
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Outline

Field theory of elastic/tethered/polymerized membranes

Graphene as a membrane

Experiments

Graphene Kirigami & Metamaterials

Simulations

Elastic (polymerized) membranes

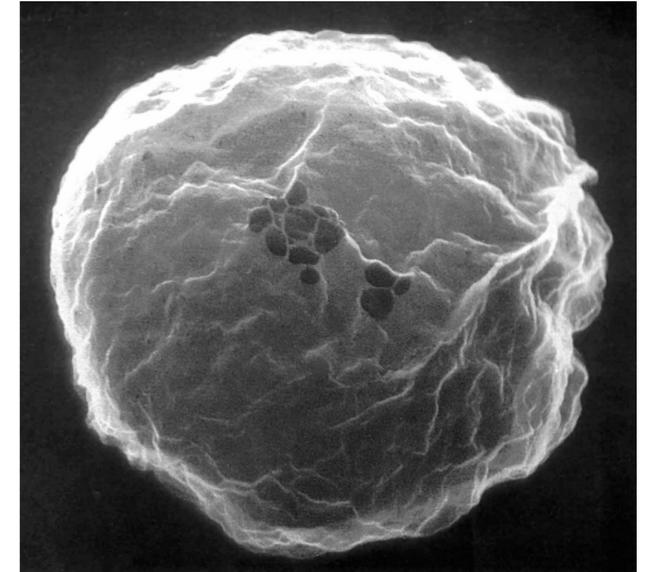
Entropically-stabilized phases



Bowick et al. (1996)

$$E = E_{el} + E_{bend}$$

↑
shear (μ) + compression (K)



RBC Ghost: Steck (77)

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

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

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

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

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

Nelson-Peliti (1987)

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

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

∫ out the phonons

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

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

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

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

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

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

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

Calculate perturbatively in Y

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

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

Power counting

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

IR Stiffening!

$\kappa \rightarrow \kappa_R(\vec{q} + \vec{k})$ 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

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

Order from Disorder!

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

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

$$\kappa_R(q) \sim q^{-\eta}$$

$$\mu(q) \sim q^{\eta_u}; \lambda(q) \sim q^{\eta_u}$$

$$\eta_u = 2(1 - \eta) \quad \text{Ward identities (remnant rotational symmetry)}$$

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

$$\eta = 0.72(4) \quad \text{MJB et al. (MC)}$$

Poisson Ratio

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

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

Flat phase fixed point

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

$$\implies \nu = -1/3 \quad \text{Auxetic}$$

MJB, Falcioni, Gitter and Thorleifsson (1997)

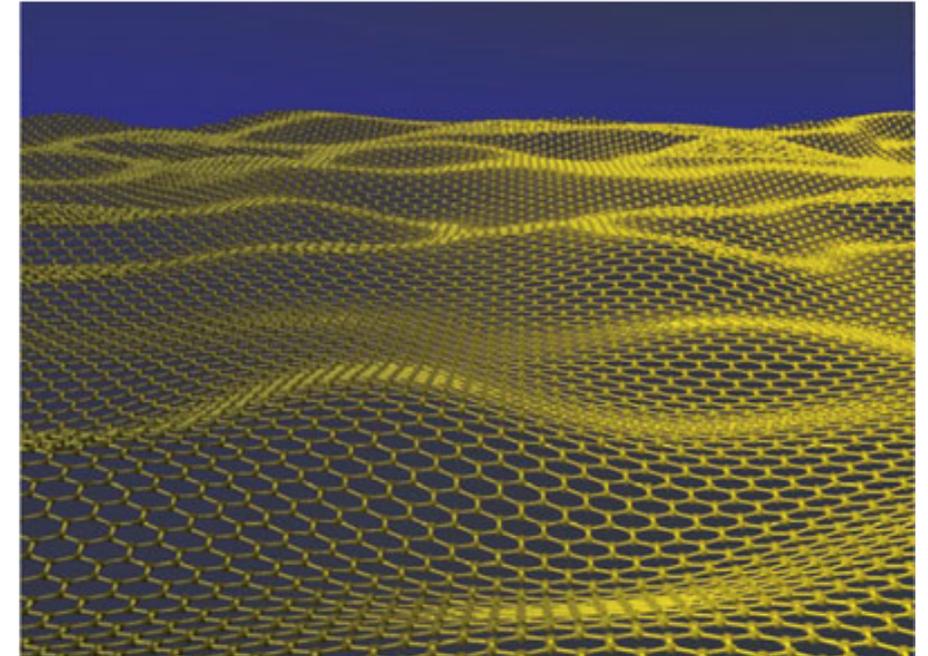
Graphene as Atomic Paper

$$Y \approx 20\text{eV}\text{\AA}^{-2} \quad \kappa_0 \approx 1.2\text{eV} \quad k_B T \approx 1/40\text{ eV}$$

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

$$\kappa_R(l)/(k_B T) = \kappa_0/(k_B T) + \nu K(l)$$

$$\nu K = \text{Foppl-von Karman \#} = Y l^2 / \kappa_0$$



200 μm sheet of graphene $\nu K \approx (L/h)^2 = 10^{12}$ cf. paper $\nu K \approx 10^6$

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

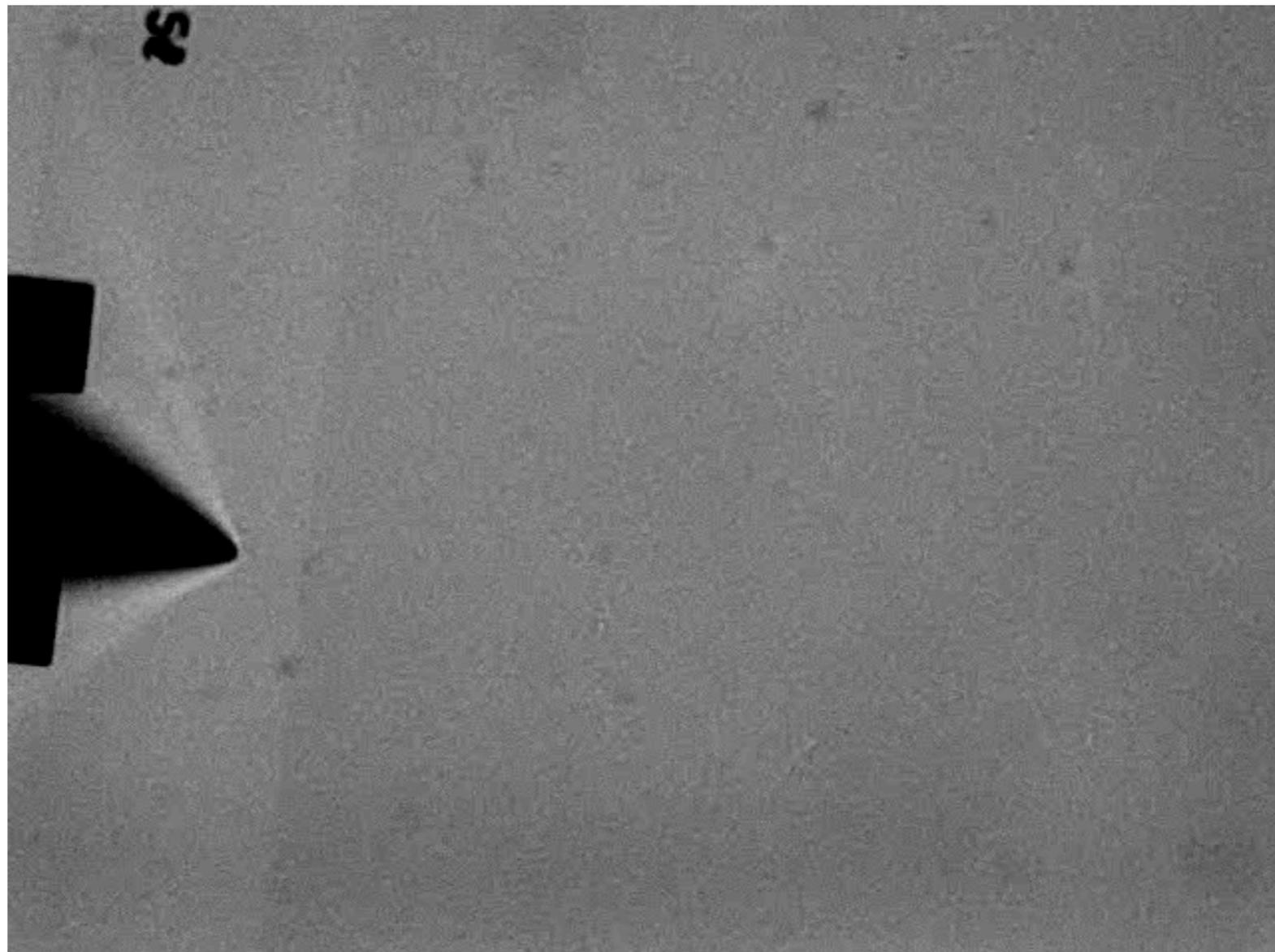
Fopply graphene is self-stiffening to bend via *soft* thermal fluctuations of a *hard* material

