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Active biological adhesion

Luca Bellino, Giuseppe Florio, Stefano Giordano, Lev Truskinovsky, Giuseppe Puglisi

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Politecnico
di Bari

Dipartimento di Scienze
dell'Ingegneria
Civile e dell'Architettura

Active biological adhesion

G. Puglisi

COST Workshop on Advances in numerical modelling of adhesion and friction
Trento 18-19 Nov. 2019

Cohoperations



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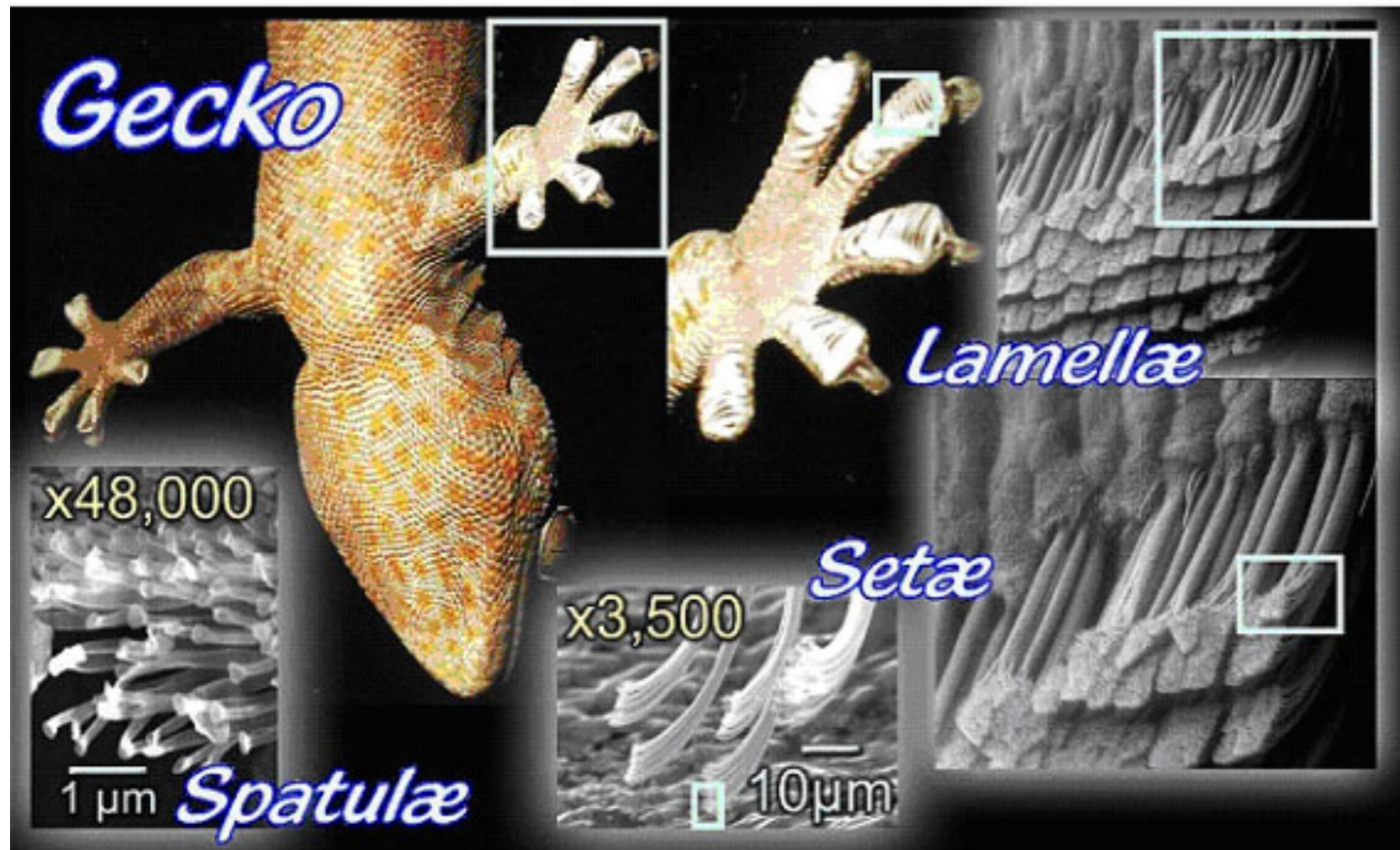


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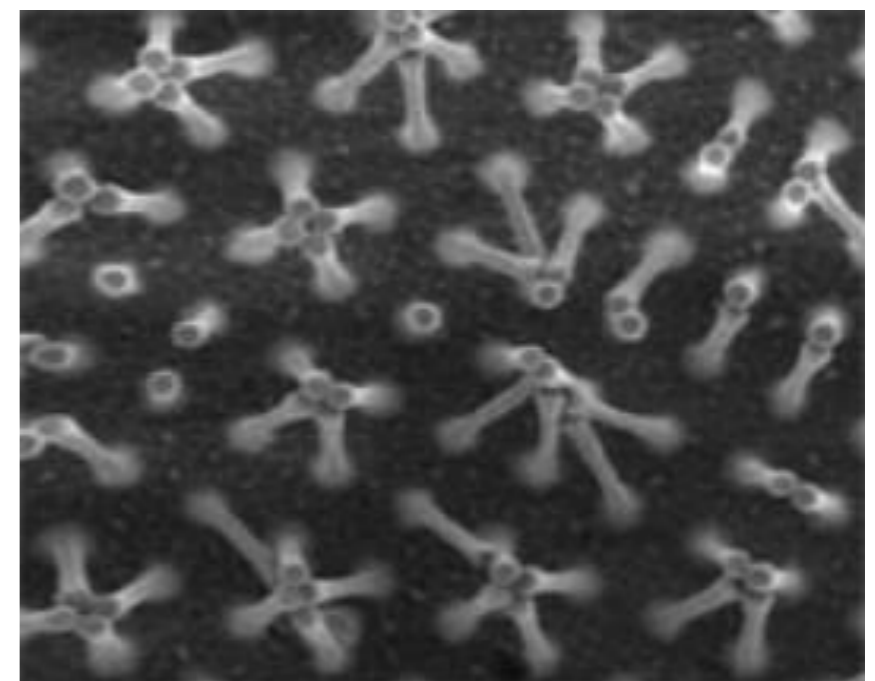
Fibrillar Adhesion: Gecko



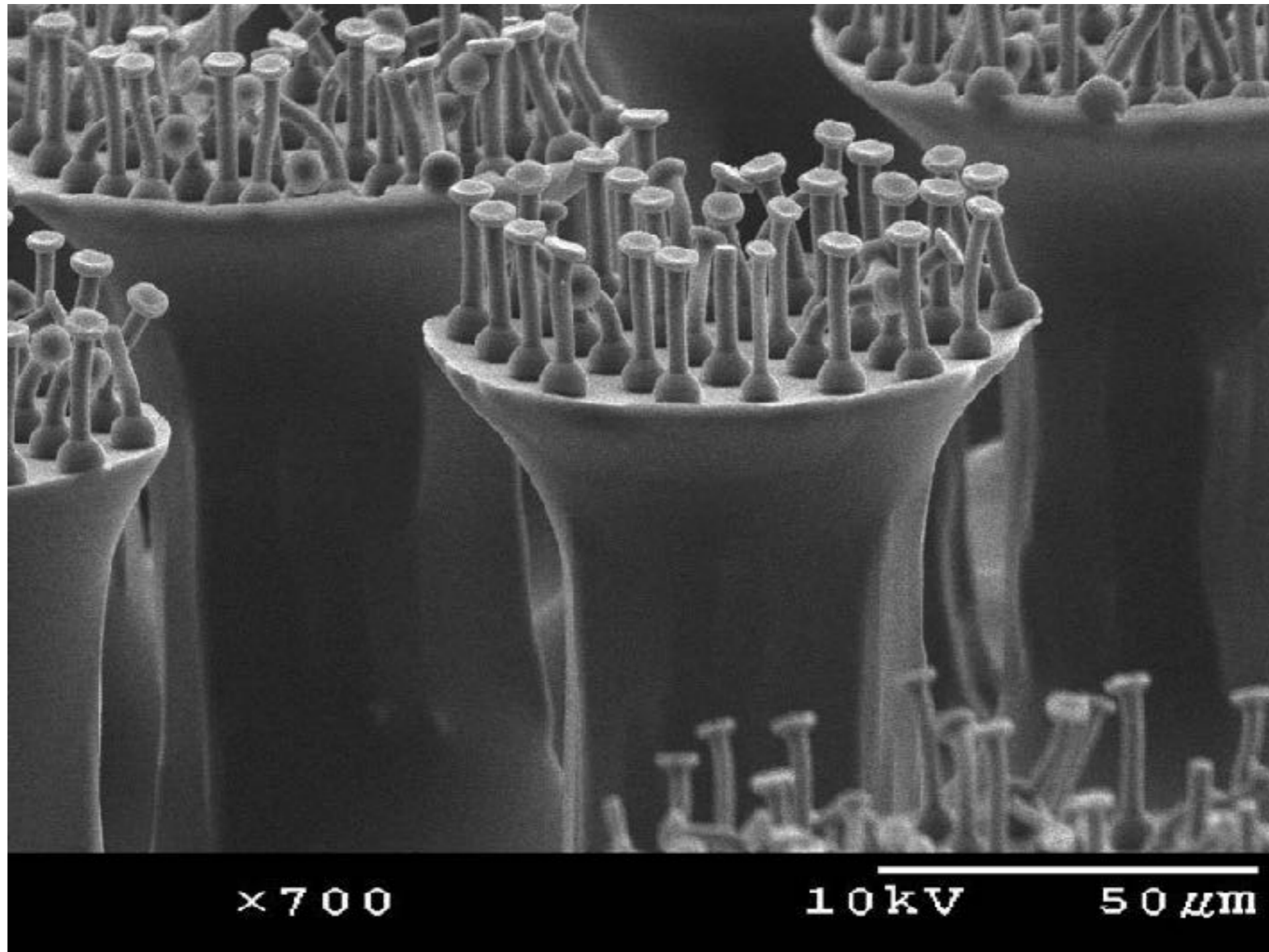
K. Autumn, N. Gravish,
*Gecko adhesion: evolutionary
nanotechnology*,
Philosophical Transaction of the
Royal Society, 2008.

Aristotele, Historia Animalum

*“It can run up and down a tree in any way,
even with the head downwards,
like the gecko-lizard” (Aristotele, 350B.C.)*

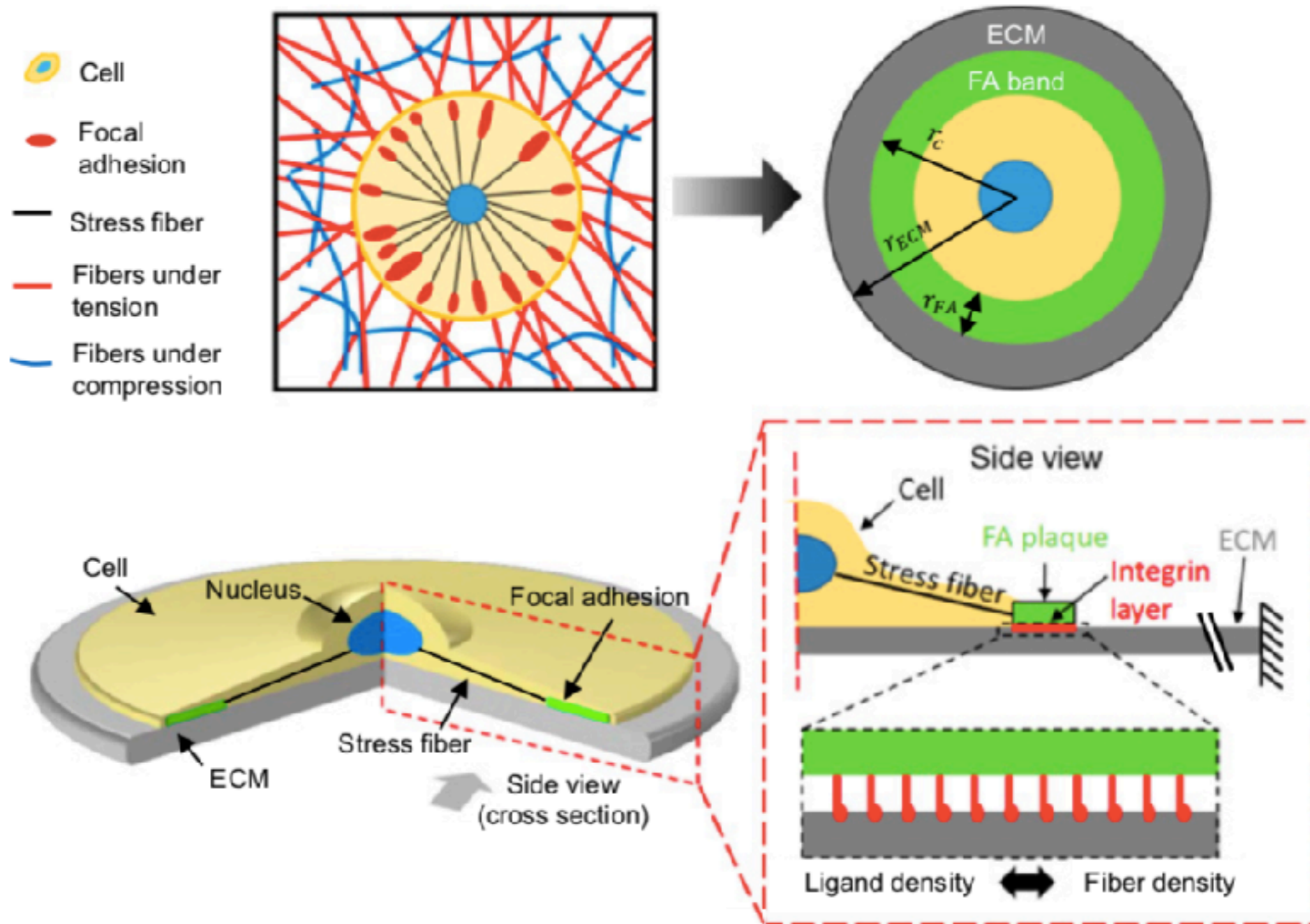


Bio-inspired Materials

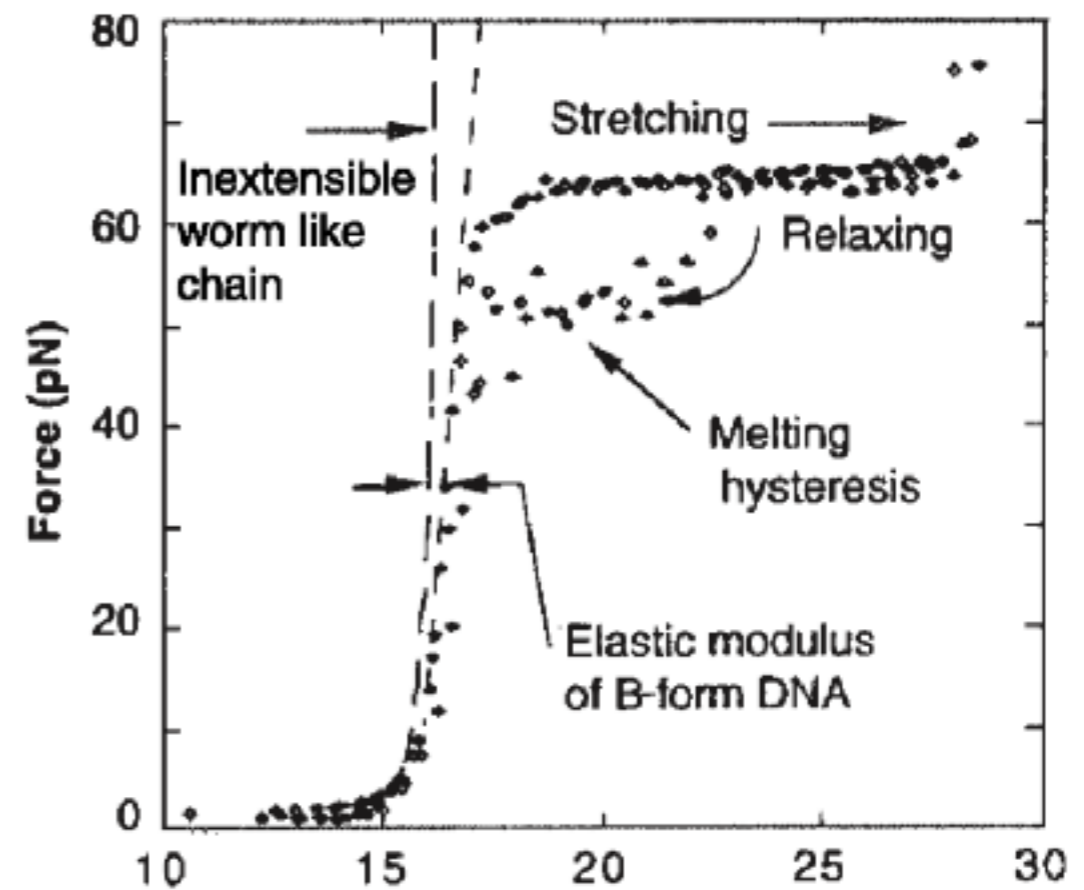
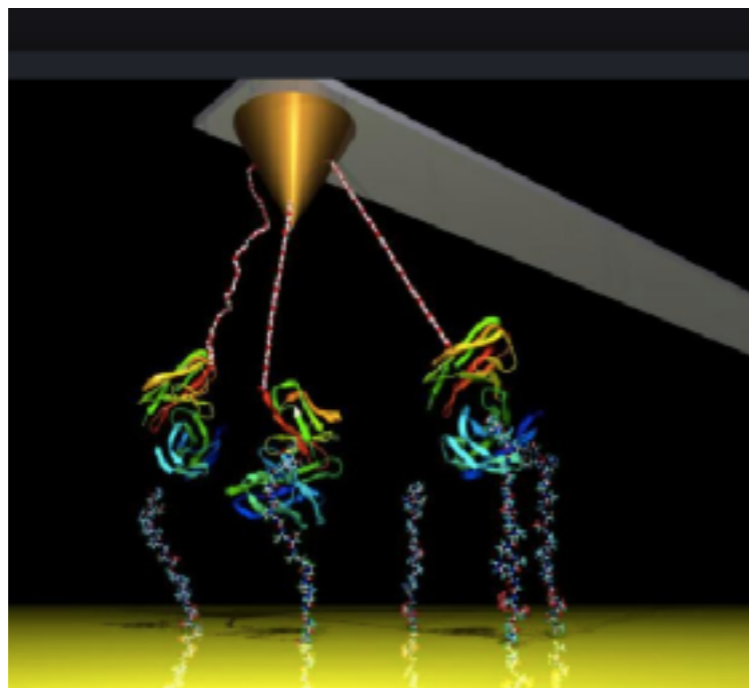
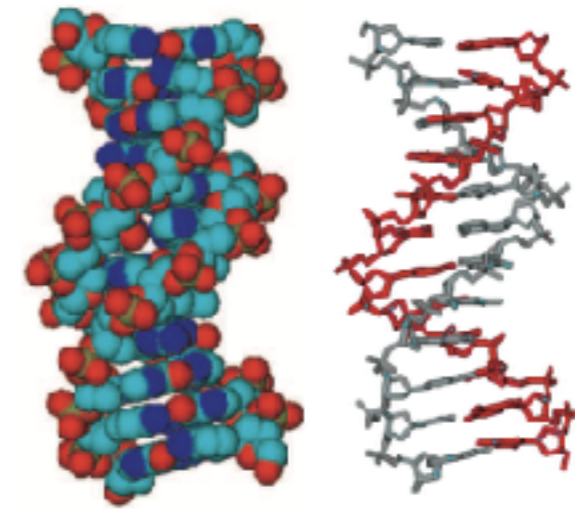
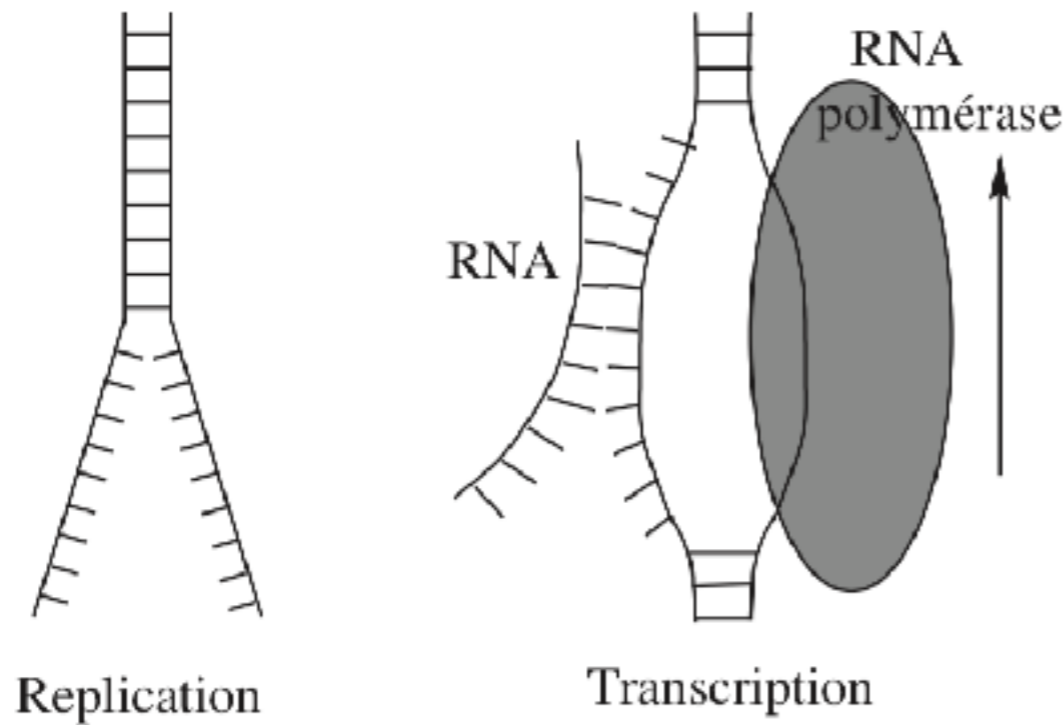