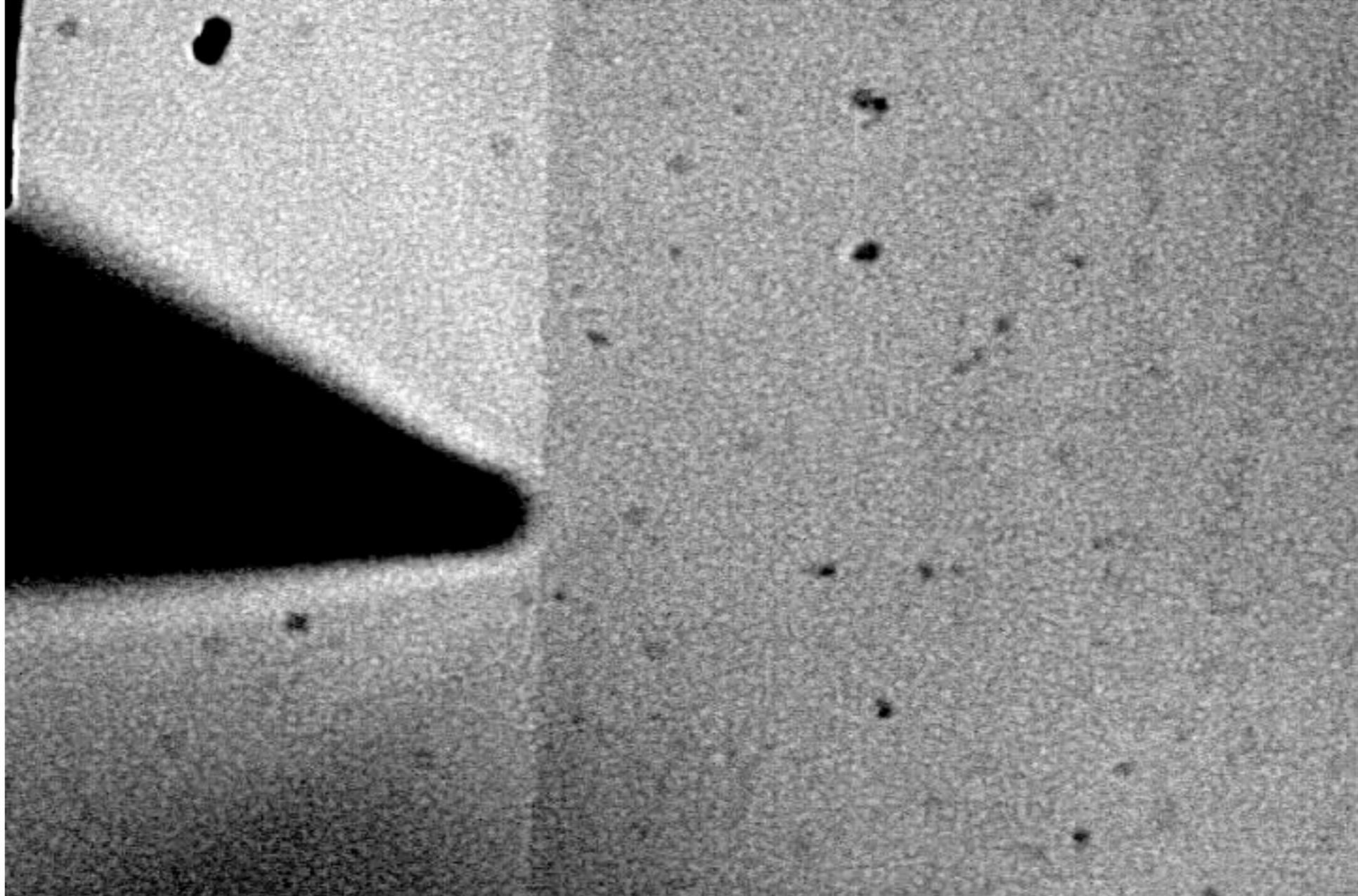
$$\frac{\kappa_R(l)}{\kappa_0} \approx \left(\frac{l}{l_{th}} \right)^\eta$$

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

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

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



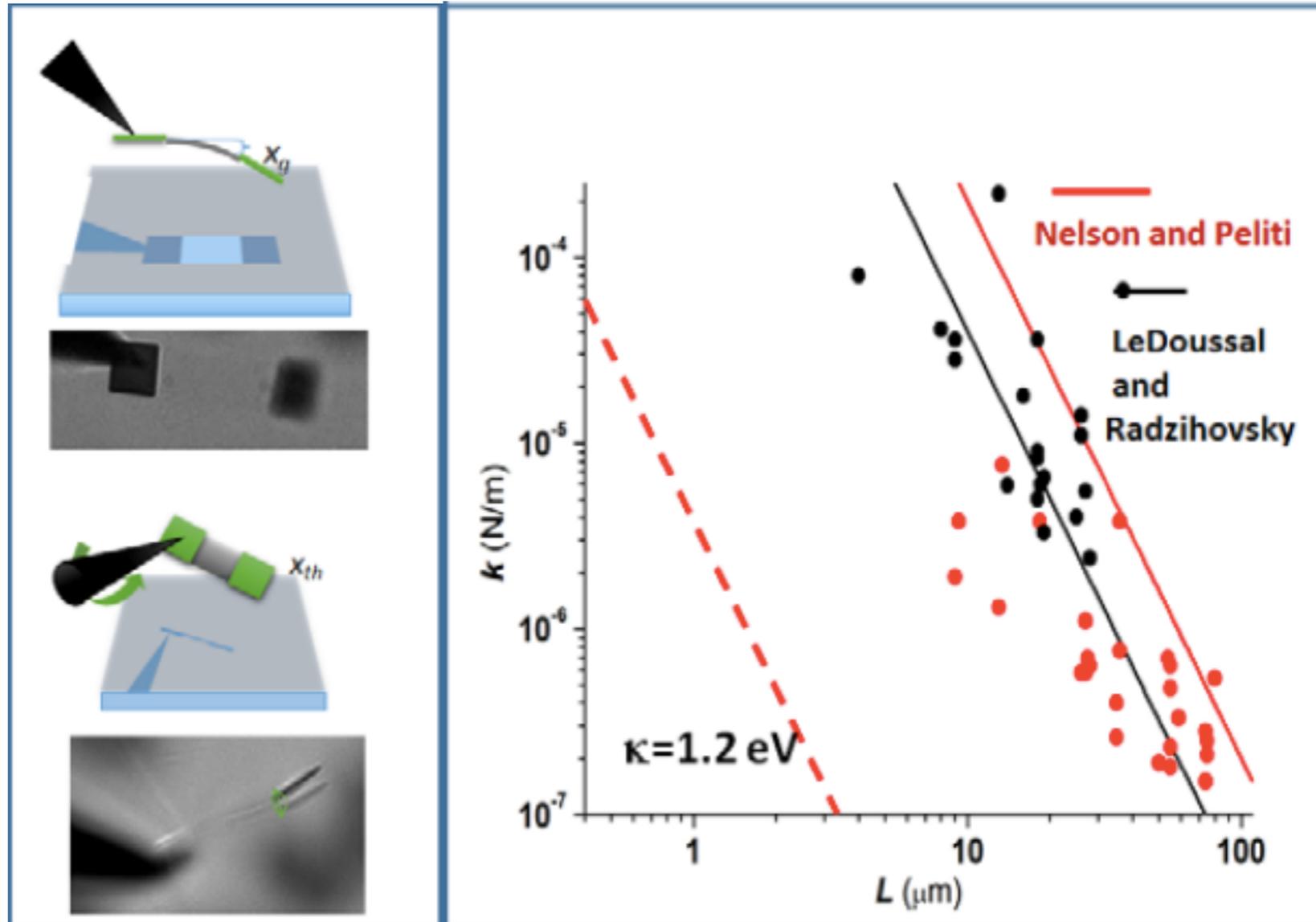


Melina Blees (McEuen group, Cornell)



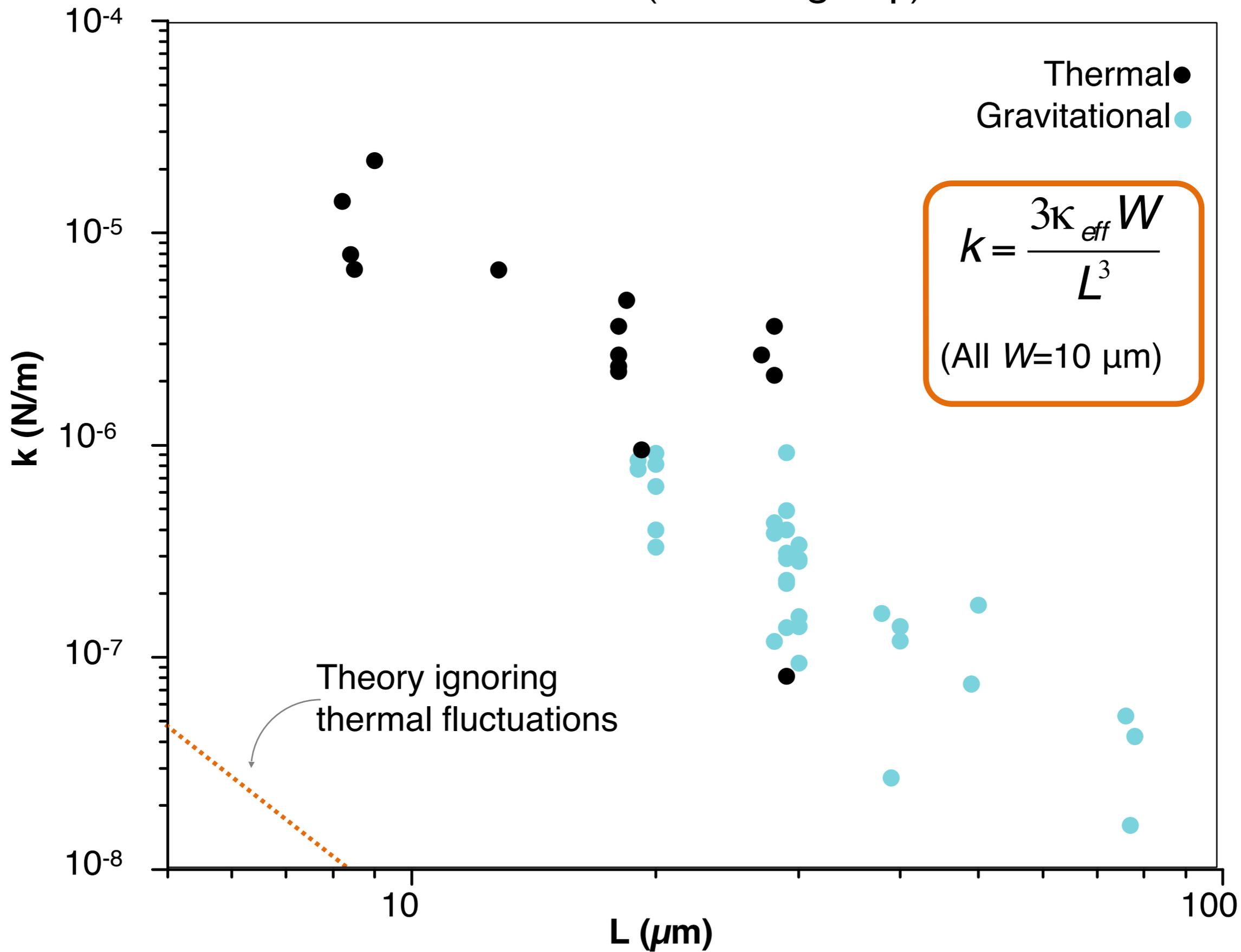
McEuen group

Bending Rigidity Measurements



McEuen group

from Melina Bles (McEuen group)