Dry fibrillar adhesives allow gecko-like robots to climb smooth, vertical surfaces. The NanoRobotics Lab created a synthetic version of the gecko's toes, consisting of microscopic fibers with special tips that allow them to stick to surfaces (courtesy of Wikimedia Commons).

Cell adhesion

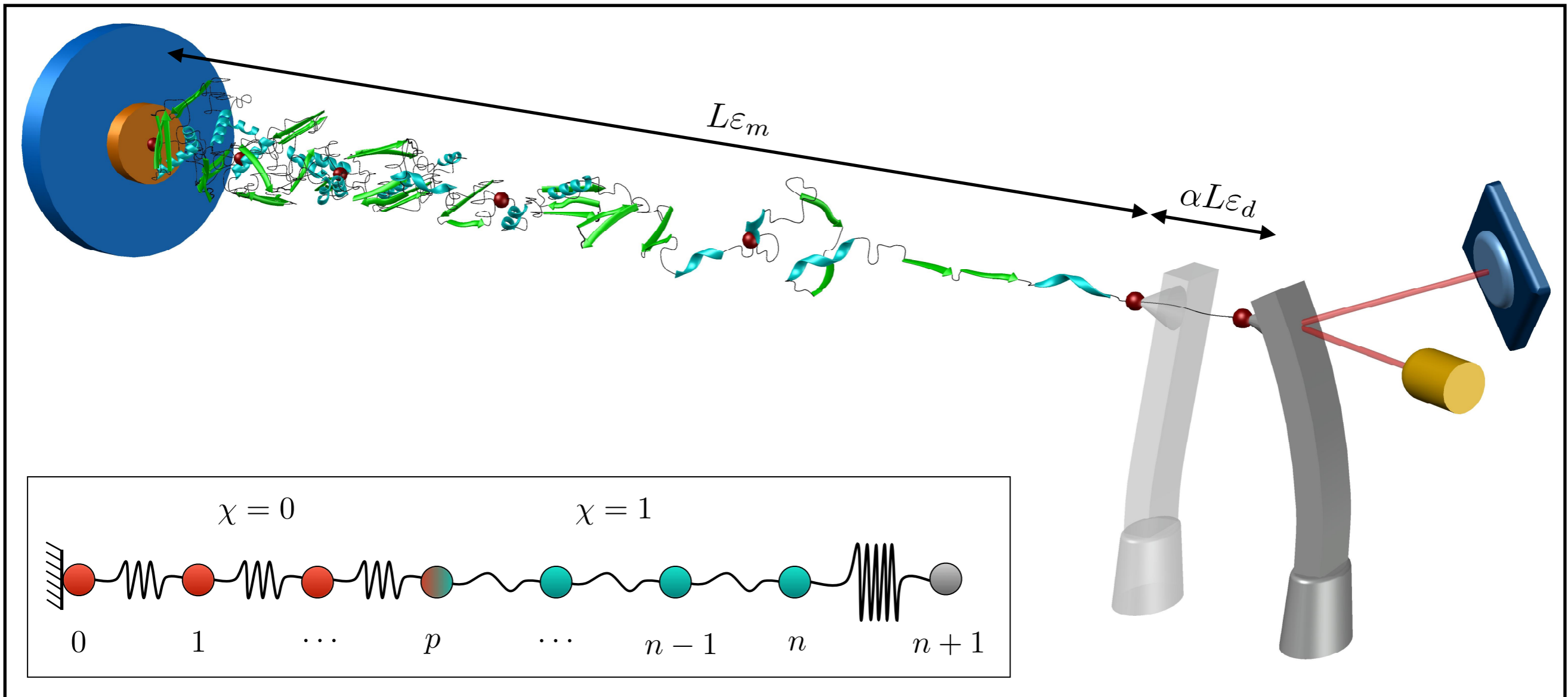


DNA, Proteins unfolding



M. Peyrard, A. R. Bishop, Statistical Mechanics of a Nonlinear Model for DNA Denaturation, PHYSICAL REVIEW LETTER 62, 2755 (1989)

Molecule Unfolding

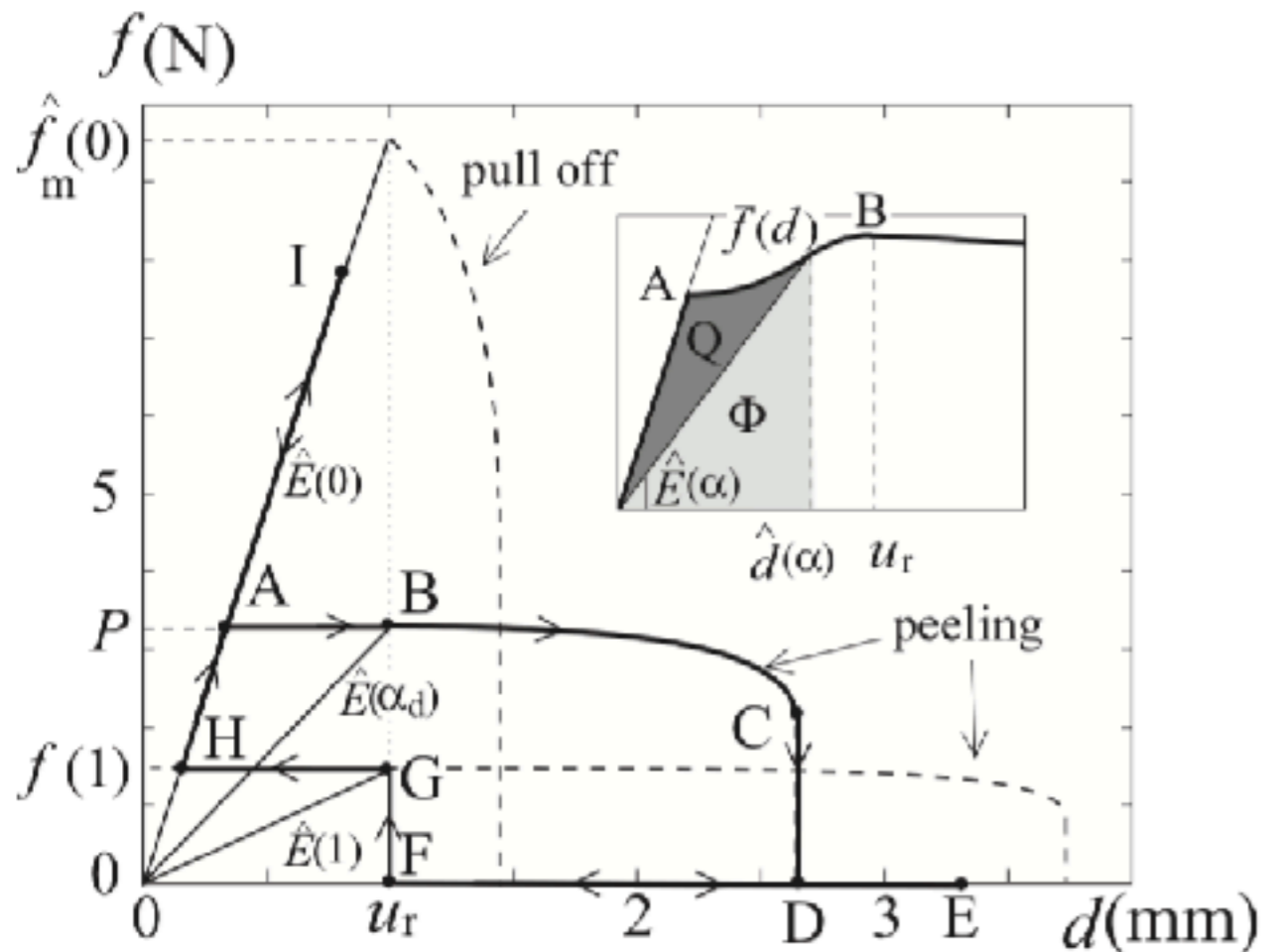


- Matthias Rief, *et al.* Reversible Unfolding of Individual Titin Immunoglobulin Domains by AFM Science **276**, 1109 (1997)
- G. Florio, G.P, *Unveiling the influence of device stiffness in single macromolecule unfolding.* Scientific Reports **9** (2019), p. 4997
- L. Bellino, G. Florio, G.P, *The influence of device handles in single molecule experiments,* Soft Matter **15**, 8680-8690, 2019
- D. De Tommasi, N. Millardi, GP, G. Saccomandi G. An energetic model for macromolecules unfolding in stretching experiments, J R Soc Interface **10**, 20130651, 2013

Important open questions: elasticity of the adhering layer

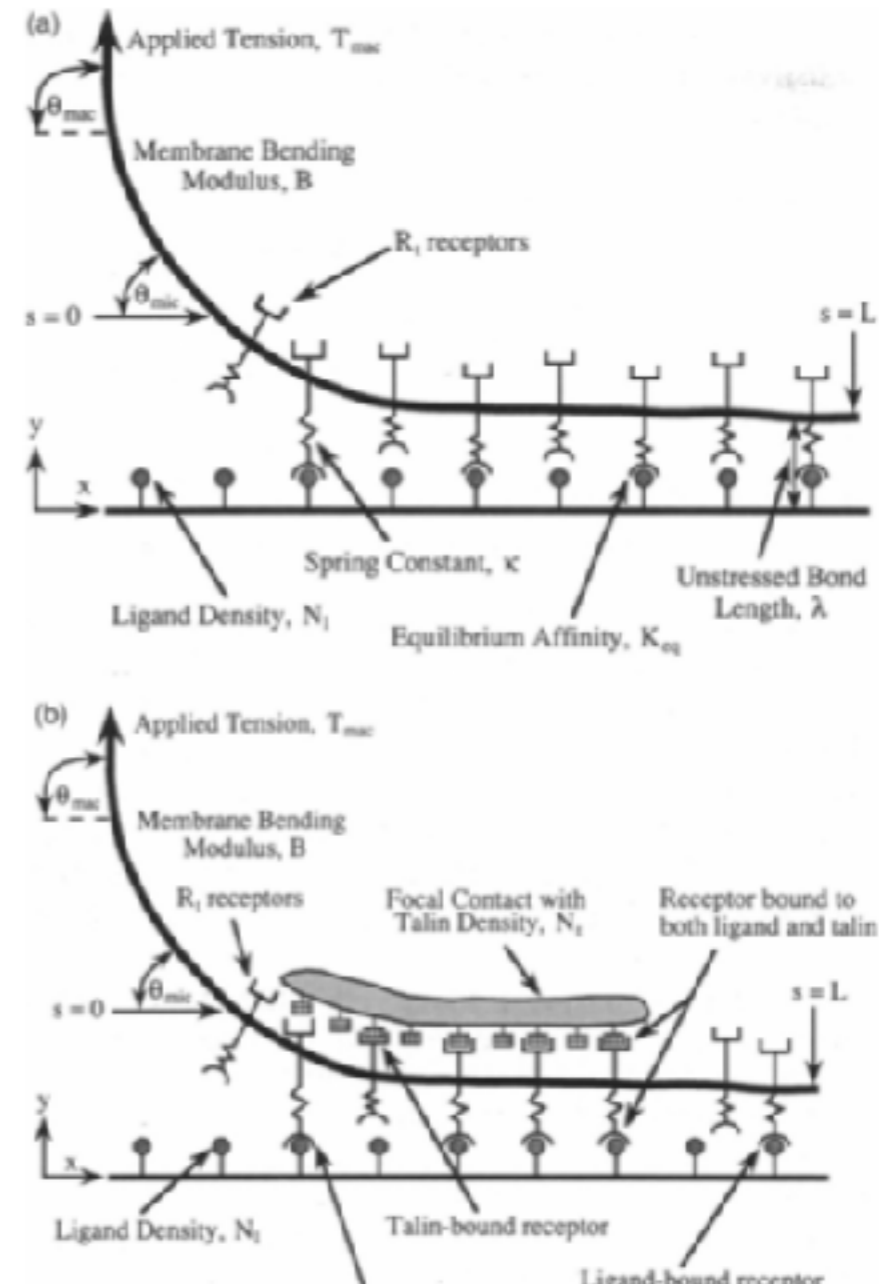


Gecko adhesion/decohesion asymmetry



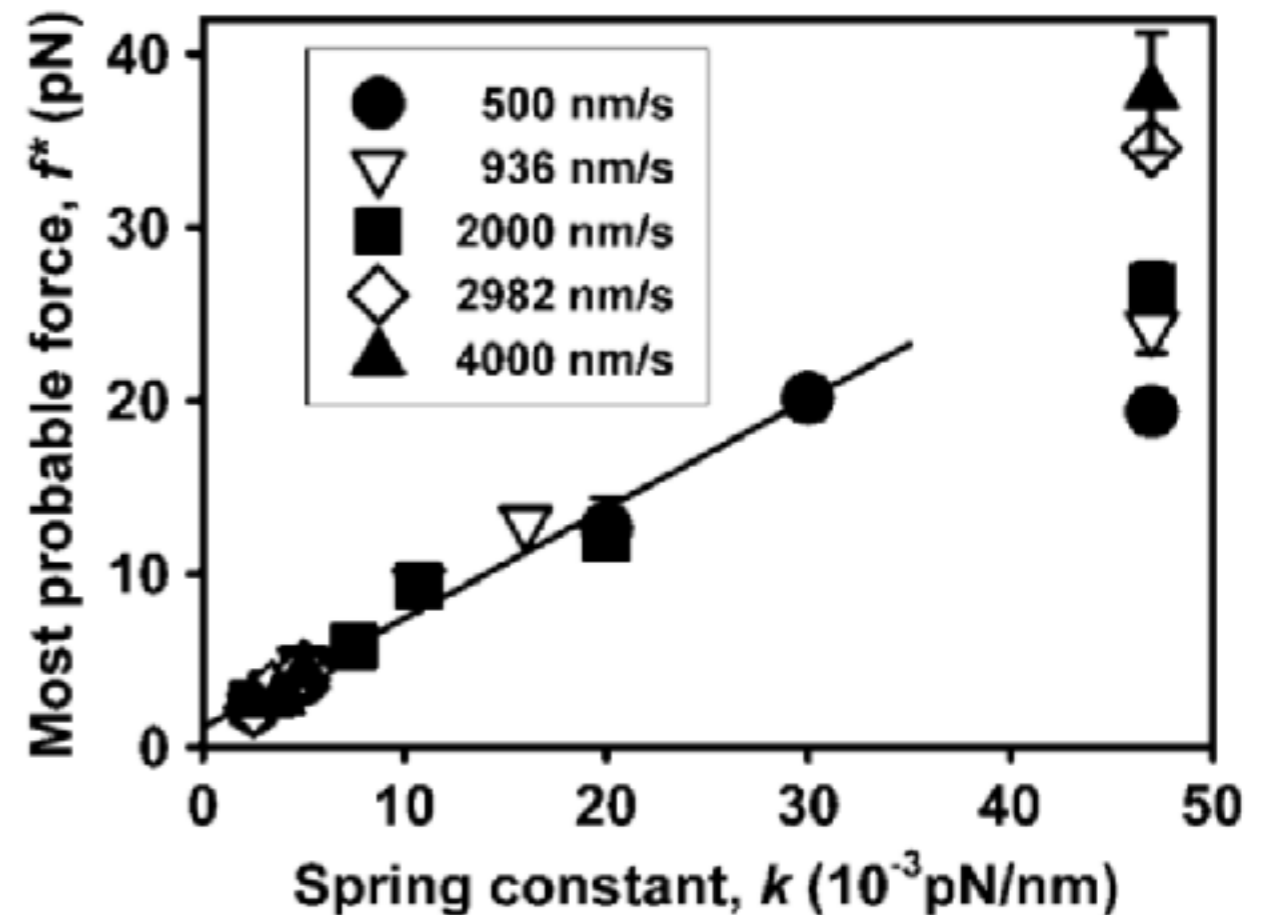
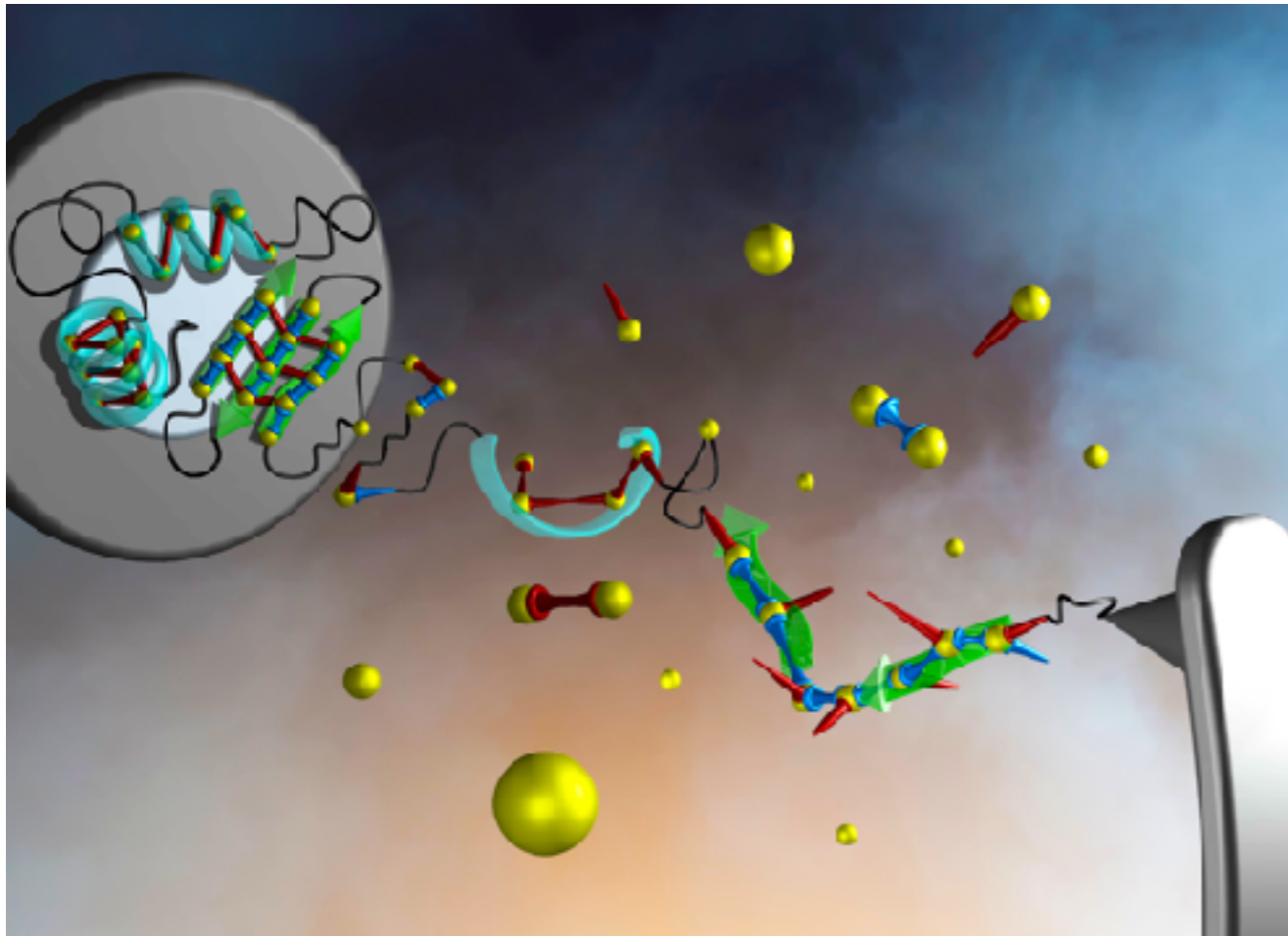
GP and L. Truskinovsky. Cohesion-decohesion asymmetry in gecko. *PHYSICAL REVIEW E* 87, 032714 (2013)