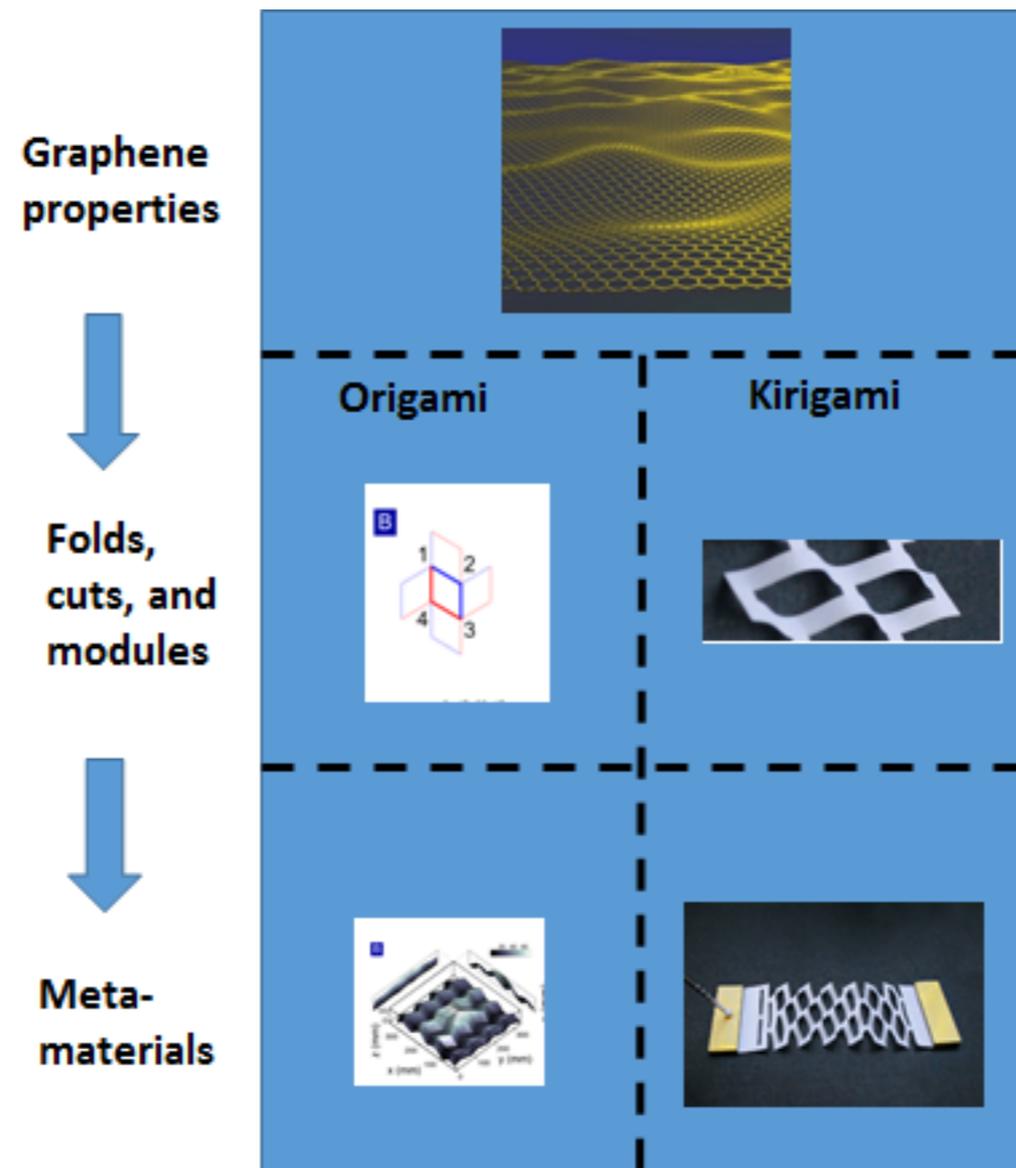


Graphene Kirigami

w/ Itai Cohen, Paul McEuen and David Nelson

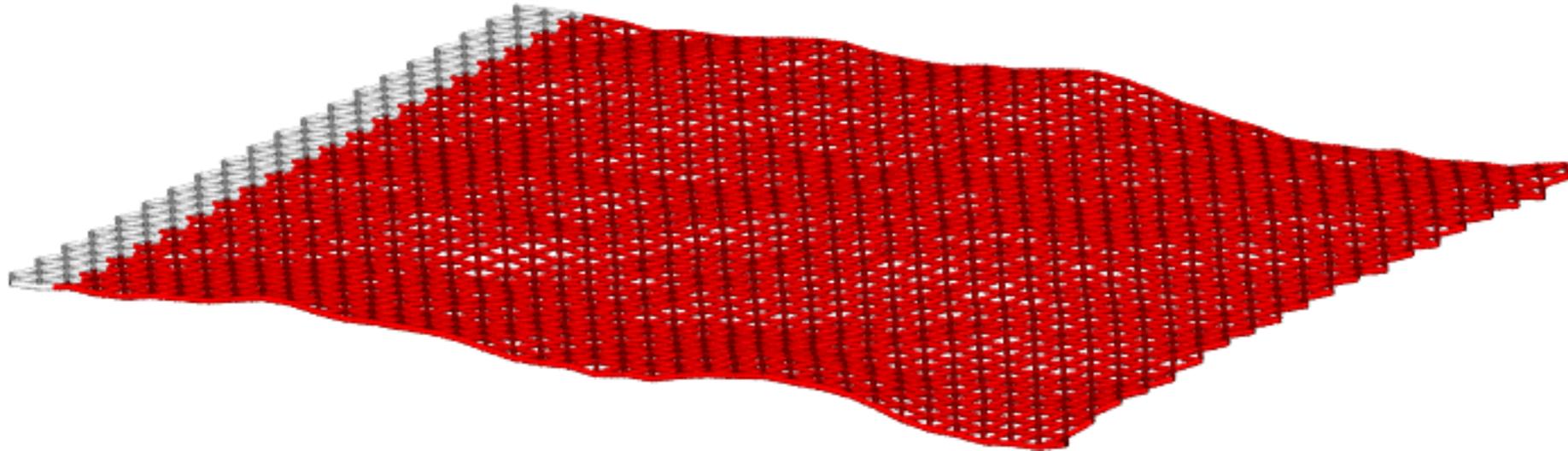
Graphene material properties depend on the geometry through thermal fluctuations