Cellular motion and growth



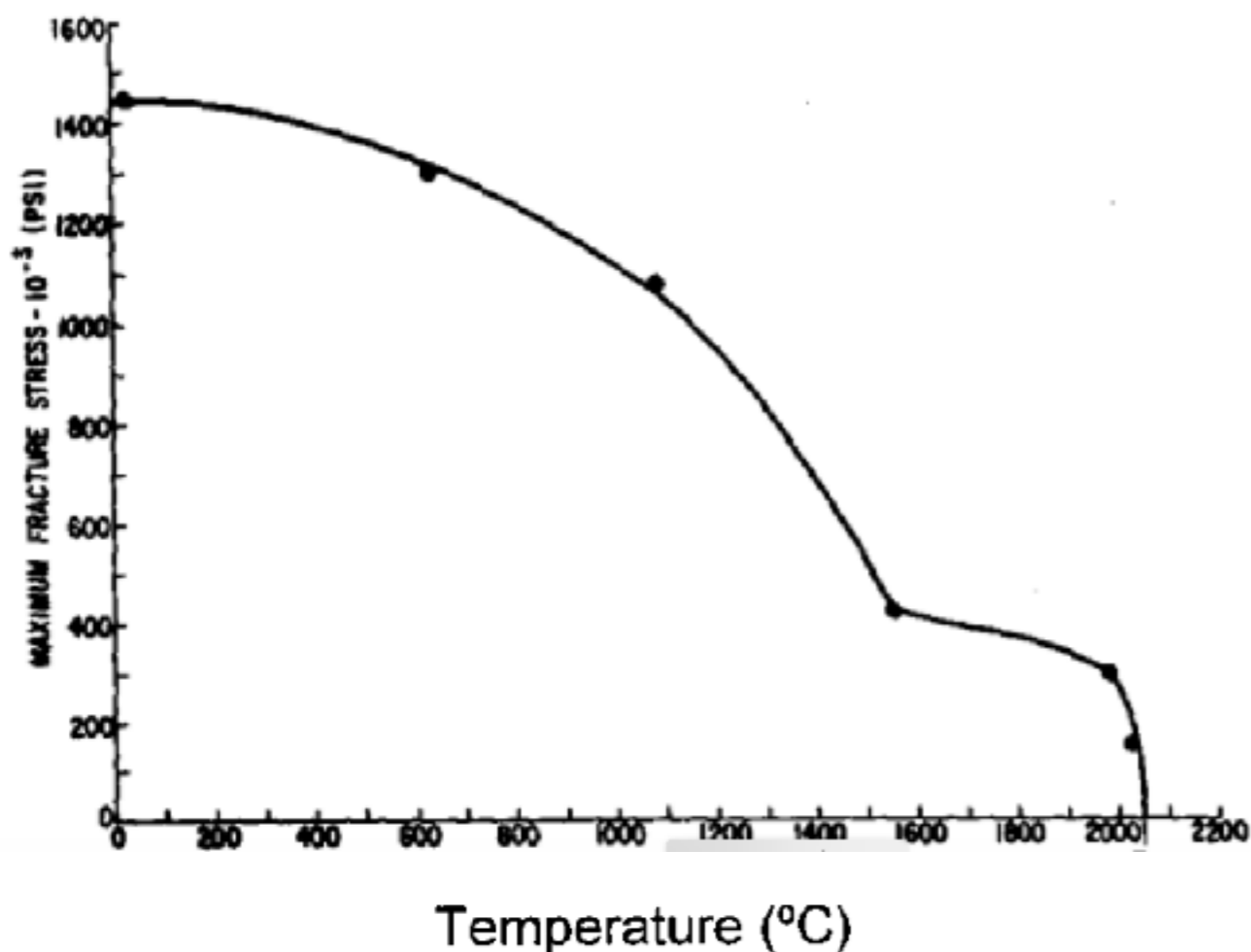
Ward MD1, Hammer DA. A theoretical analysis for the effect of focal contact formation on cell-substrate attachment strength. *Biophys J.* 1993, 64(3), 936-59.

Important open questions: stiffness of the loading device

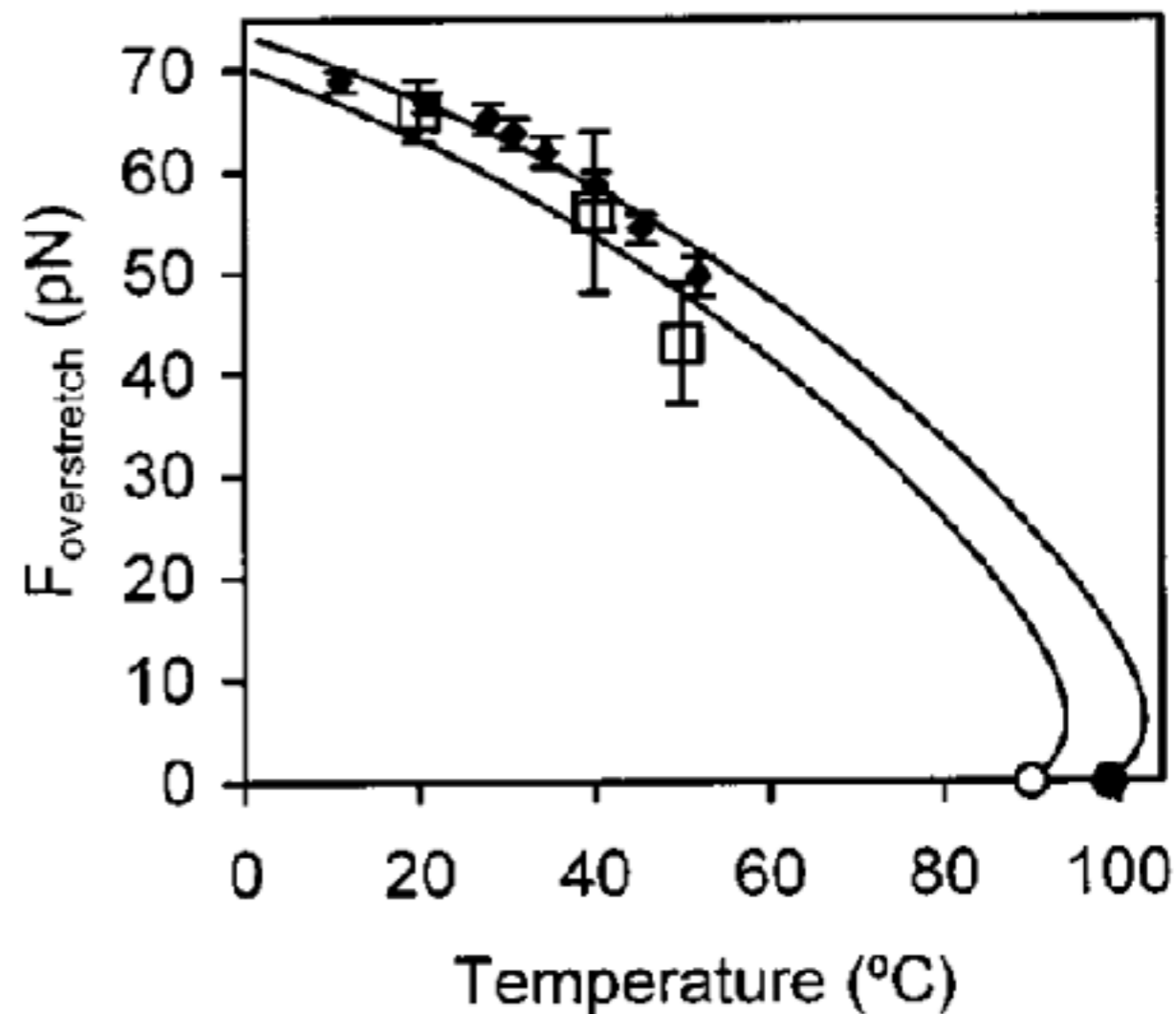


- Zhanget, Y. *et al.* Low spring constant regulates P-Selectin-PSGL-1 bond rupture. *Biophys. Jour.* **95**, 5439–5448 (2008).
- G. Florio, G.P, *Unveiling the influence of device stiffness in single macromolecule unfolding.* Scientific Reports 9 (2019), p. 4997.
- L. Bellino, G. Florio, G.P, *The influence of device handles in single molecule experiments,* Soft Matter **15**, 8680-8690, 2019.

Important open questions: temperature effects

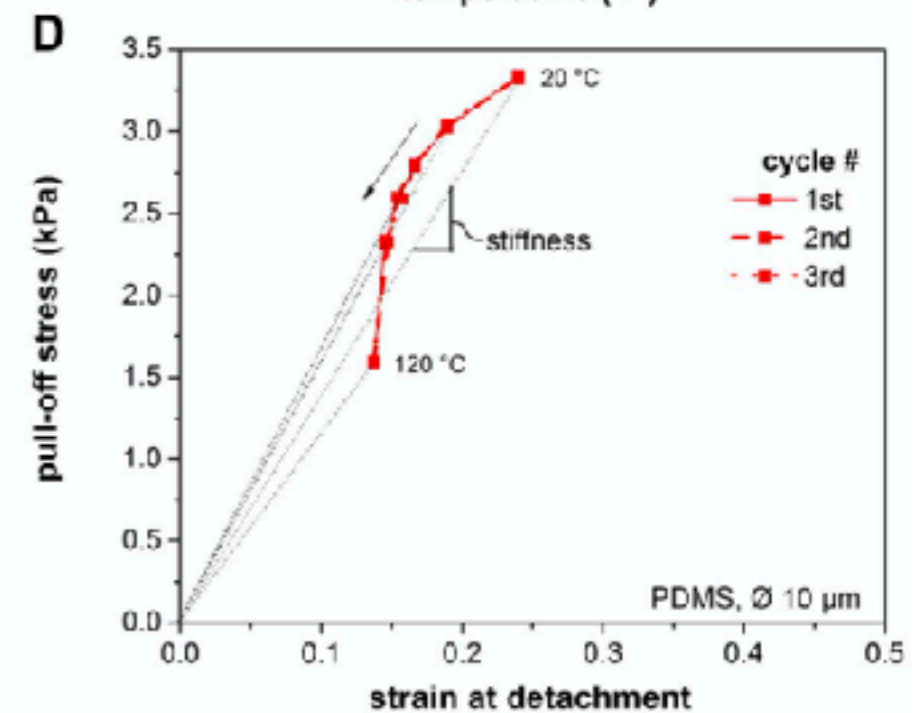
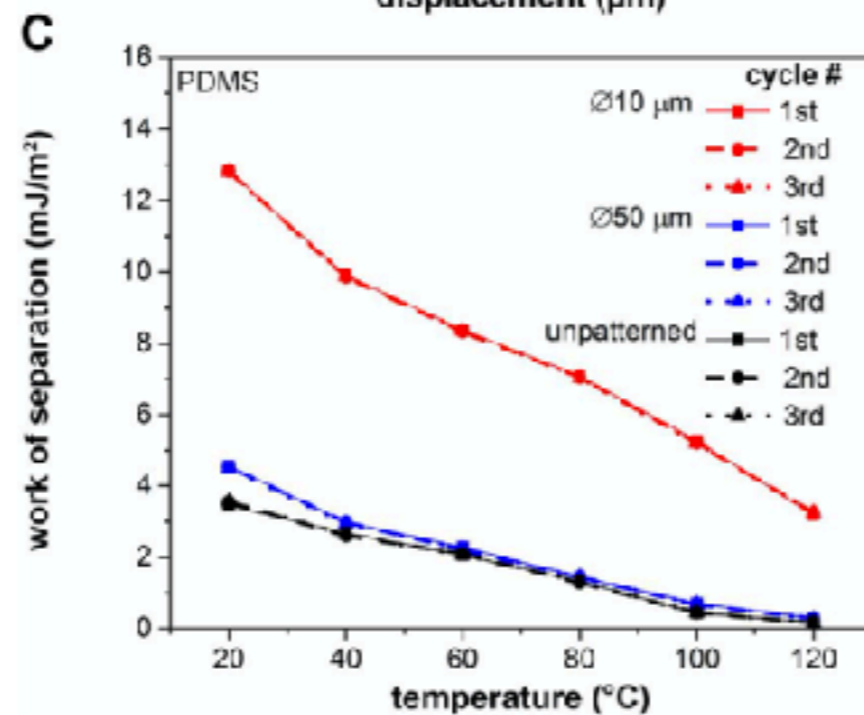
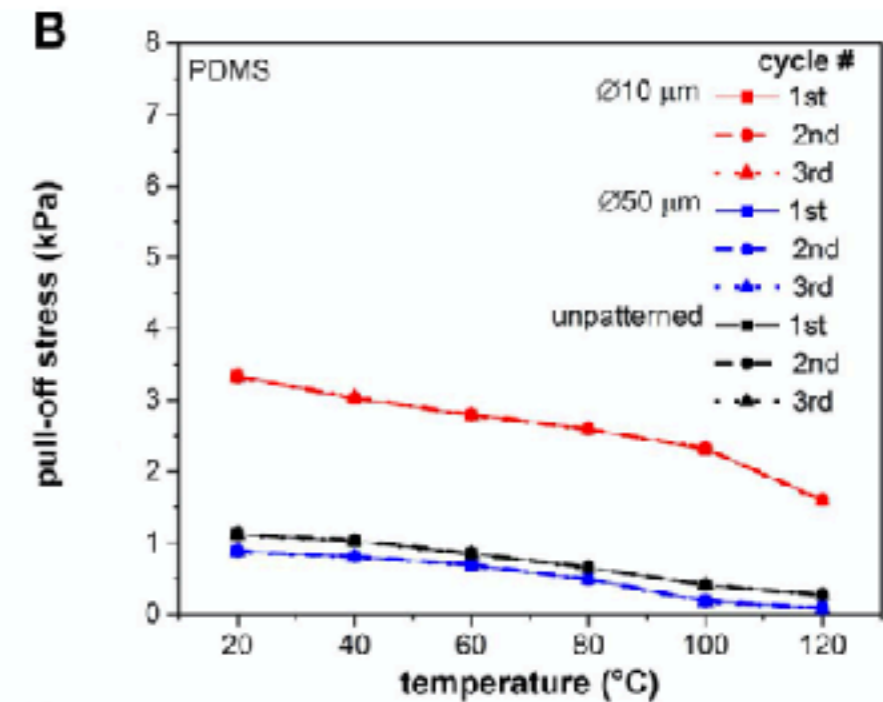
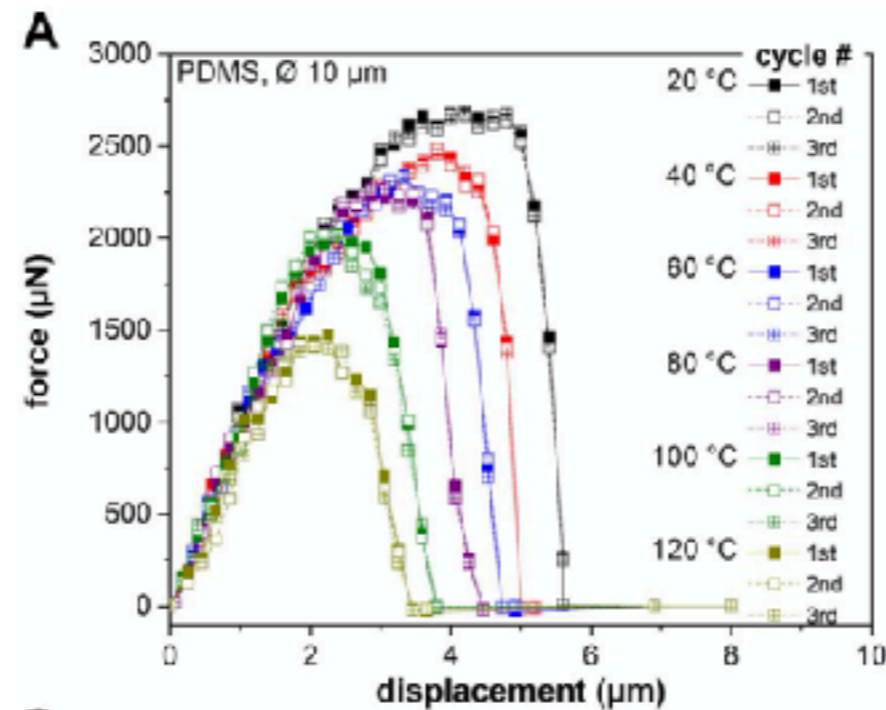
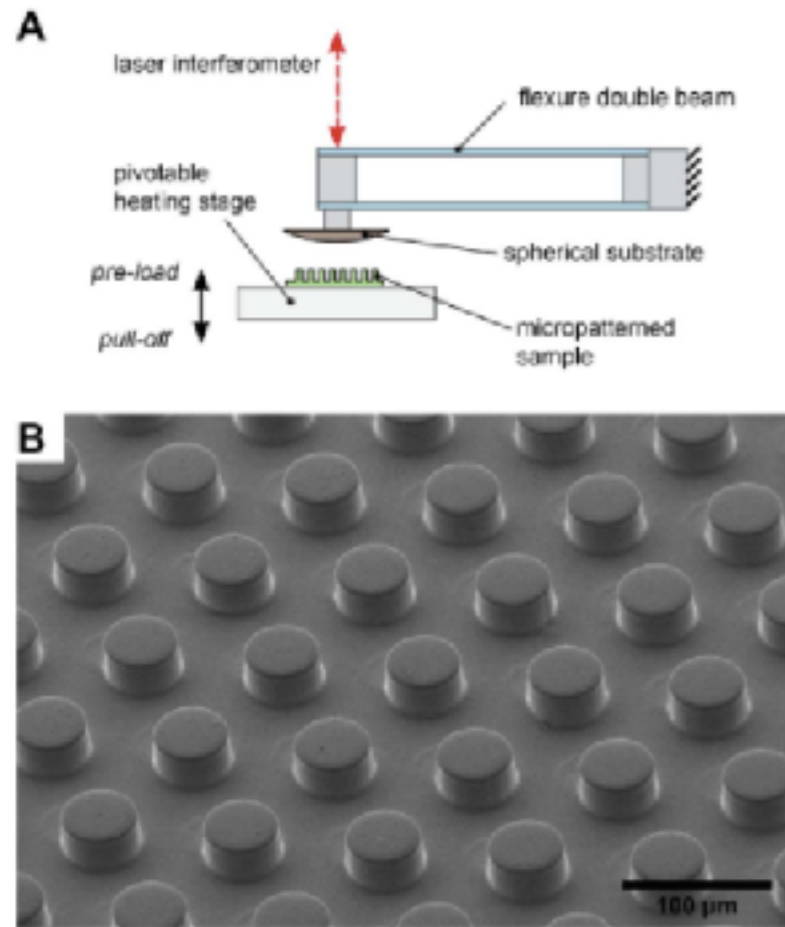