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

MD simulations

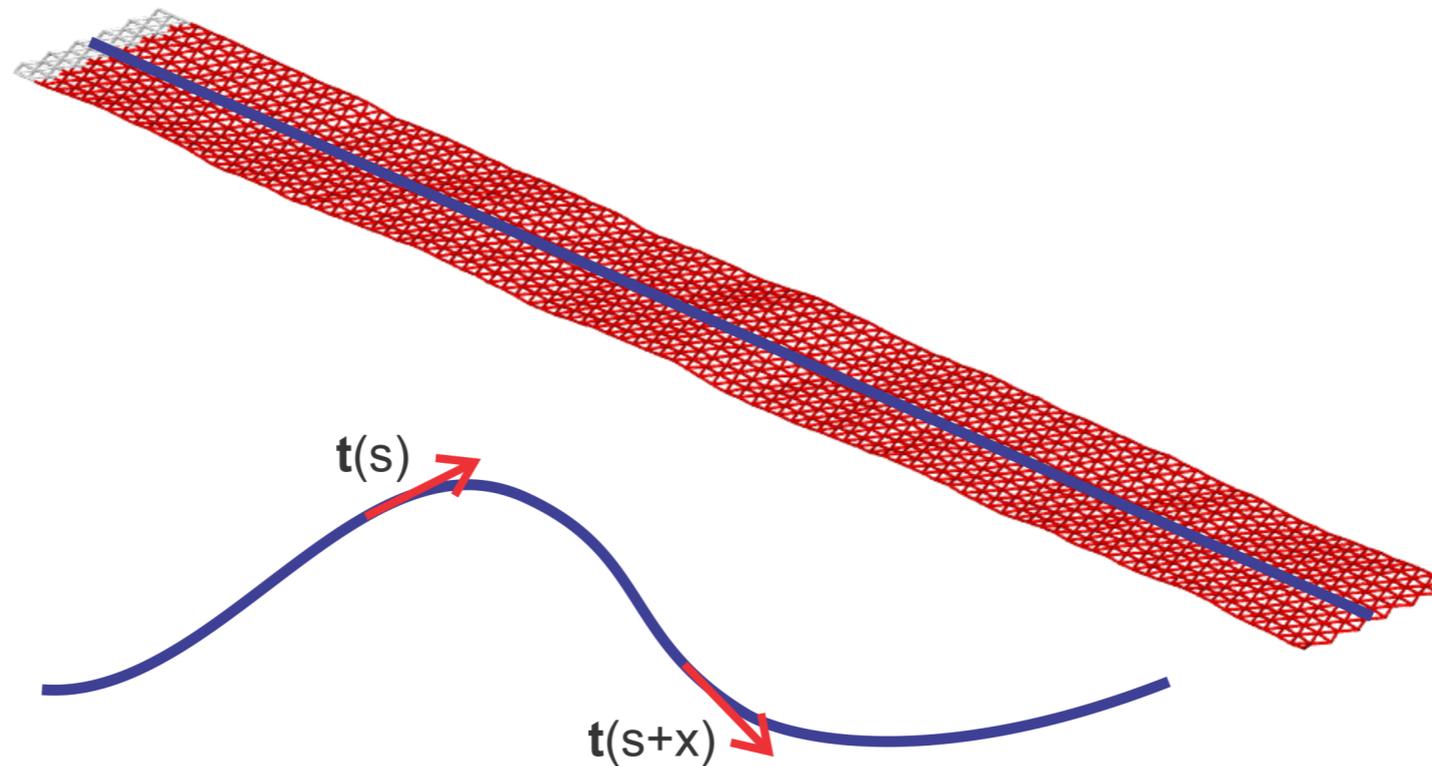


$W=10, L=100$



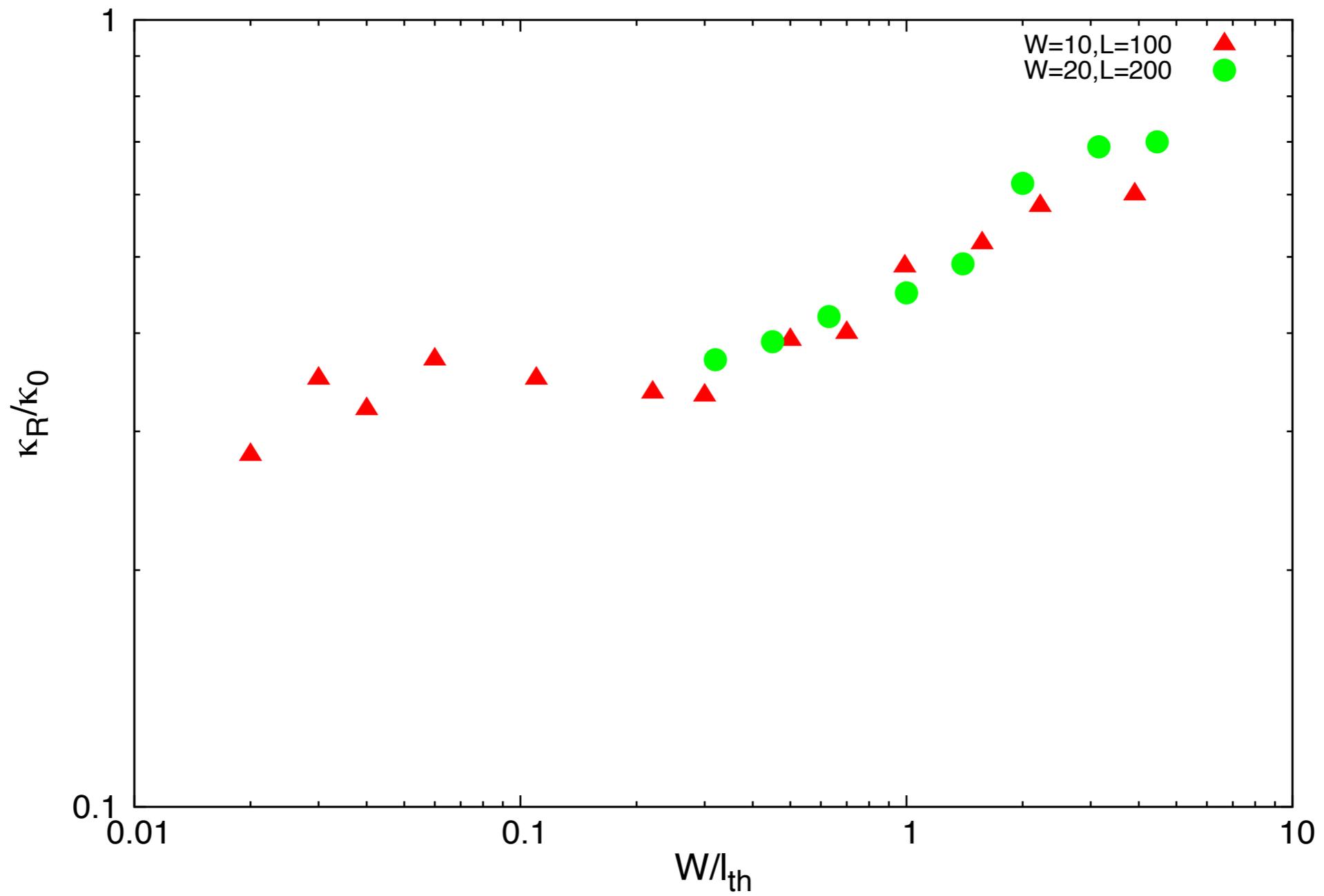
$W=10, L=200$

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



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

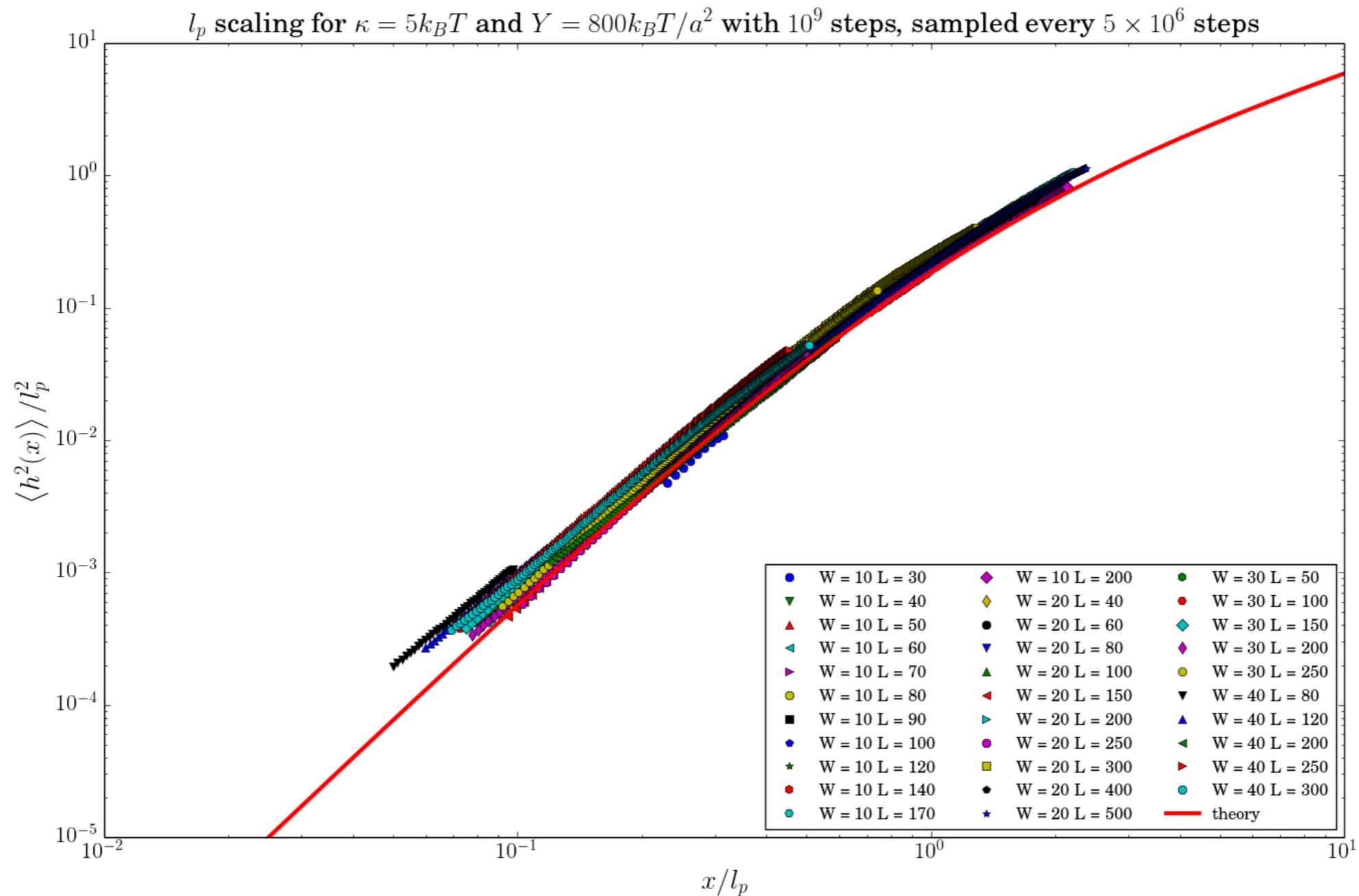