S. S. Brenner Mechanical Behavior of Sapphire Whiskers at Elevated Temperatures. *Journal of Applied Physics* 33, 33 (1962)



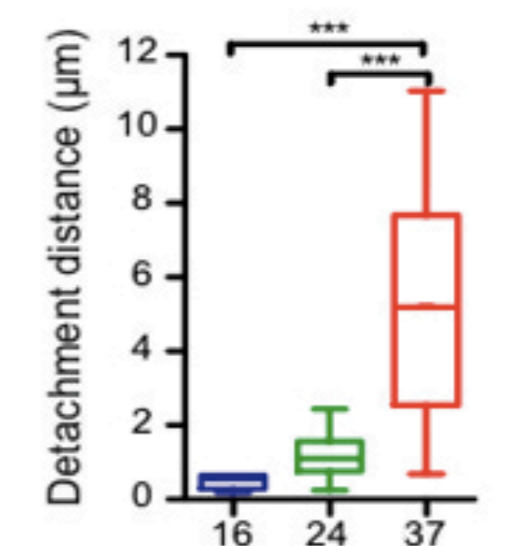
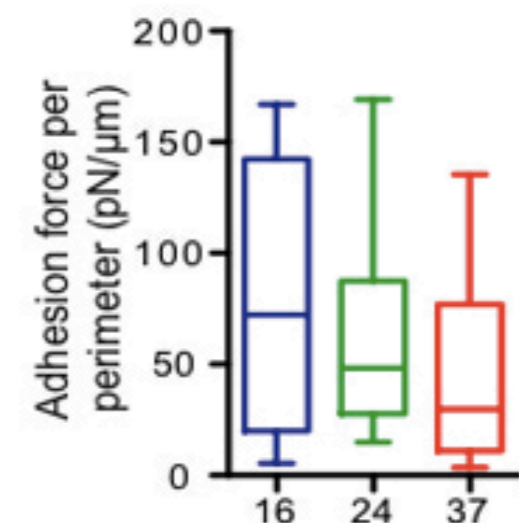
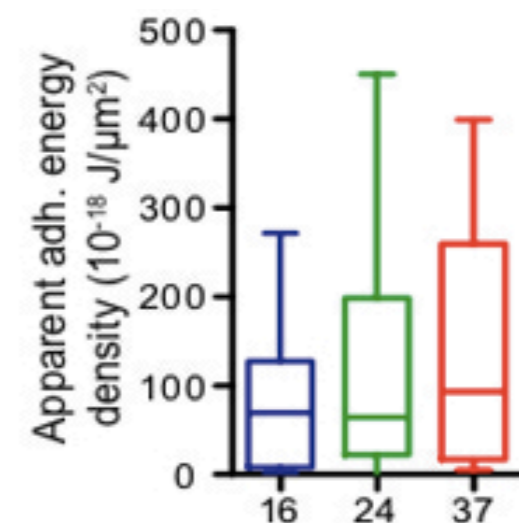
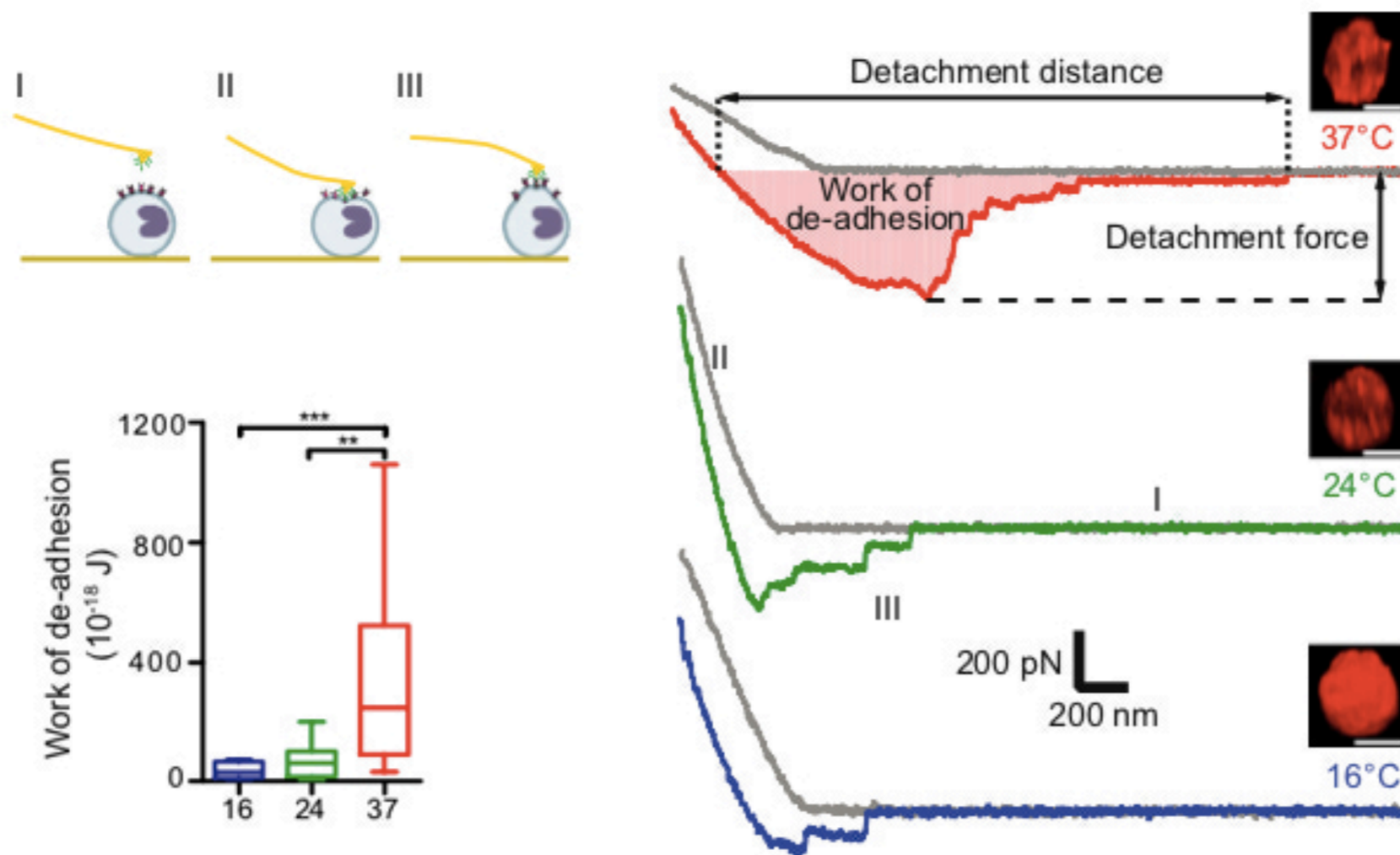
C. Williams, I. Rouzina, A. Bloomfield, Thermodynamics of DNA Interactions from Single Molecule Stretching Experiments, *Acc. Chem. Res.* 35, 159–166, 2002

Important open questions: temperature effects



V. Barreau, D. Yua, R. Hensel, E. Arzta, Elevated temperature adhesion of bioinspired polymeric micropatterns to glass. *Journal of the Mechanical Behavior of Biomedical Materials*, 76 (2017) 110–118

Important open questions: temperature effects



Felix Rico, Calvin Chu, Midhat H. Abdulreda, Yujing Qin, and Vincent T. Moy. Temperature Modulation of Integrin-Mediated Cell Adhesion. *Biophysical Journal* **99** 2010 1387–1396

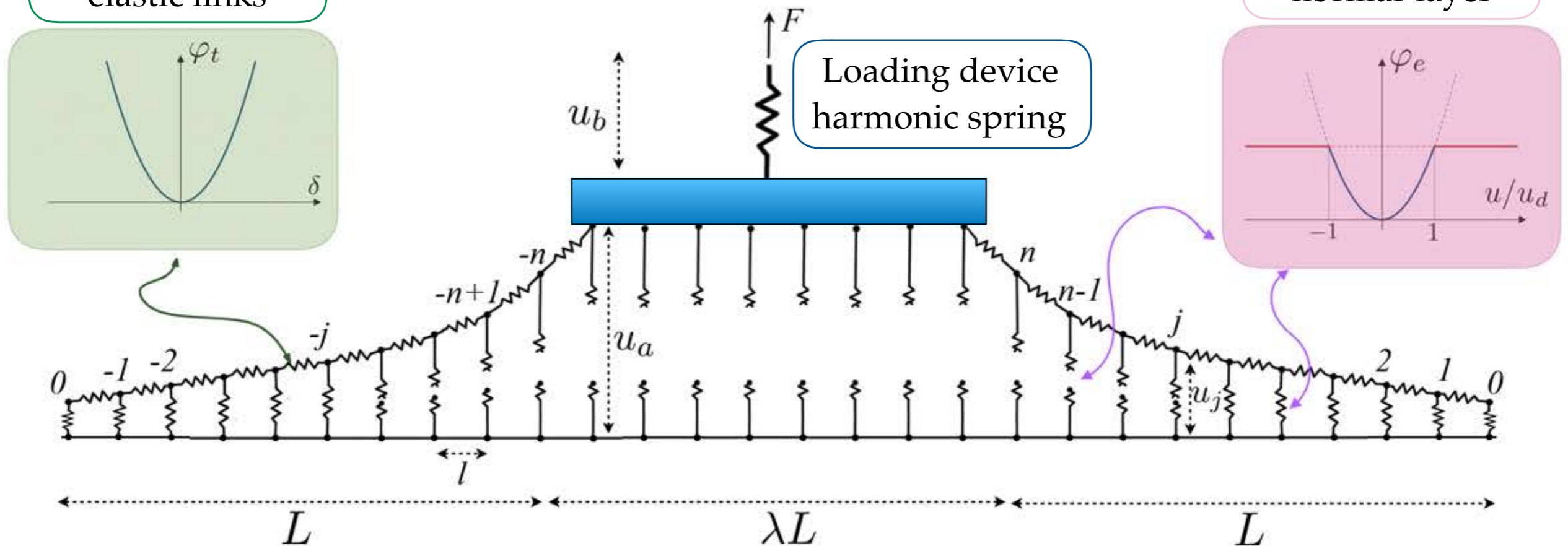
Model



Adhering layer
elastic links

Adhesive
fibrillar layer

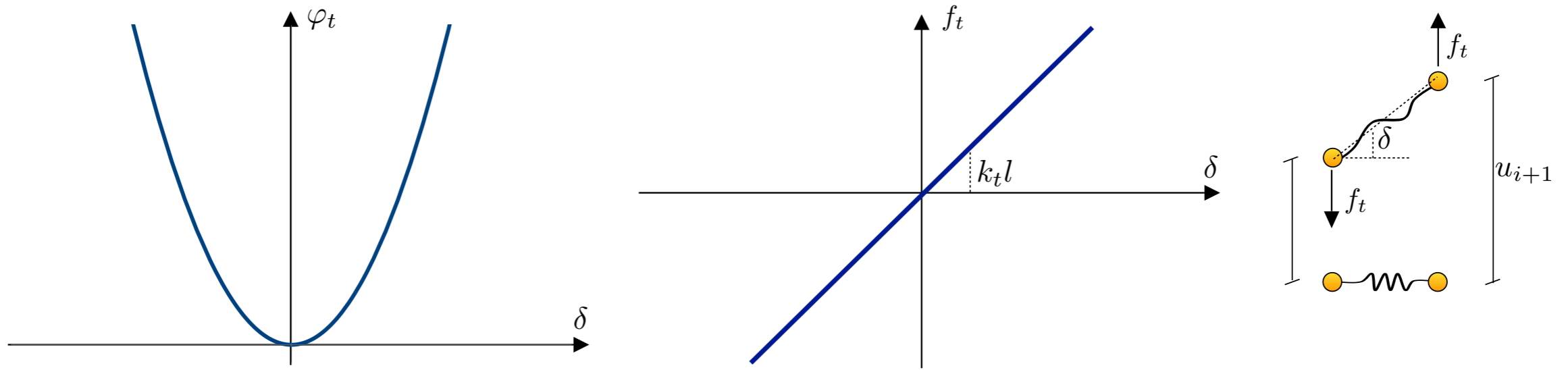
Loading device
harmonic spring



Model

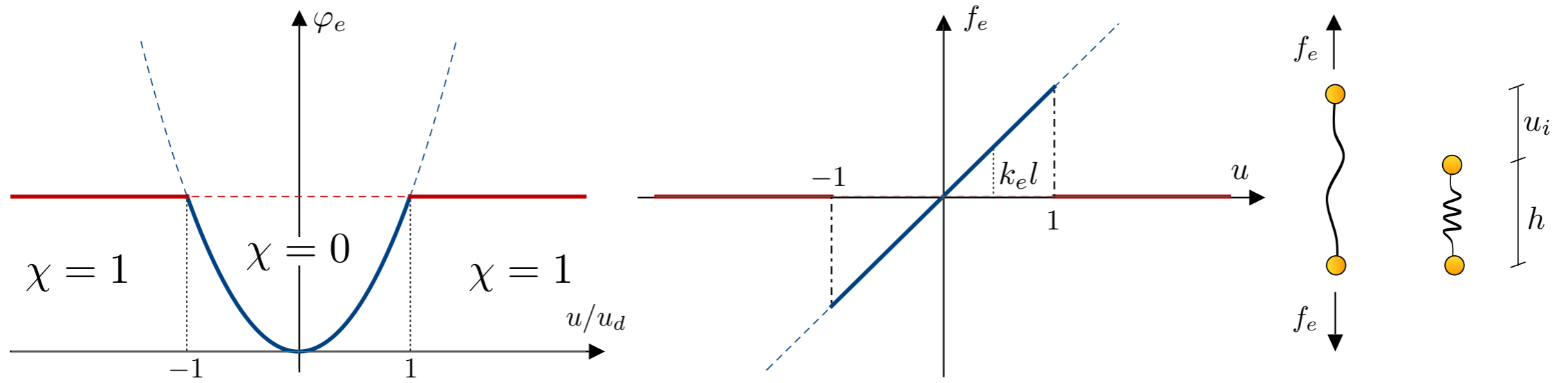


$$\varphi_t(\delta) = \frac{lk_t}{2} \gamma^2$$



$$\varphi_e(u) = \frac{lk_e}{2} [(1 - \chi(u))u^2 + \chi(u)] \quad \chi = \chi(u) = \begin{cases} 0, & \text{if } u \leq u_d, \\ 1, & \text{if } u > u_d, \end{cases}$$

attached fibril
detached fibril



$$nh = \frac{H}{k_e l} = \frac{1}{2} \sum_{j=l,r} \sum_{i=0}^n \left[\nu^2 (w_{i+1}^j - w_i^j)^2 + (1 - \chi_i^j)(w_i^j)^2 + \chi_i^j \right] + \frac{\lambda}{2} [(1 - \chi_a)w_a^2 + \chi_a] + \frac{\xi}{2} w_b^2$$

Adhering layer
 Adhesive fibrils
 Loaded fibrils
 Loading device

$$w_i = \frac{u_i}{u_d}, w_a = \frac{u_a}{u_d}, w_b = \frac{u_b}{u_d},$$

... non-dimensional displacements

$$w_a + w_b = \delta := \frac{d}{u_d}, w_o^l = w_o^r = 0$$

... boundary conditions

$$w_{n+1} = w_{-(n+1)} = w_a$$

... compatibility conditions

Main non-dimensional parameters

$$\nu = \sqrt{\frac{k_t}{k_e}} \frac{u_d}{l}$$

adhering vs adhesive

$$\xi = \frac{k_{dev} u_d^2}{L k_e}$$

loading device vs adhesive

Energy: compact notation

$$\mathbf{w}^j = \begin{pmatrix} w_1^j \\ \dots \\ w_n^j \end{pmatrix}, \quad \boldsymbol{\chi}^j = \begin{pmatrix} \chi_1^j \\ \dots \\ \chi_n^j \end{pmatrix}, \quad j = l, r, \mathbf{i}_1 \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix}, \quad \mathbf{i}_n \begin{pmatrix} 0 \\ 0 \\ \dots \\ 1 \end{pmatrix},$$

$$\mathbf{B}^j = \begin{bmatrix} 2\nu^2 + 1 - \chi_1^j & -\nu^2 & & & & & \mathbf{0} \\ -\nu^2 & 2\nu^2 + 1 - \chi_2^j & -\nu^2 & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\nu^2 & 2\nu^2 + 1 - \chi_{n-1}^j & -\nu^2 & \\ \mathbf{0} & & & & -\nu^2 & 2\nu^2 + 1 - \chi_n^j & \end{bmatrix}, \quad j = l, r.$$

$$nh(\mathbf{w}^l, \mathbf{w}^r, \boldsymbol{\chi}^l, \boldsymbol{\chi}^r, w_a, w_b) = \sum_{j=l,r} \left(\frac{1}{2} \mathbf{B}^j \mathbf{w}^j \cdot \mathbf{w}^j + (n - p^j) - \nu^2 w_a \mathbf{w}^j \cdot \mathbf{i}_n \right) + \frac{\xi}{2} w_b^2 + \lambda [(1 - \chi_a) w_a^2 + \chi_a^2] + \nu^2 w_a^2$$

Variational approach: Griffith

$$\min_{\mathbf{w}^l, \mathbf{w}^r, \boldsymbol{\chi}^l, \boldsymbol{\chi}^r, w_a, w_b} h(\mathbf{w}^l, \mathbf{w}^r, \boldsymbol{\chi}^l, \boldsymbol{\chi}^r, w_a, w_b) - f(w_a + w_b - \delta).$$

f Lagrange multiplier, force applied by the loading device (AFM, ancilla molecule, adhering cell,...)