Following Panyukov & Rabin PRE **62** (2000) $l_p \approx 2W\kappa_R/k_B T$



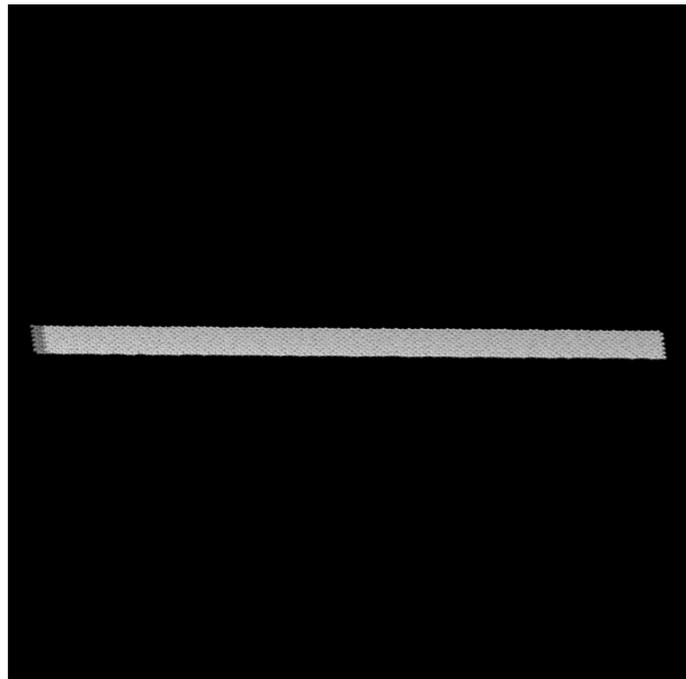
$$\kappa_R/\kappa_0 \sim \left(\frac{W}{l_{th}}\right)^\eta$$

Height Fluctuations

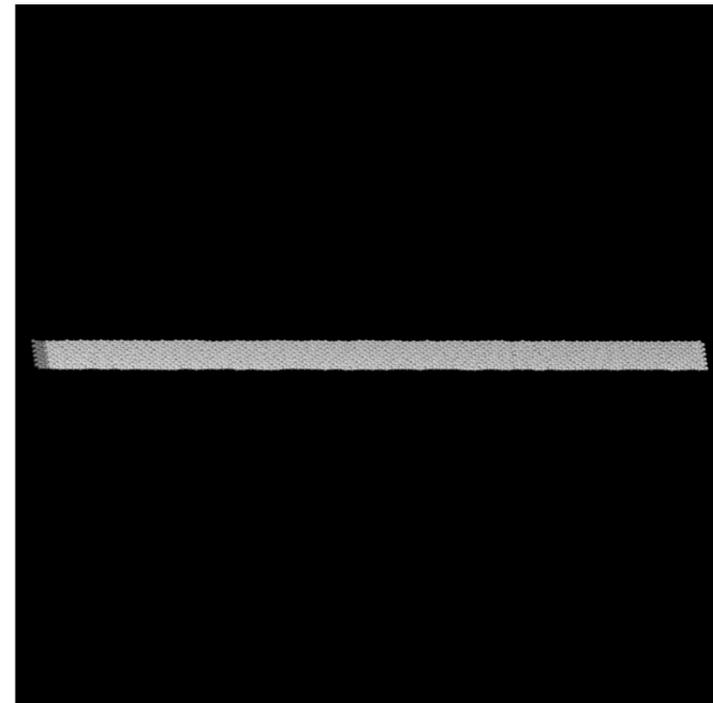
$$\Phi(x) = \frac{1}{W} \int dy \langle h^2(x, y) \rangle / l_p^2 \quad \Phi(x) \sim (x/l_p)^3 \quad (x > W)$$