Equilibrium: Euler-Lagrange equations

$$w^j = \nu^2 w_a (\mathbf{B}^j)^{-1} i_n, \quad j = l, r \quad \dots \text{ adhesive system equilibrium}$$

$$w_a = \frac{f + \nu^2 (w_n^l + w_n^r)}{\lambda(1 - \chi_a) + 2\nu^2}, \quad \dots \text{ action-reaction principle}$$

$$w_b = \frac{f}{\xi}. \quad \dots \text{ equilibrium loading device}$$



$$w_i^j = \nu^2 (\mathbf{B}^j)^{-1}_{i,n} w_a \quad \dots \text{ monotonic}$$

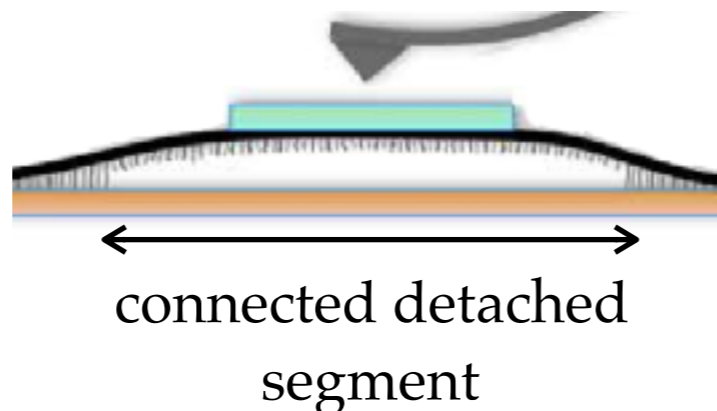


di-block solutions

$$f = k_{tot}(p)\delta,$$

$$h = \frac{\delta^2}{2k_{tot}(p)} + 2(n - p),$$

$$k_{tot}(p) = \frac{\xi k(p)}{\xi + k(p)}.$$



$$k(p) = \nu^2 [1 - \nu^2 \mathbf{B}_{n,n}^{-1}(p)] = \frac{2\nu^2}{n - p + a(p)},$$

$$a(p) = \left(1 - \frac{\sinh[p\bar{\lambda}]}{\sinh[(p+1)\bar{\lambda}]} \right),$$

$$\cosh \bar{\lambda} = 1 + \frac{1}{2\nu^2}.$$

Metastable Configurations: Hysteresis

$$f = k_{tot}(p)\delta, \quad \dots \text{equilibrium force-displacement relation}$$

$$h = \frac{\delta^2}{2k_{tot}(p)} + 2(n-p), \quad \dots \text{equilibrium energy-displacement relation}$$

$$k_{tot}(p) = \frac{\xi k(p)}{\xi + k(p)}. \quad \dots \text{effective global elastic modulus}$$

$$w_i = a(p) \frac{\cosh[(1+i)\lambda] - \cosh[(1-i)\lambda]}{2 \sinh \lambda \sinh[(1+p)\lambda]} \frac{k_{tot}(p)\delta}{2\nu^2}, \quad i = 1, \dots, p \quad \dots \text{attached segment}$$

$$w_i = \left(\frac{\nu^2}{k(p)} - (n+1-i) \right) \frac{k_{tot}(p)\delta}{2\nu^2}, \quad i = p, \dots, n+1. \quad \dots \text{detached segment}$$

$$\delta \in (\delta_m(p), \delta_M(p)) := \left(\frac{\nu^2}{a(p) k_{tot}(p)}, \frac{\nu^2}{(a(p)-1) k_{tot}(p)} \right). \quad \dots \text{metastability domain}$$

Global minima: reversible adhesion

$$\delta = \delta_{\text{Max}}(p) := \frac{1}{\nu\xi} \sqrt{\frac{(\xi b(p) + \nu^2)(\xi b(p+1) + \nu^2)}{b(p) - b(p+1)}}, \quad p = 0, \dots, n-1,$$

$$b = b(p) := n - p + a(p). \quad \frac{d\delta_{\text{Max}}(p)}{dp} < 0.$$



Coherent propagation

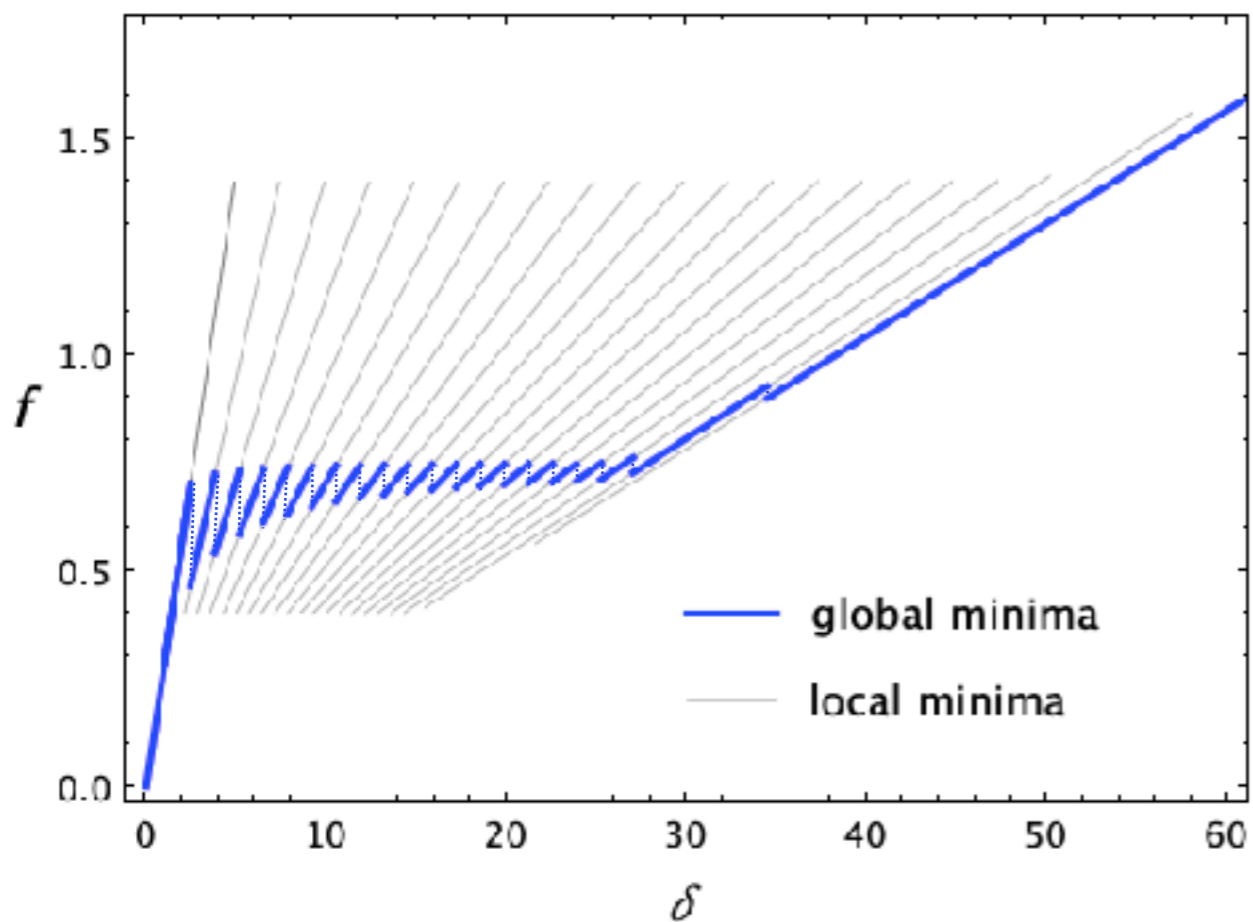
$$\begin{array}{lll} \delta < \delta_{\text{Max}}(n-1) & \text{if } p = n & \text{(fully attached)} \\ \delta \in [\delta_{\text{Max}}(p), \delta_{\text{Max}}(p-1)] & \text{if } 0 < p < n & \text{(partially detached)} \\ \delta > \delta_{\text{Max}}(0) & \text{if } p = 0 & \text{(fully detached).} \end{array}$$

$$f \in [f_m(p), f_M(p)] \quad \text{where} \quad f_m(p) := \bar{k}(p)\delta_{\text{Max}}(p), \quad f_M(p) := \bar{k}(p)\delta_{\text{Max}}(p-1).$$

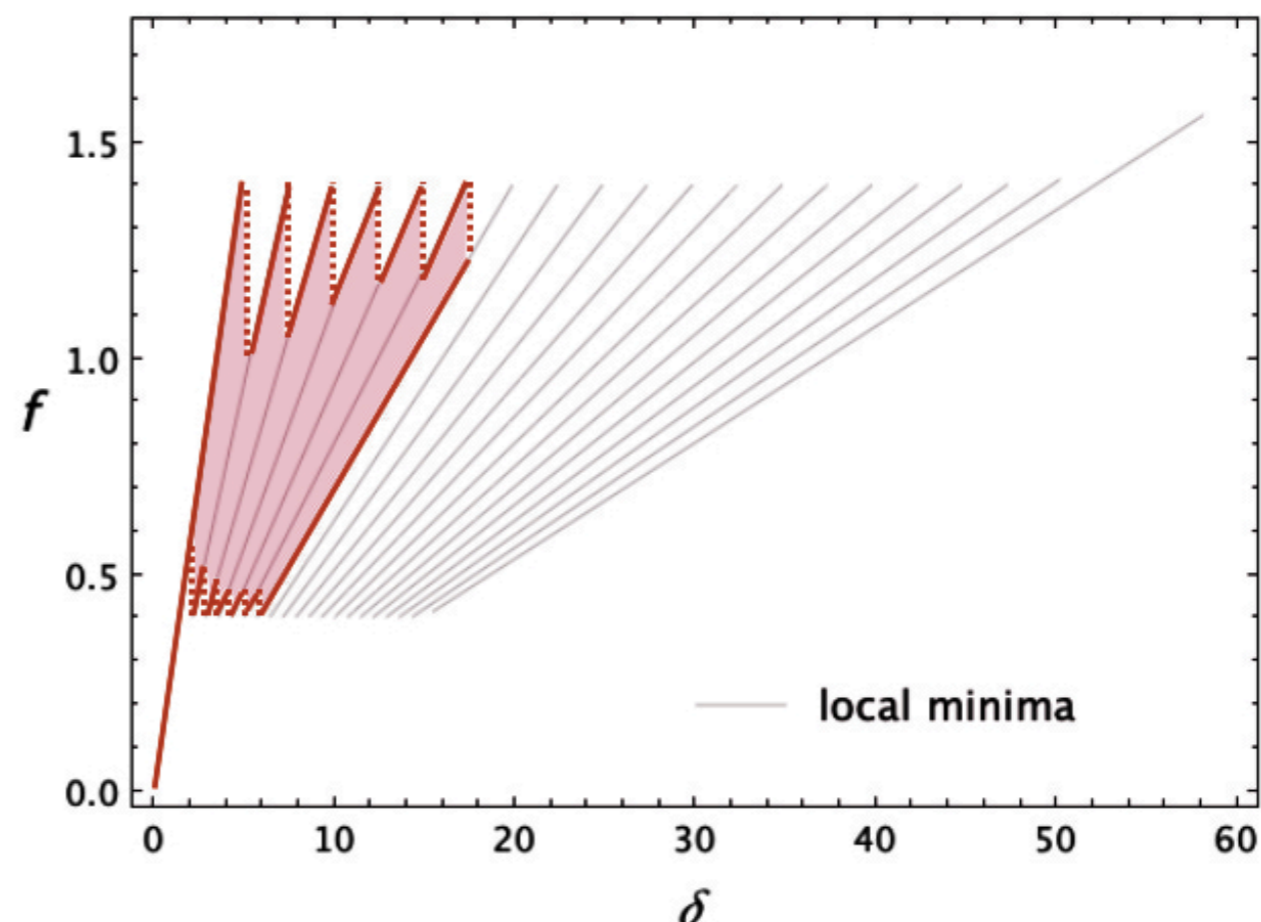


$f_M(n)$... maximum adhesion force

Maximum delay vs Maxwell conventions

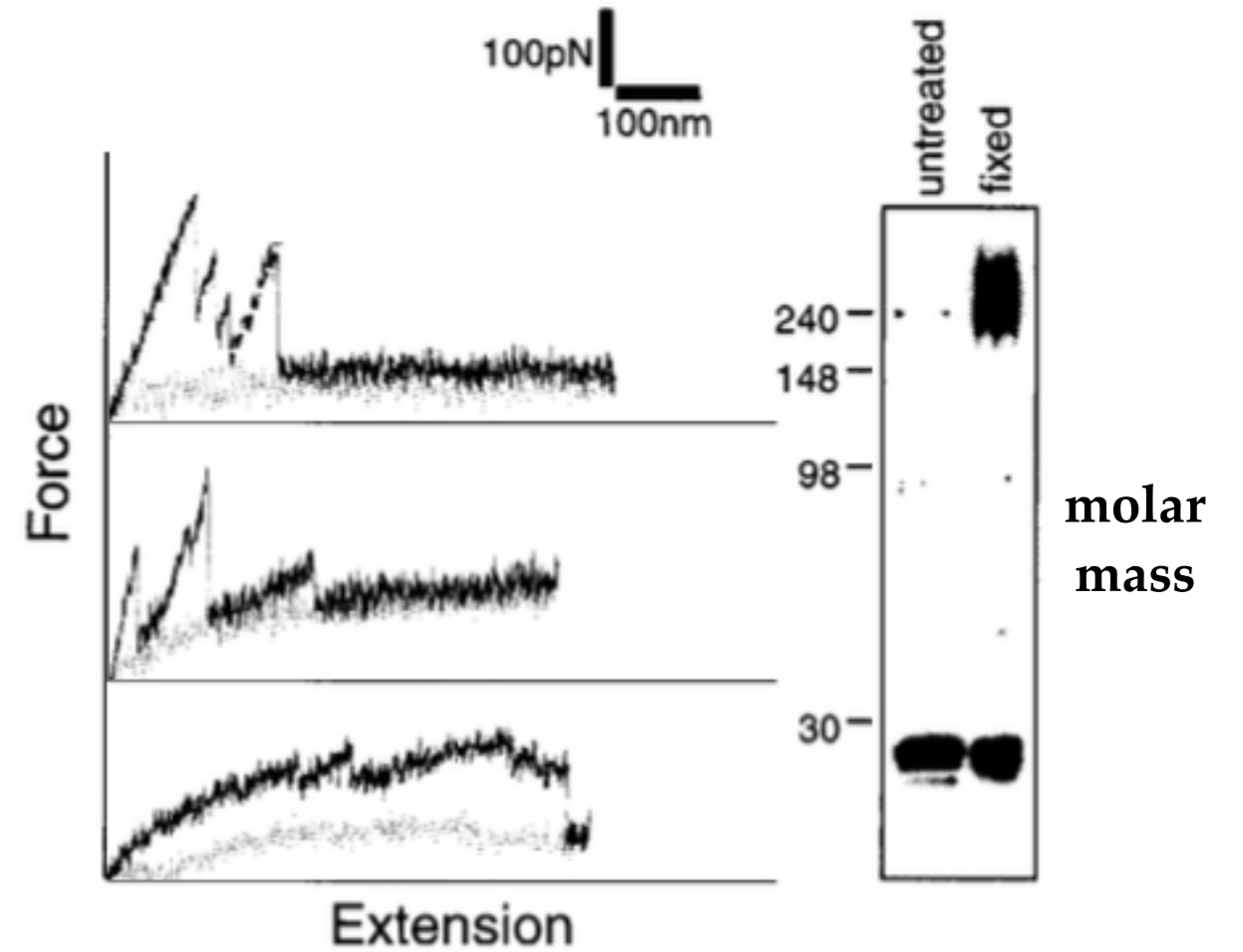
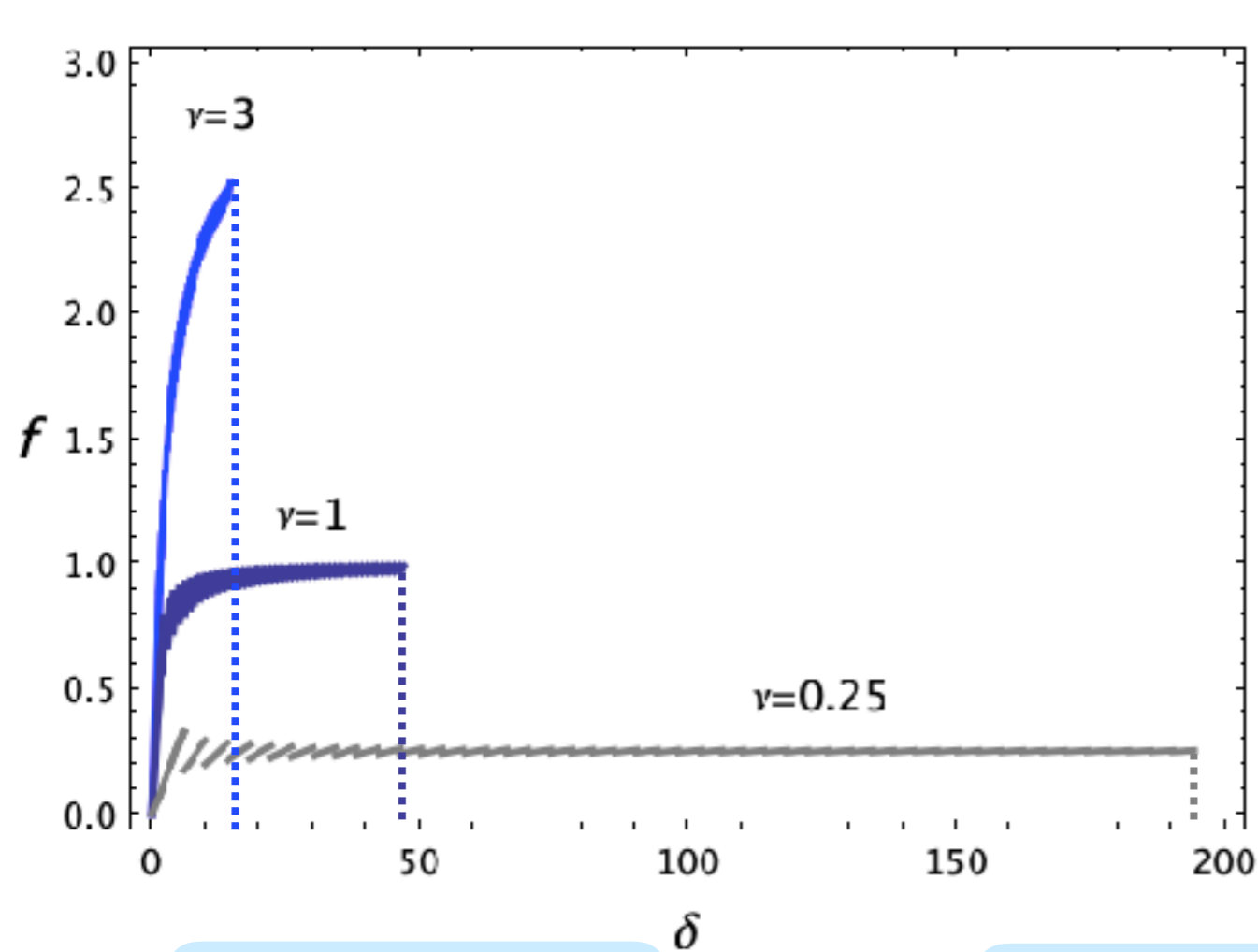


reversible adhesion

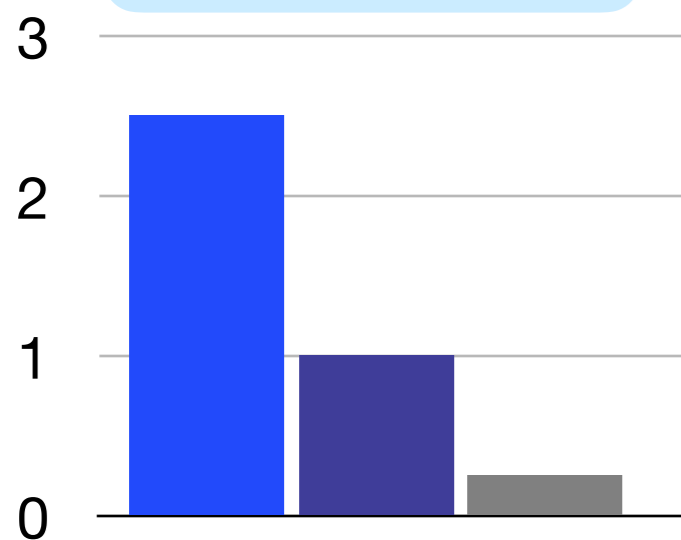


hysteresis

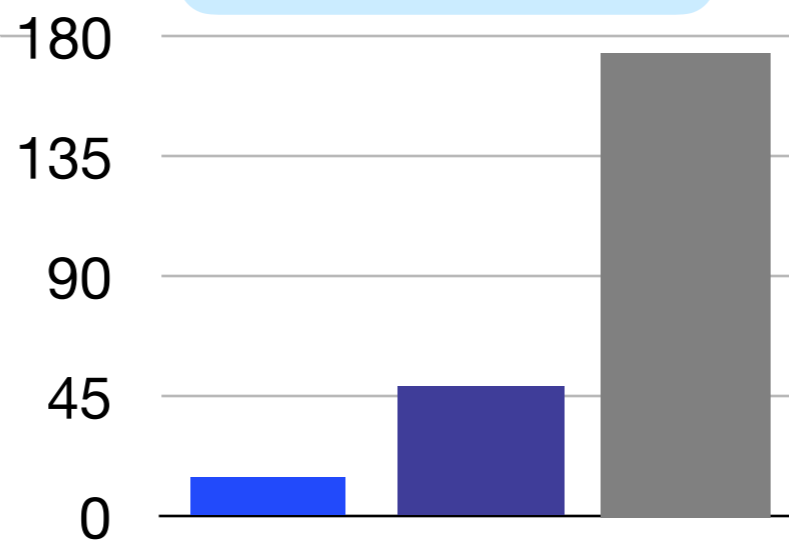
Adhering stiffness effect



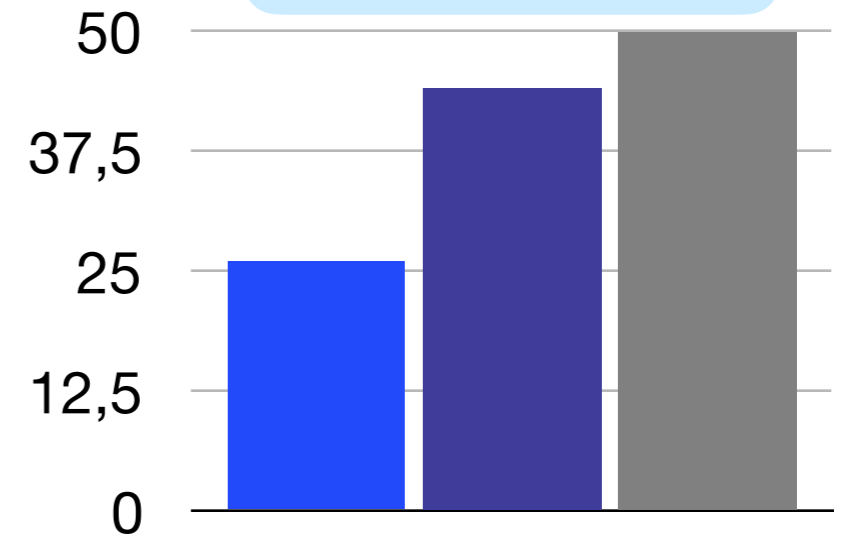
decohesion force



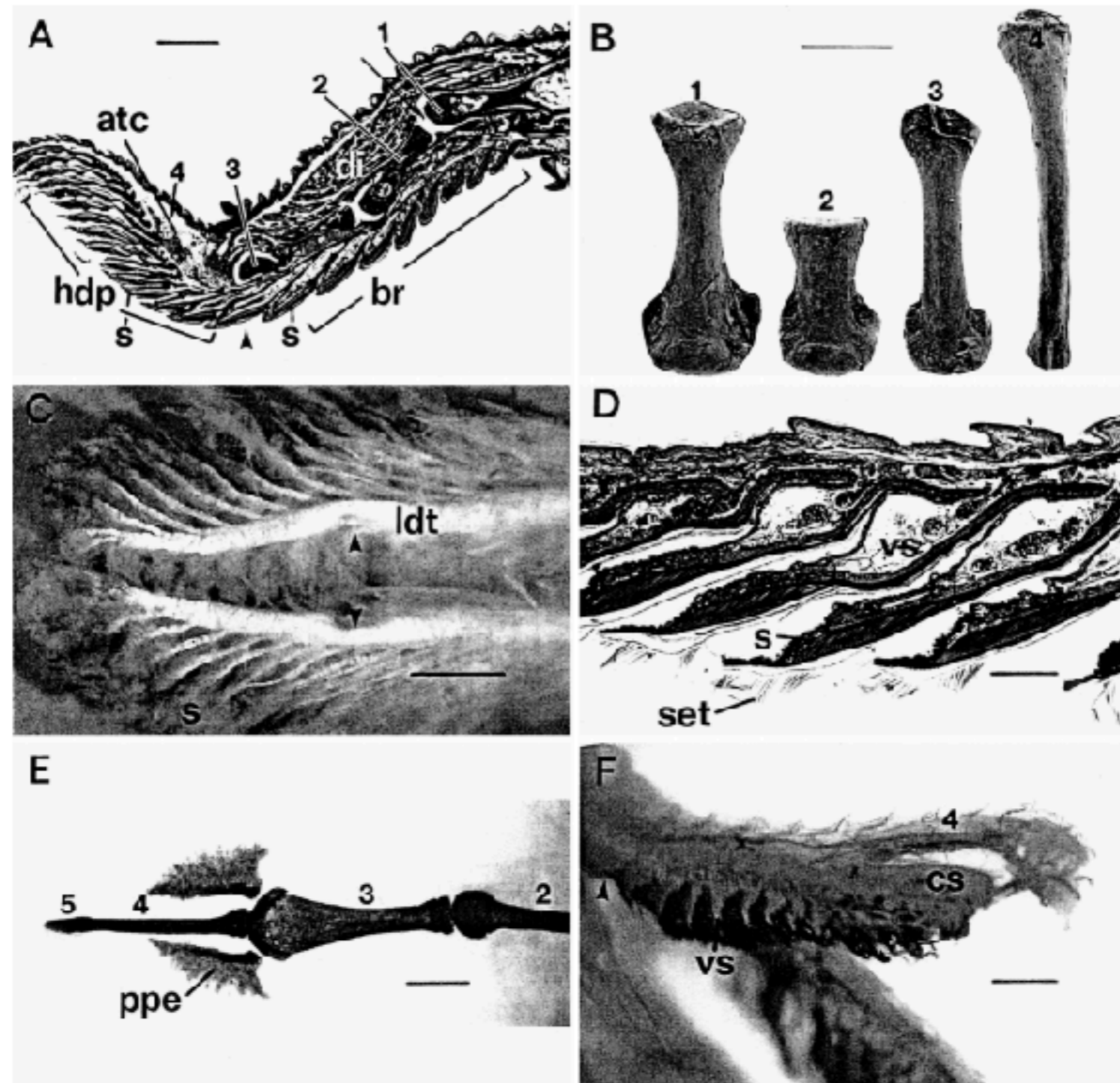
limit displacement



decohesion work



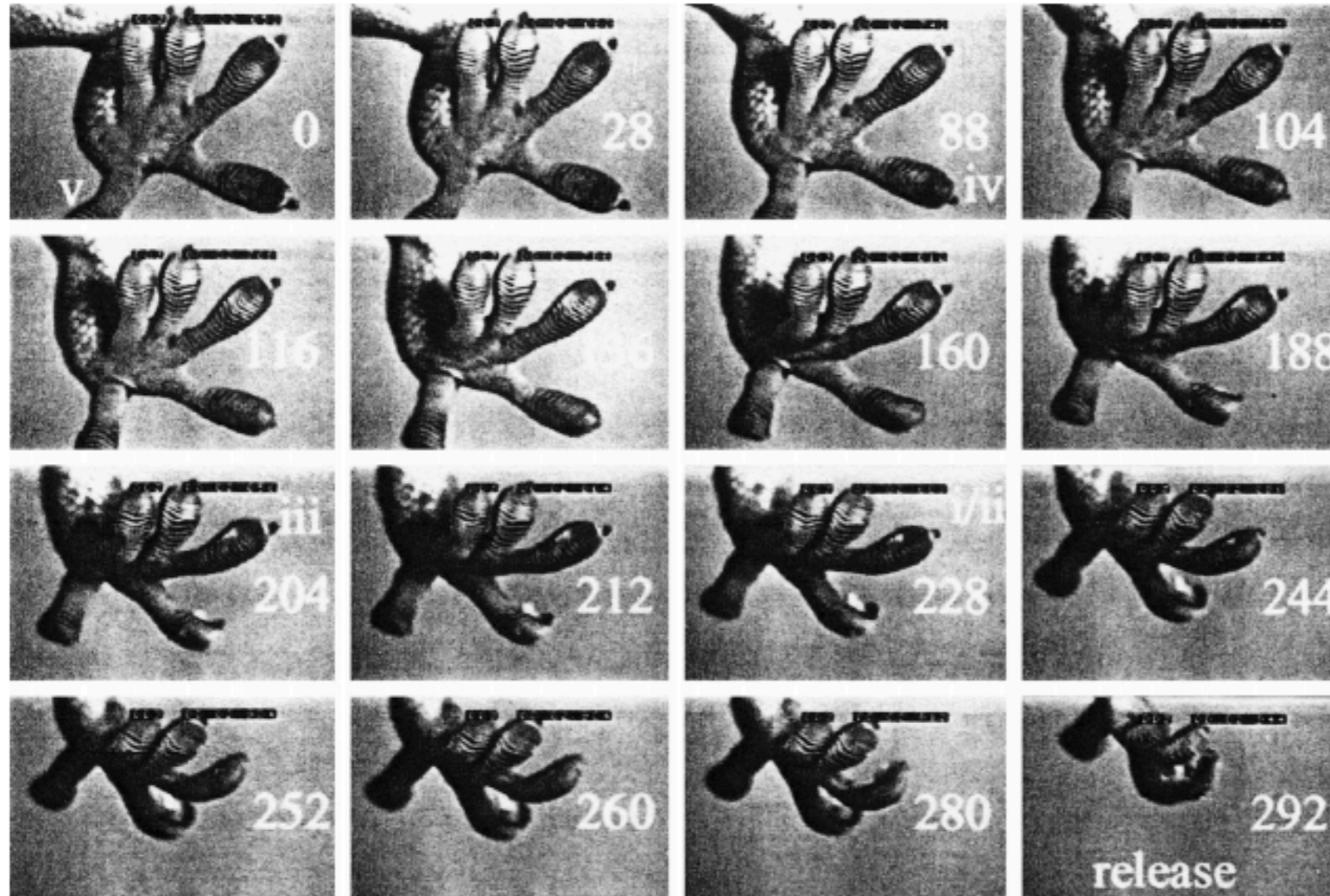
Hypothesis on gecko adhesion-decohesion asymmetry



Hypothesis on gecko adhesion-decohesion asymmetry



digital hyperextension



At the macroscale the easy release is achieved through the localization of the cohesive region

geckos (A. P. Russell, *Integr. Comp. Biol.* **42**, 1154 (2002))

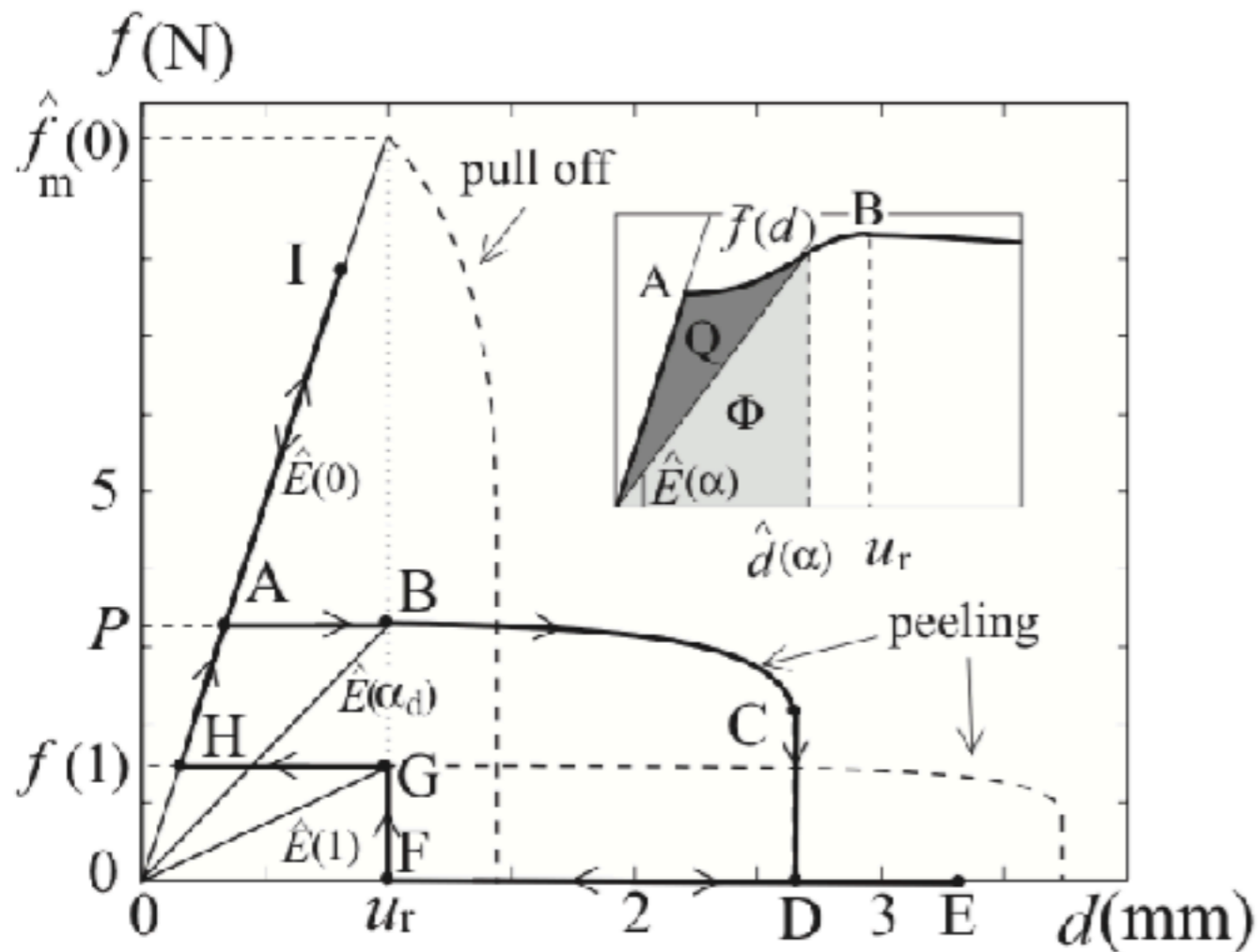
frogs (G. Hanna and W. Barnes, *J. Exp. Biol.* **155**, 103 (1991))

ants (W. Federle and T. Endlein, *Arthropod Struct. Dev.* **33**, 67 (2004)) also show that.

To simplify horizontal walking geckos keep the hyperextended state and start activating the attachment mechanism only at sufficiently high slope requiring stronger adhesion

(A. P. Russell and T. E. Highman, *Proc. R. Soc. London, Ser. B* **276**, 3705 (2009))

Hypothesis on gecko adhesion-decohesion asymmetry



external work

$$W = \int_{P/\hat{E}(0)}^{\hat{d}(\alpha)} \bar{f}(\tilde{d}) d\tilde{d} > 0$$

elastic energy

$$\|\Phi\| = P^2/[2\hat{E}(0)] - \hat{E}^2(\alpha)\hat{d}(\alpha)/2$$

dissipation

$$Q = - \int_0^\alpha \frac{1}{2} \hat{E}'(\tilde{\alpha}) \hat{d}^2(\tilde{\alpha}) d\tilde{\alpha}.$$

decohesion: damage, peeling, path ABC

minimize dissipation → horizontal path AB

$$\|\Phi\| = Q = (P/2)[u_r - P/\hat{E}(0)] > 0.$$

adhesion: metabolic energy, reattachment, path FGH

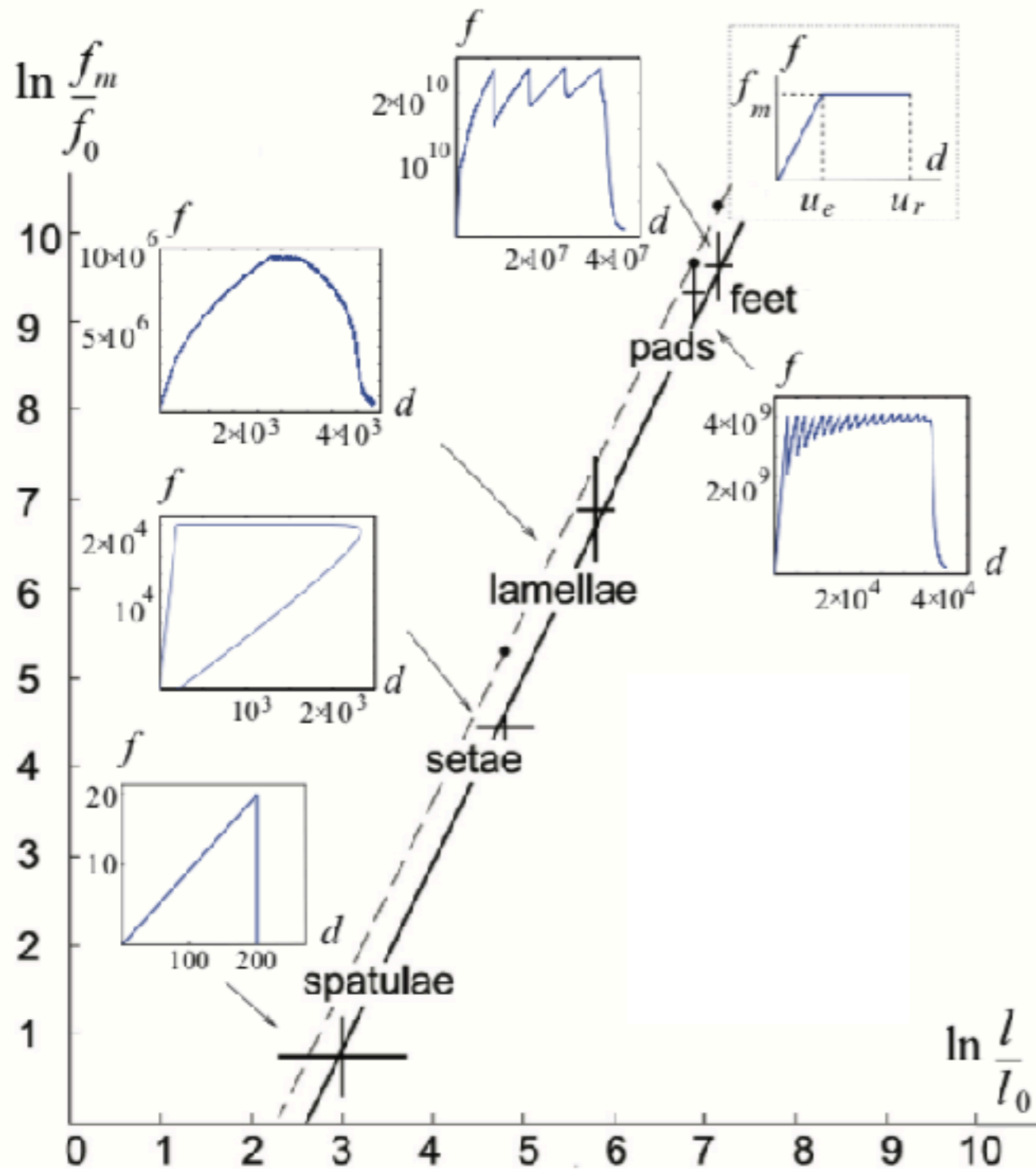
minimize metabolic energy → horizontal path GH

$$\|\Phi\| = \frac{\hat{f}_m(1)}{2} \left(\frac{\hat{f}_m(1)}{\hat{E}(0)} - u_r \right) = M < 0$$

geckos in the compliant state have a very low detaching threshold

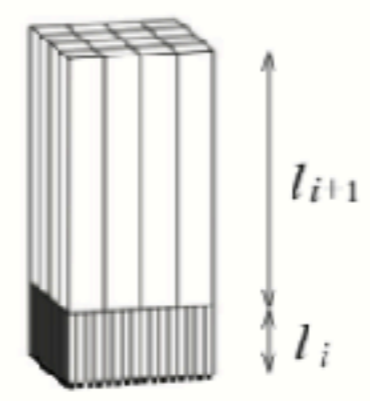
K. Autumn, in *Biological Adhesive*, edited by A. Smith and J. Callow (Springer-Verlag, Berlin, 2006).

Fractal behavior, multiscale modeling



$$f_m \sim l^\beta$$

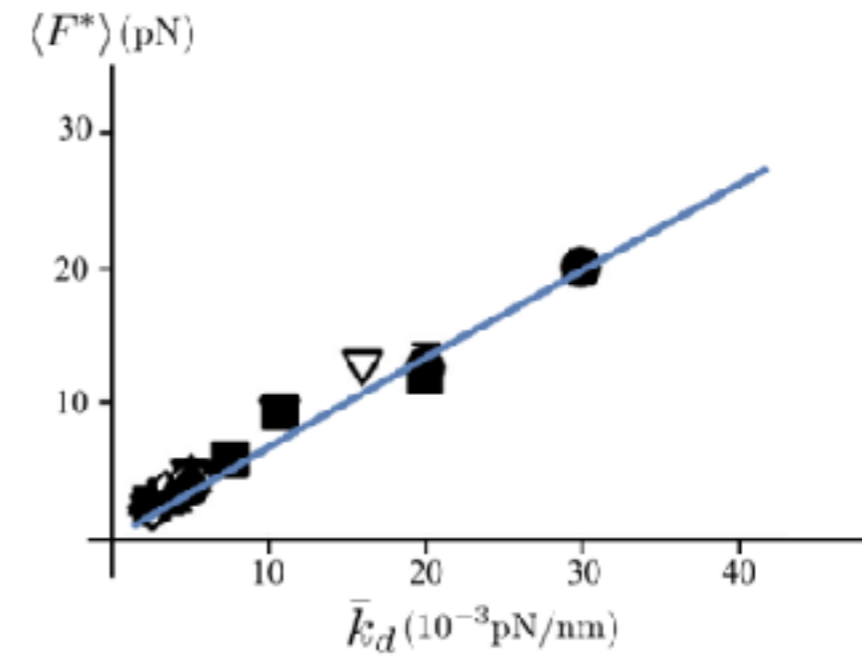
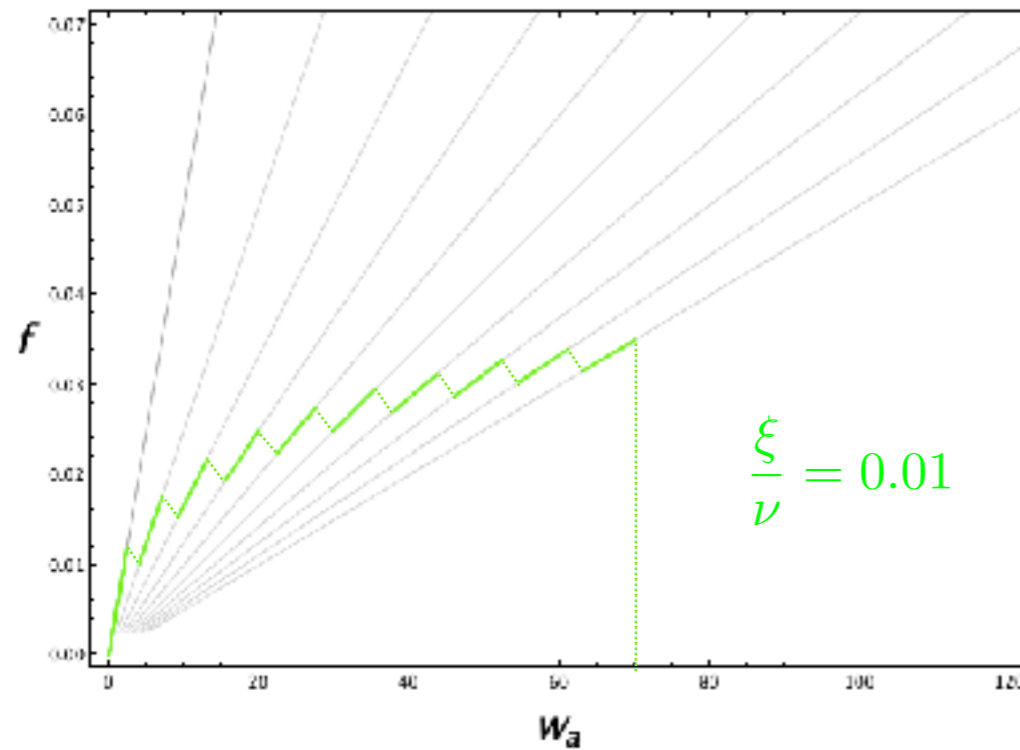
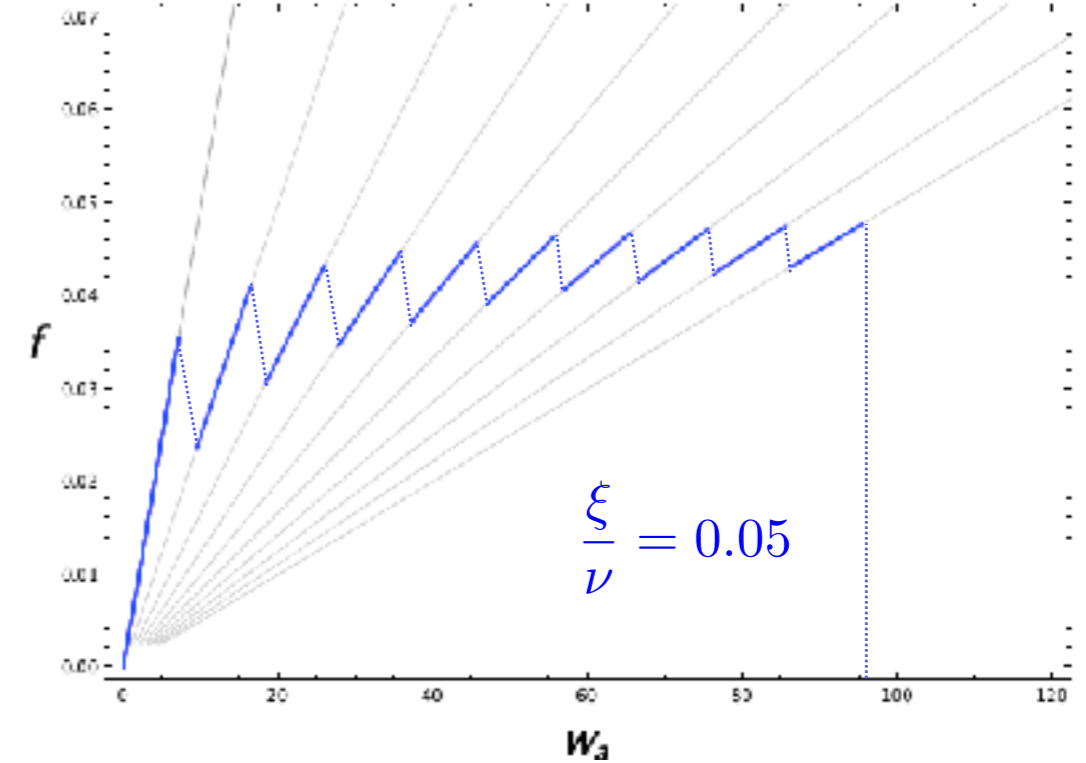
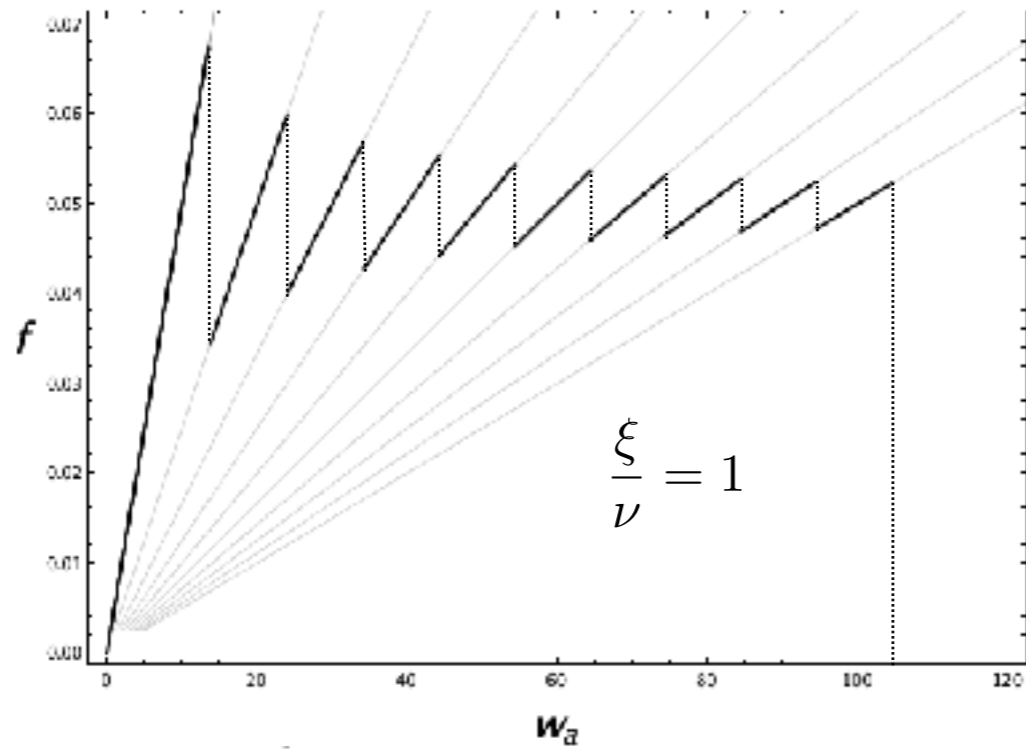
$$\beta = 2 \pm 0.5$$



$f_i = cEl_i^2$
 Euler buckling
 Selfsimilarity
 contemporary at all the scales

scale-free detachment mechanism
 ↓
 scale-generic BP model

Device stiffness effect



Rupture force $\langle F^* \rangle$ for dissociating P-selectin-PSGL-1 bond on the stiffness of the transducer

Temperature effects



Partition function

$$\mathcal{Z}_H = \left(\frac{2\pi n}{\tilde{\beta}} \right)^{n+3/2} \sum_{\chi} \Gamma_{\chi}(\tilde{\beta}, \delta), \quad \Gamma_{\chi}(\tilde{\beta}, \delta) = \frac{e^{-\frac{\tilde{\beta}}{2n}(\chi^r + \chi^l + \lambda\chi_a)} e^{-\frac{\tilde{\beta}}{2n}\xi(1 - \xi \frac{a_l a_r}{s})} \delta^2}{\sqrt{\det B^l} \sqrt{\det B^r} \sqrt{s}}$$