MD simulations of slits
w/ Emily Russell and R. Sknepnek



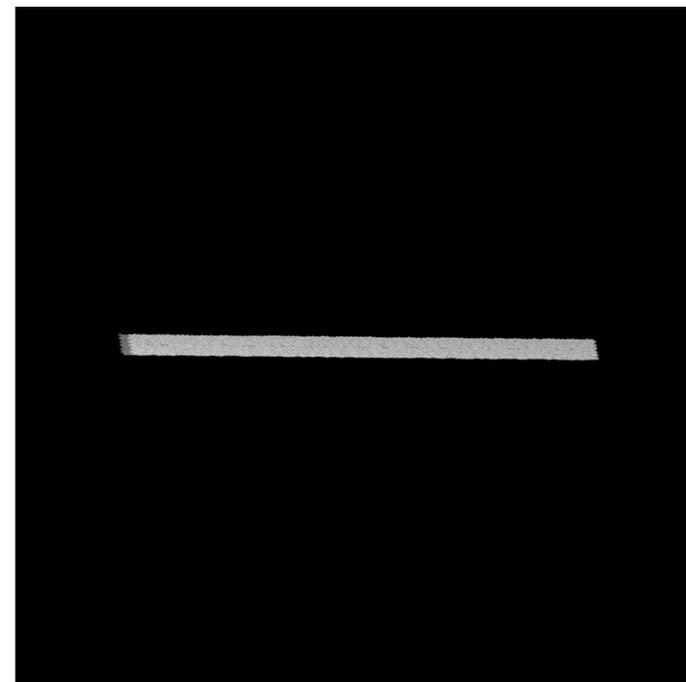
Reference Ribbon



Short slit

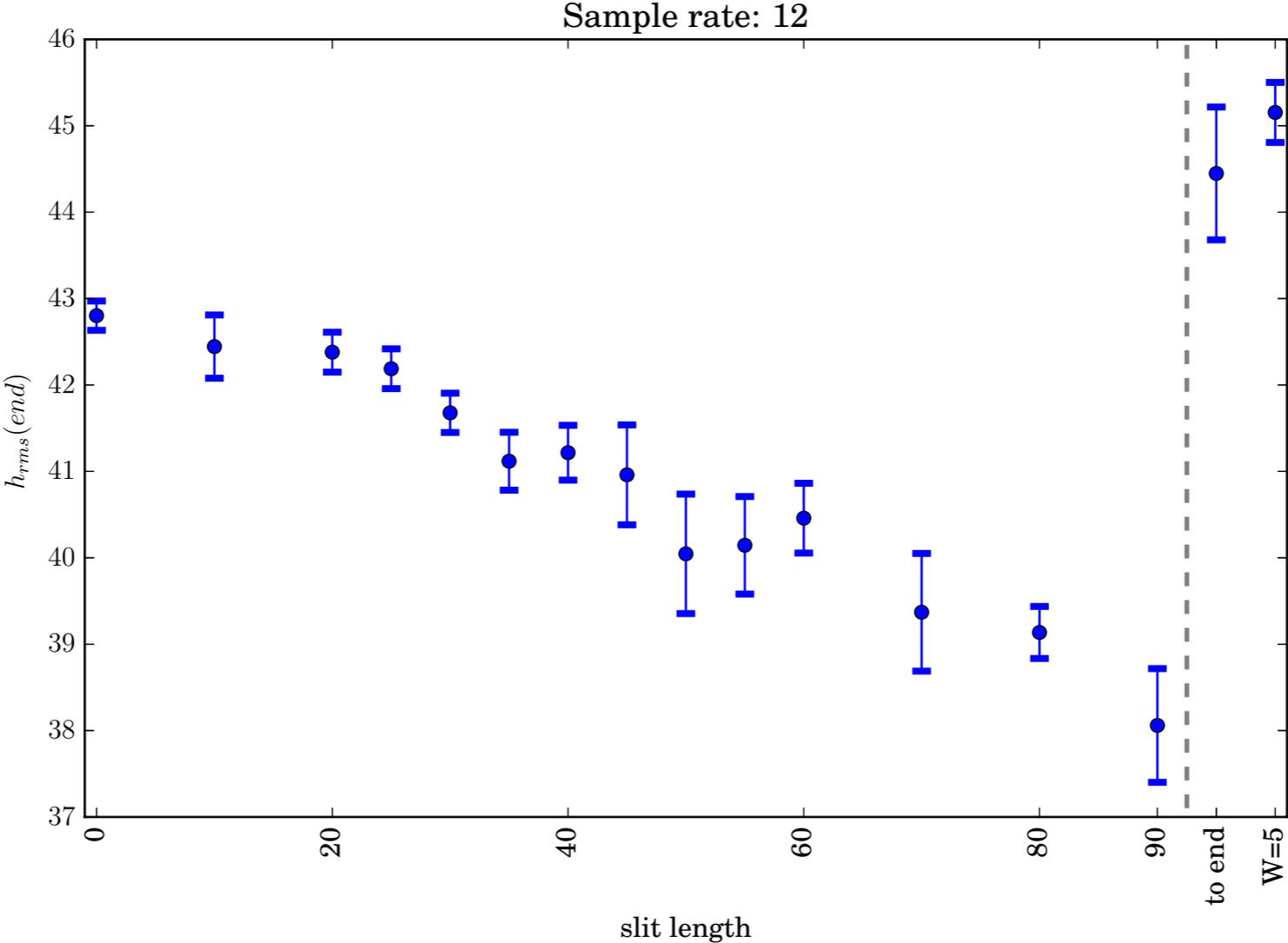


Longer slit

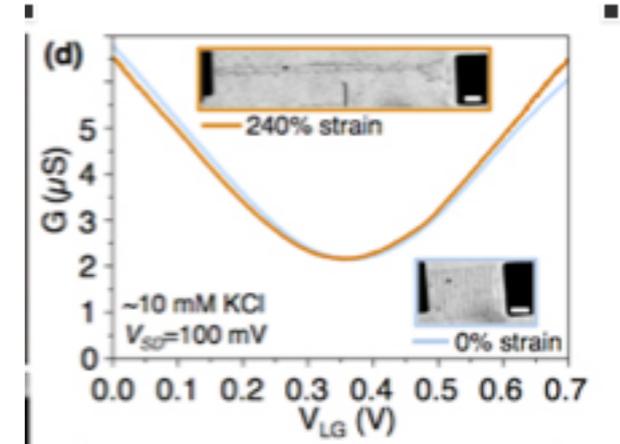
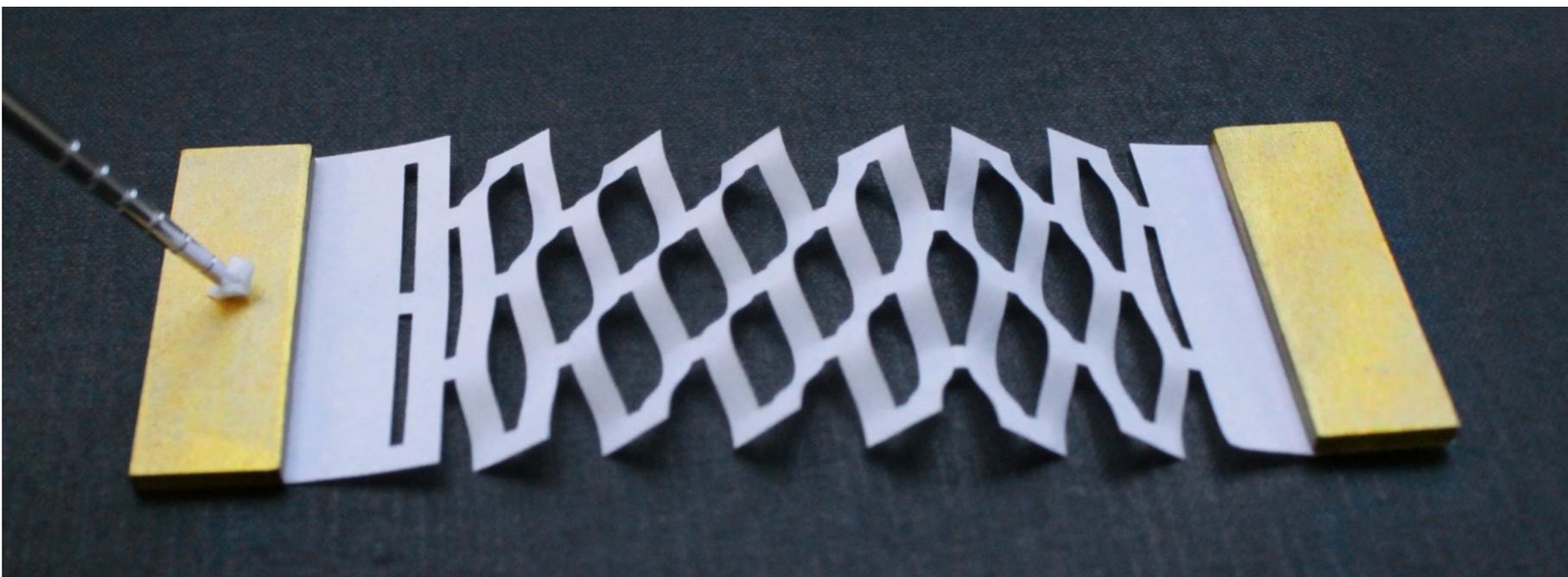
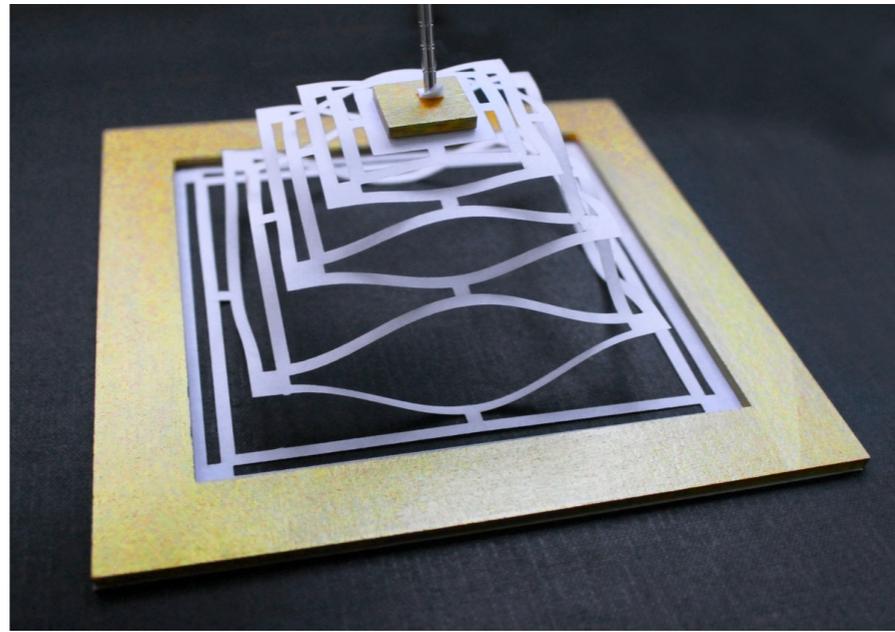
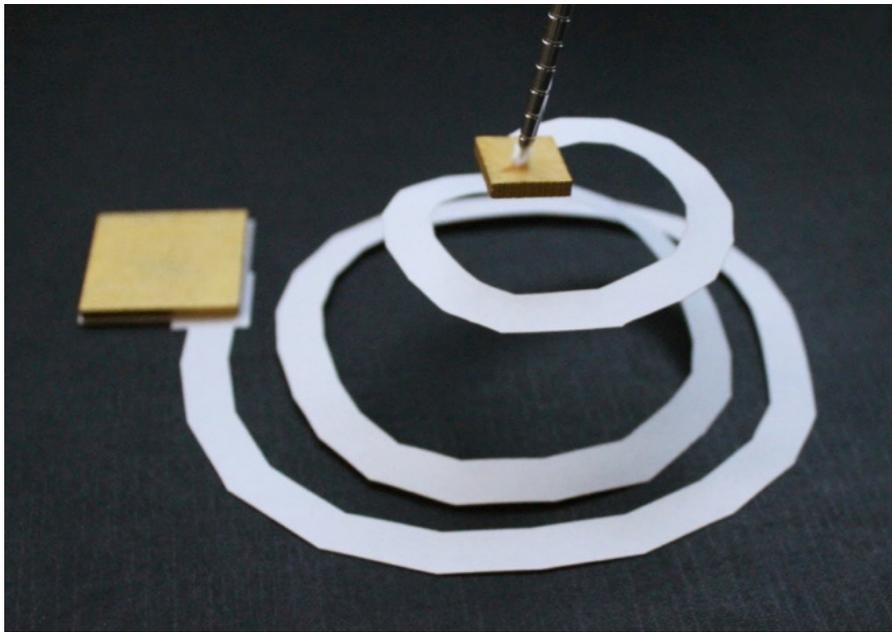