Main coefficients

$$a_j = \nu^2 \left(1 - \nu^2 (B^j)_{11}^{-1} \right)$$

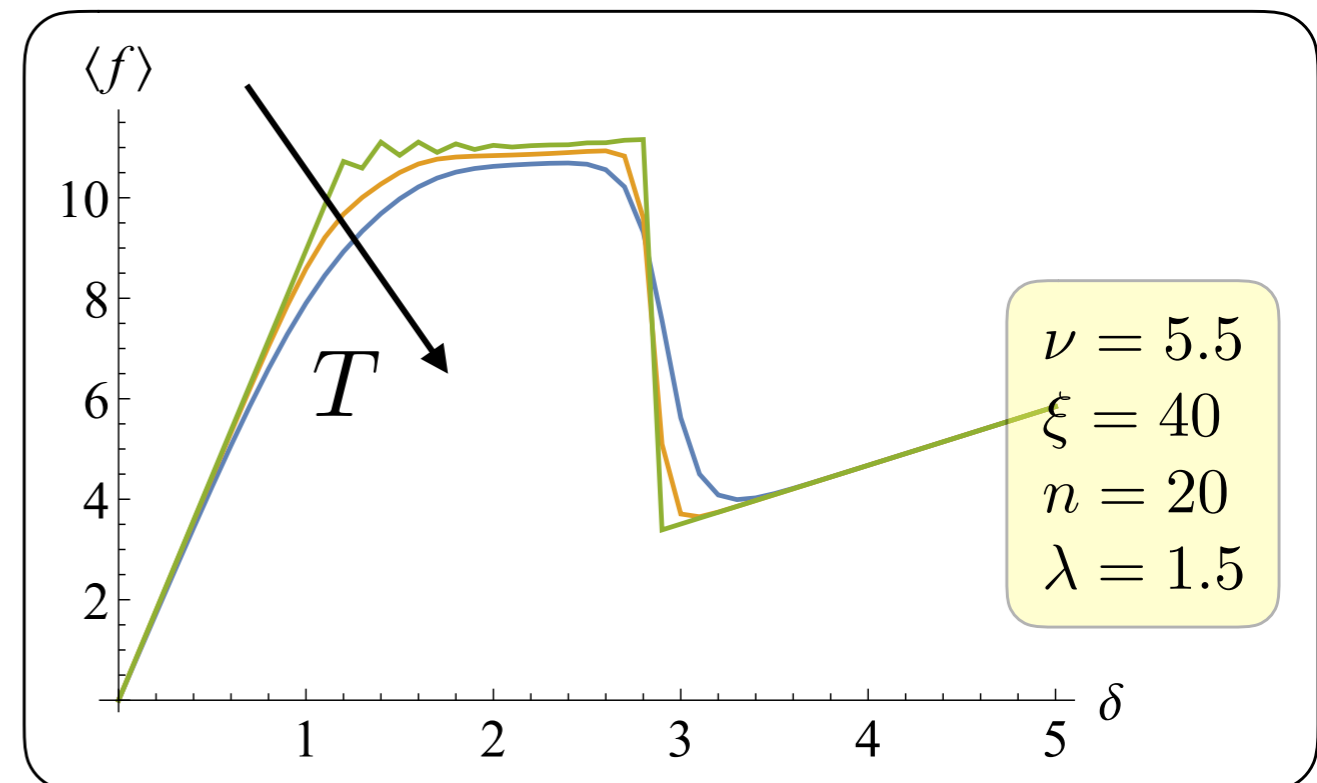
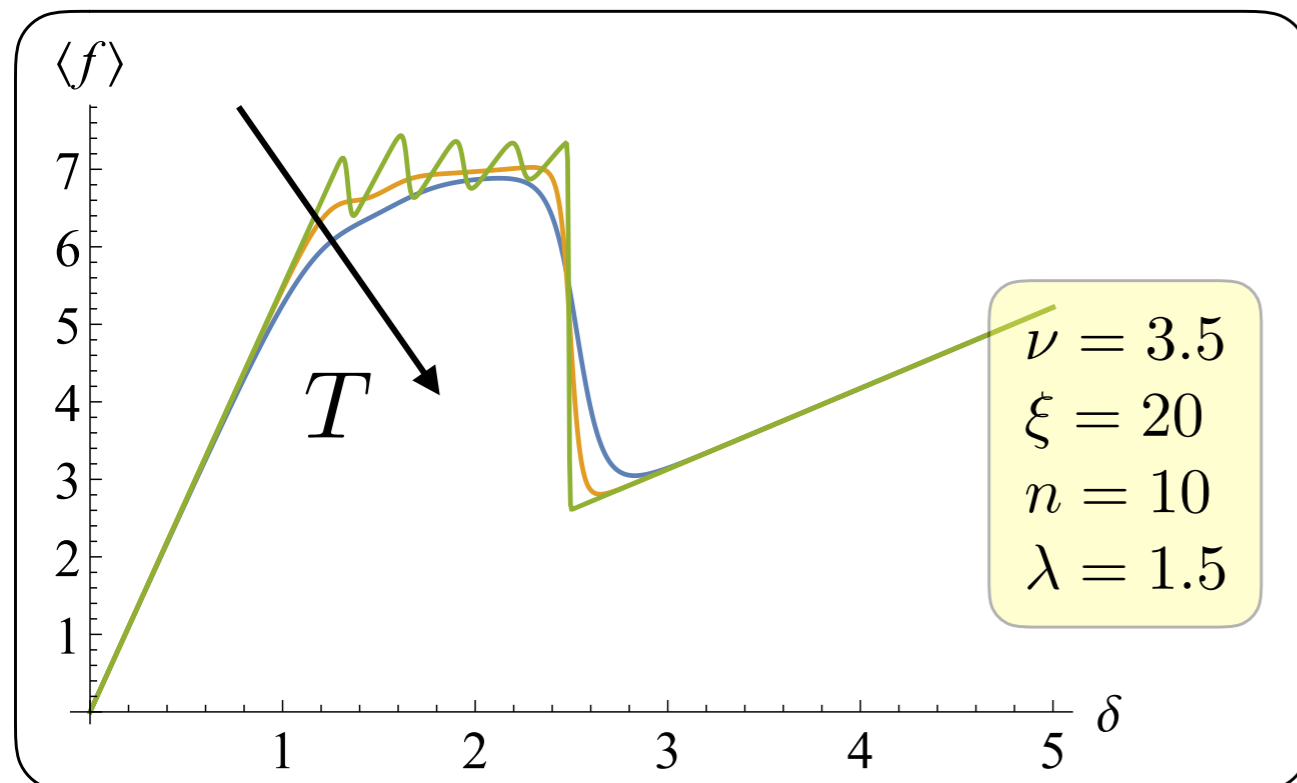
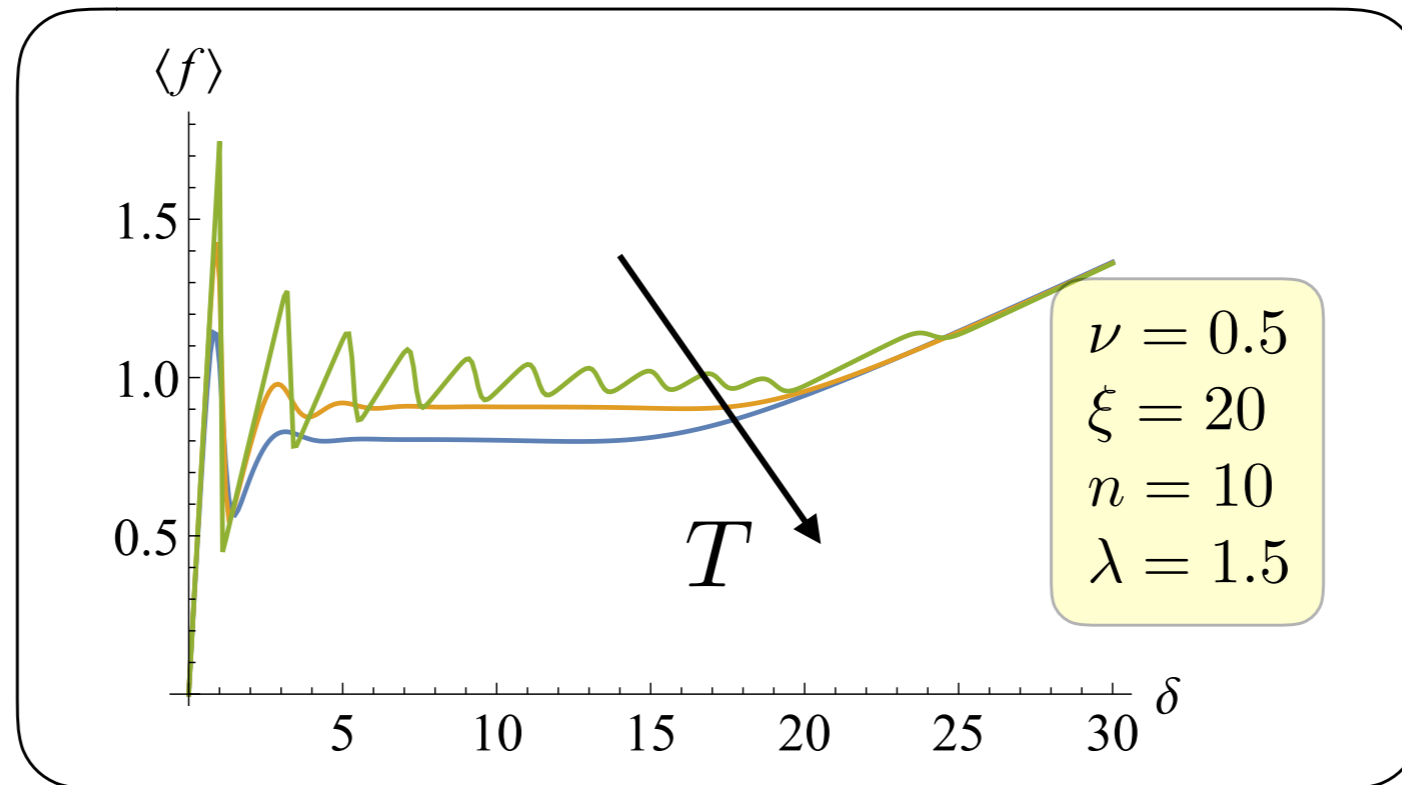
$$s = a_r a_l c - a_r \left(\nu^4 (B^l)_{1n}^{-1} \right)^2 - a_l \left(\nu^4 (B^r)_{1n}^{-1} \right)^2$$

$$c = \xi + \lambda(1 - \chi_a) + \nu^2 \left(2 - \nu^2 (B^l)_{nn}^{-1} - \nu^2 (B^r)_{nn}^{-1} \right)$$

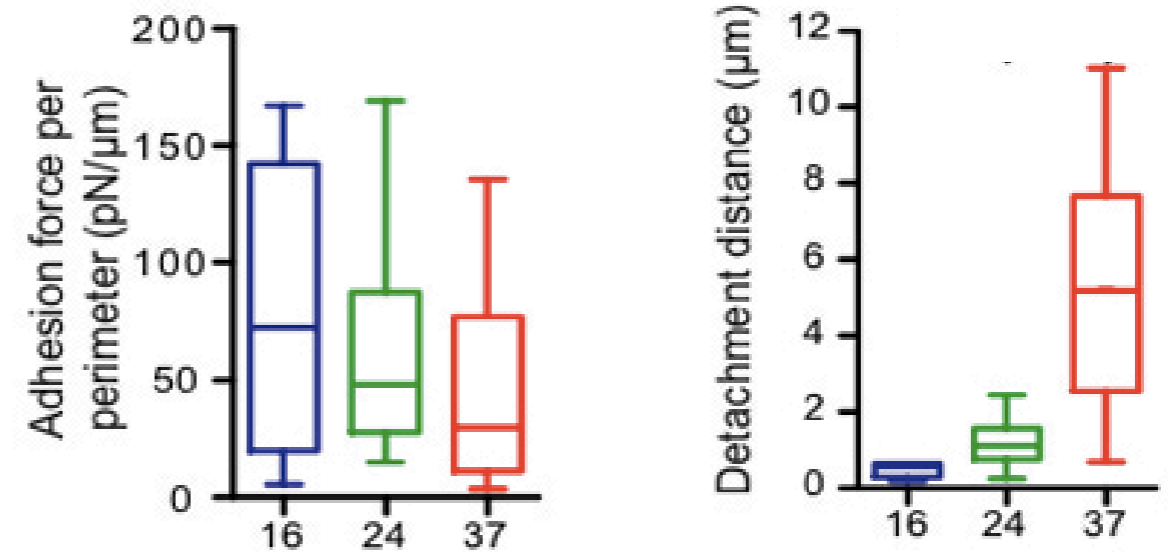
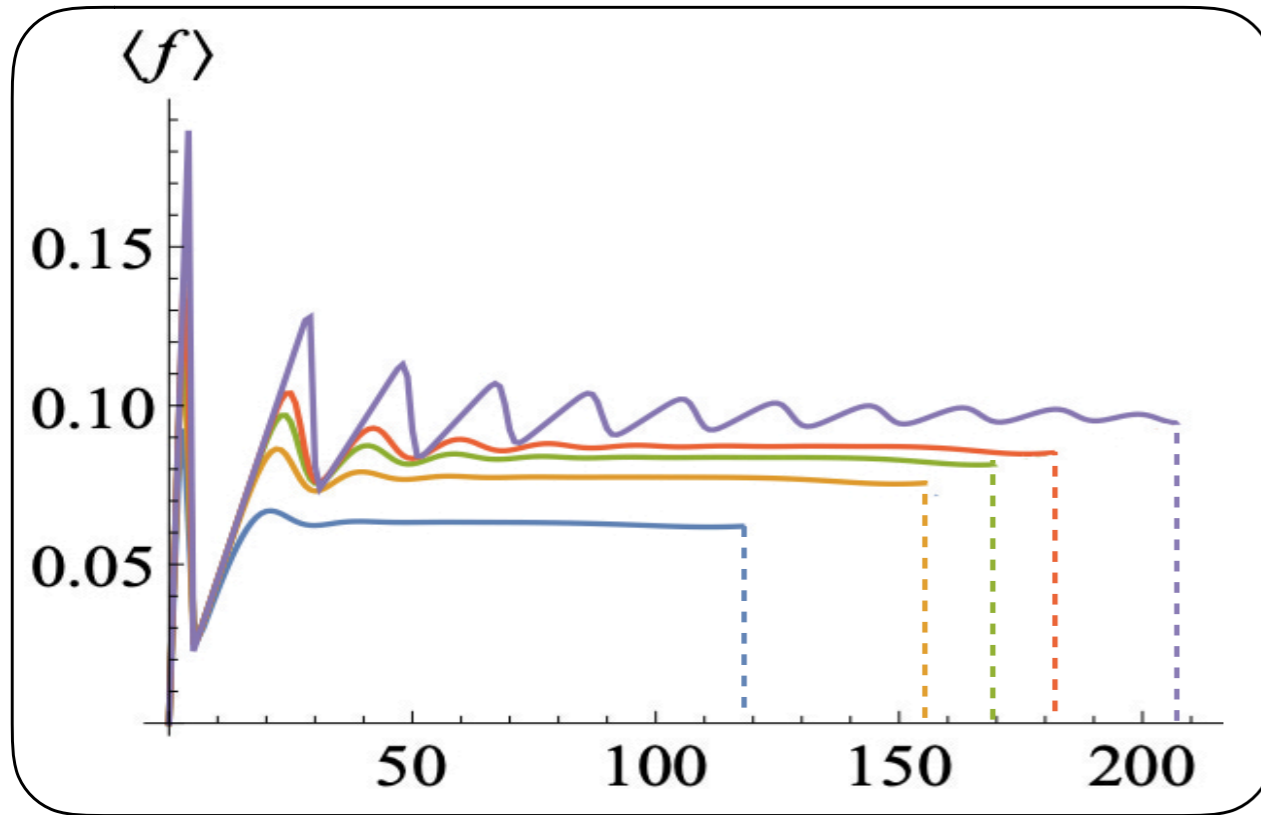
Average Force vs δ

$$\langle f \rangle = \delta \frac{\sum_{\chi} \xi \left(1 - \xi \frac{a_l a_r}{s} \right) \Gamma_{\chi}(\tilde{\beta}, \delta)}{\sum_{\chi} \Gamma_{\chi}(\tilde{\beta}, \delta)}$$

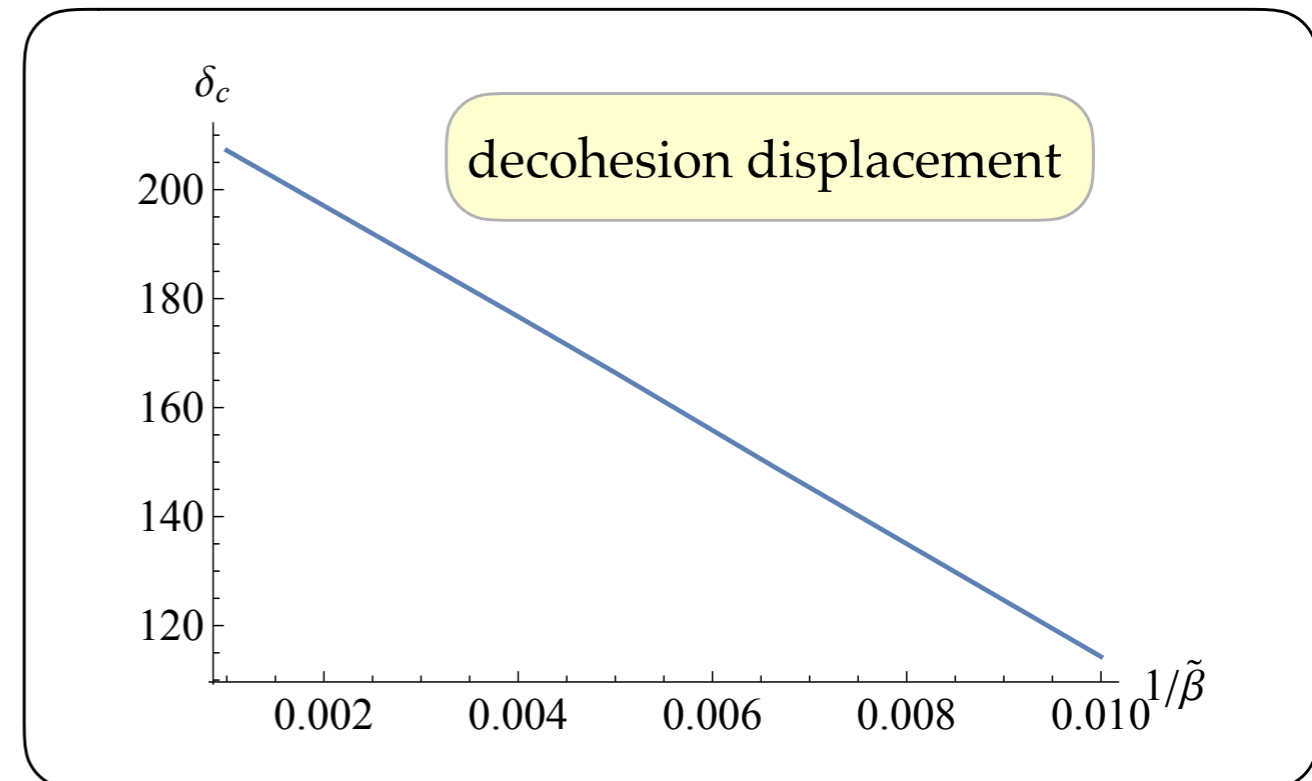
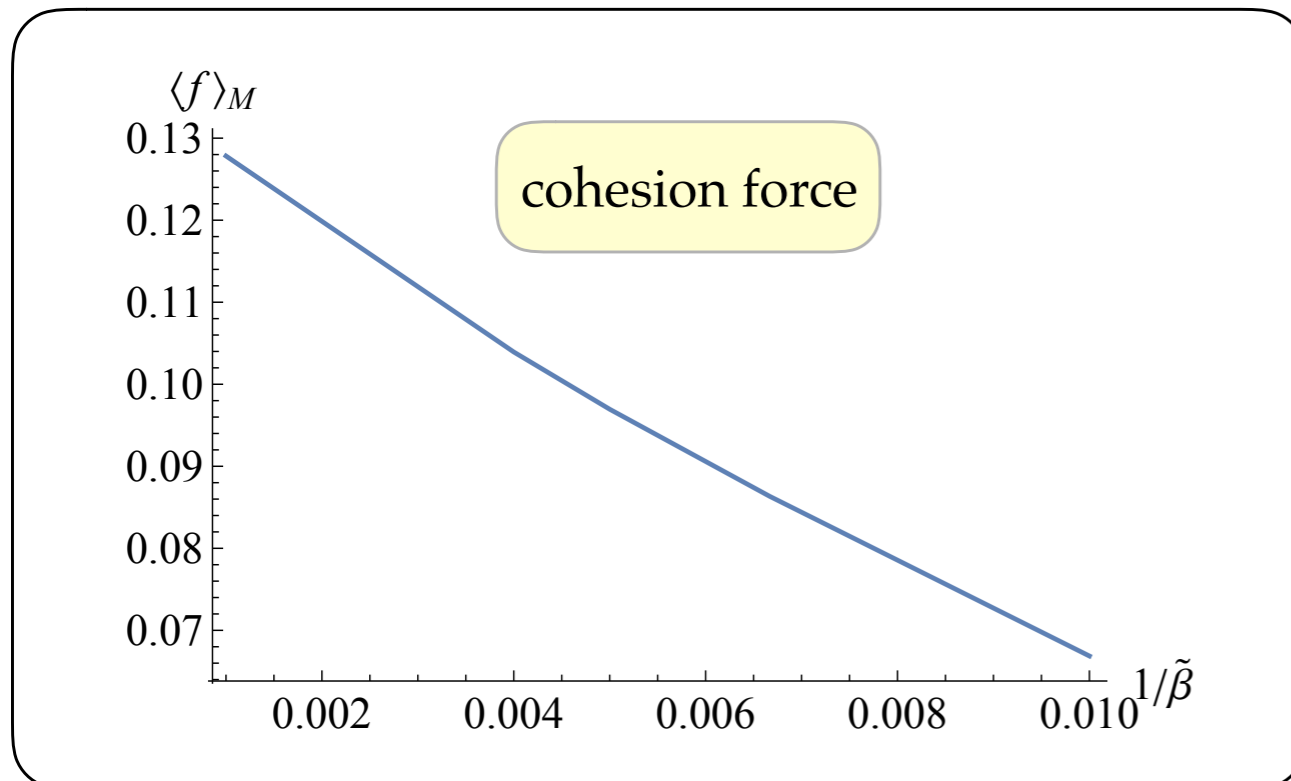
Temperature effects