End-to-end slit

RMS Height Fluctuations vs slit length



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



Conclusions

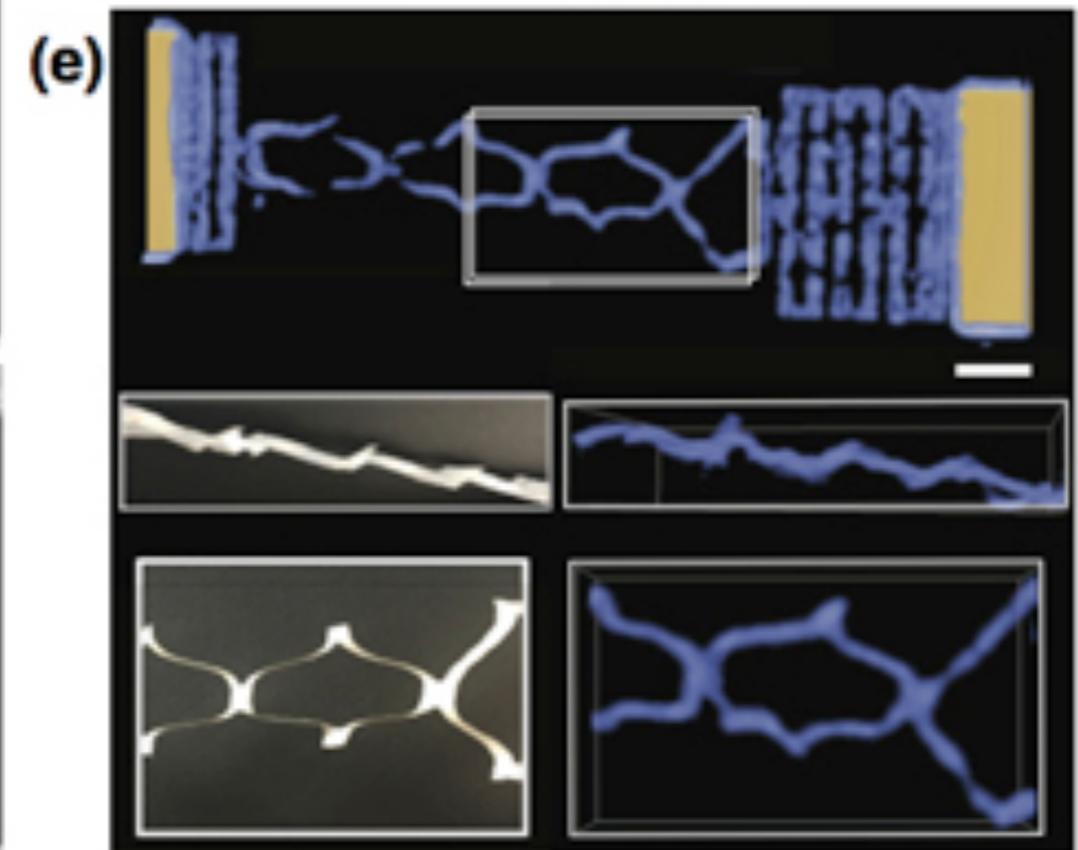
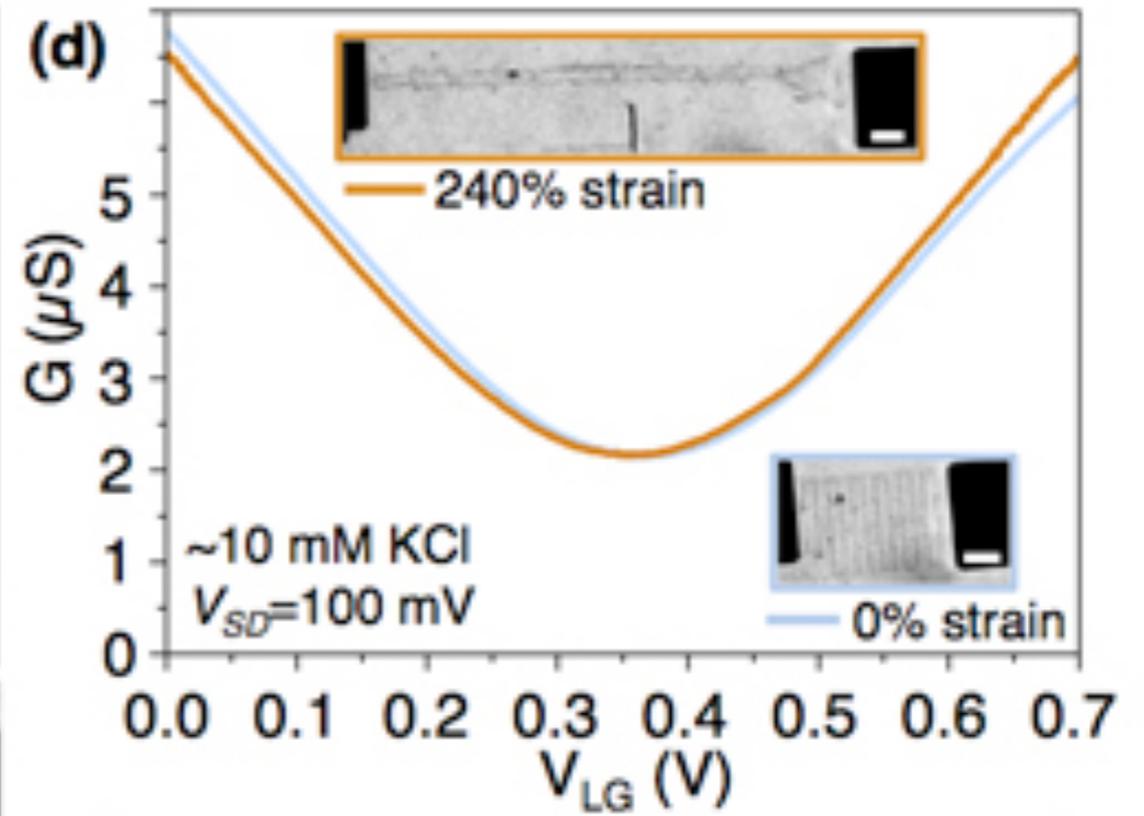
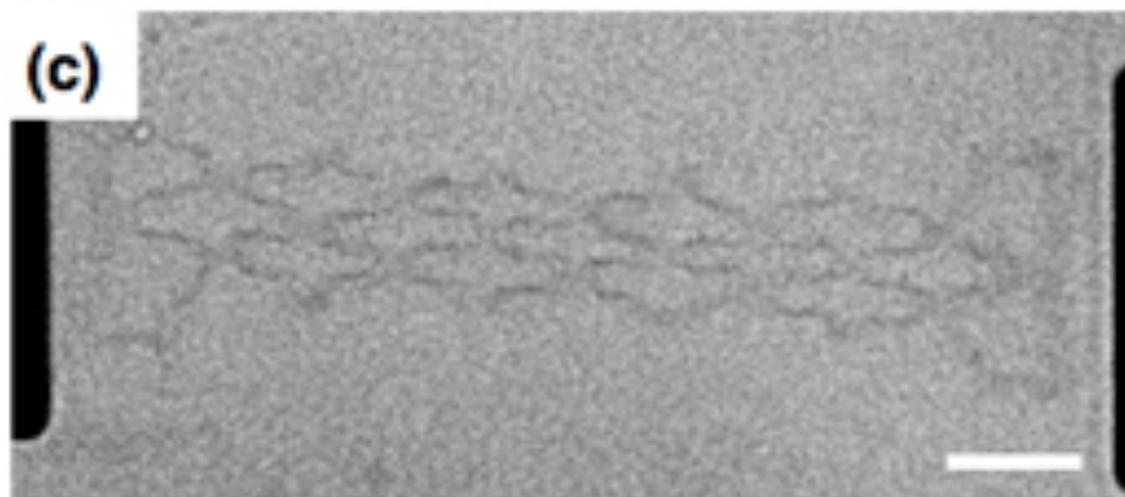
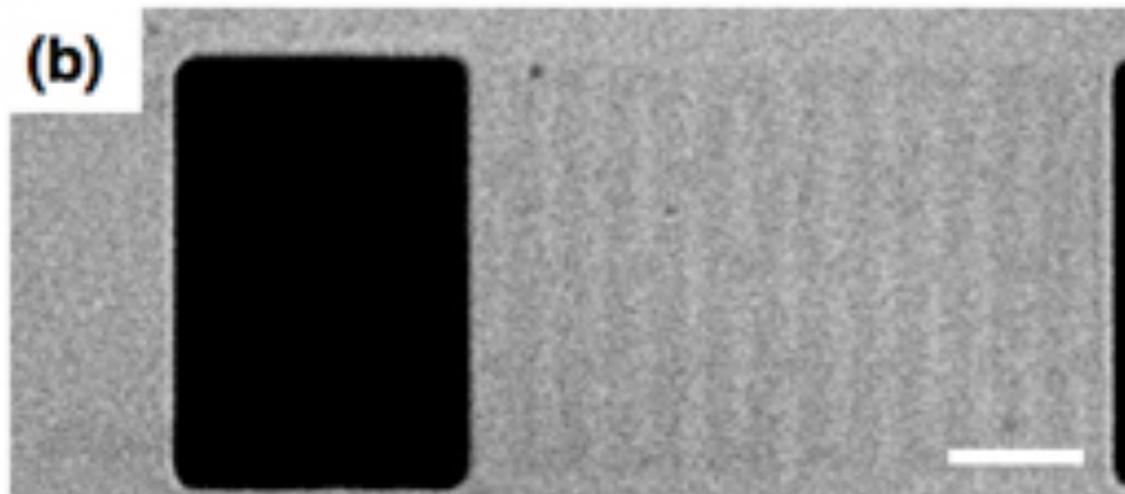
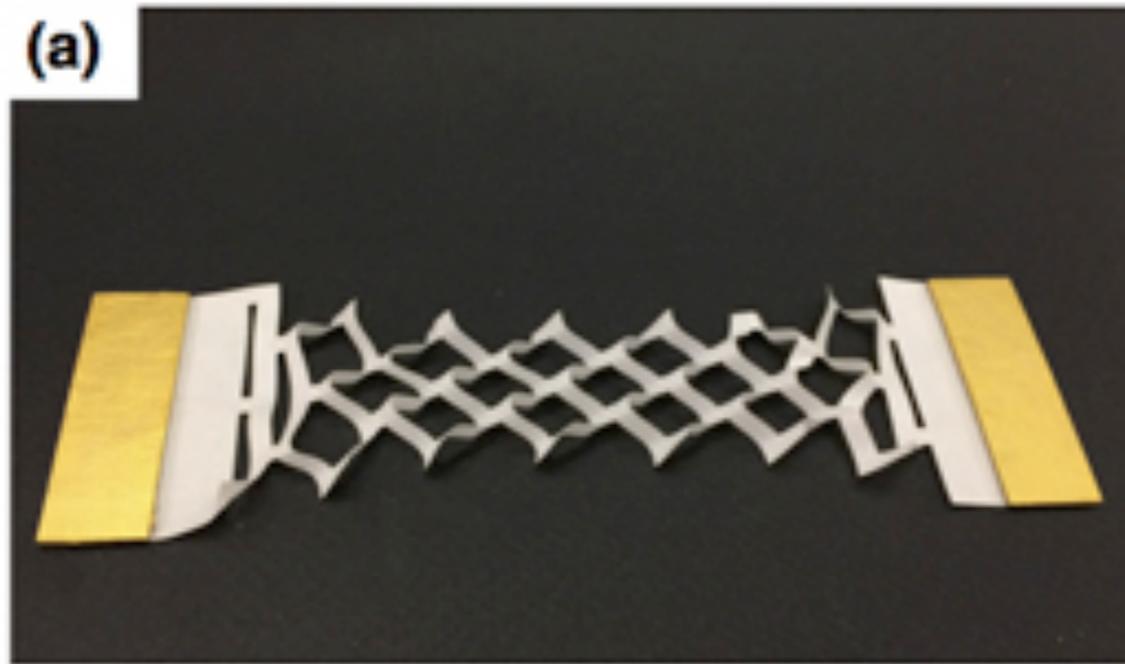
Remarkable interplay of hard and soft matter in graphene statistical mechanics

Wonderful realization of a 2d elastic membrane

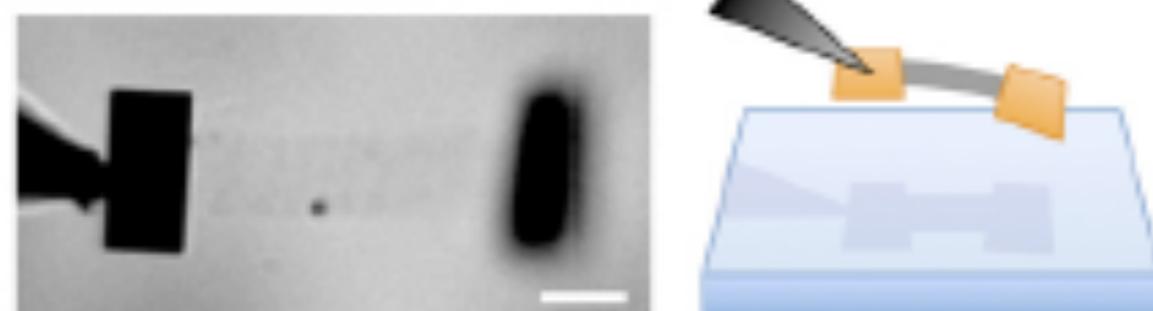
Material properties are strongly geometry dependent

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





(a) Gravitational method:



(b) Thermal method:

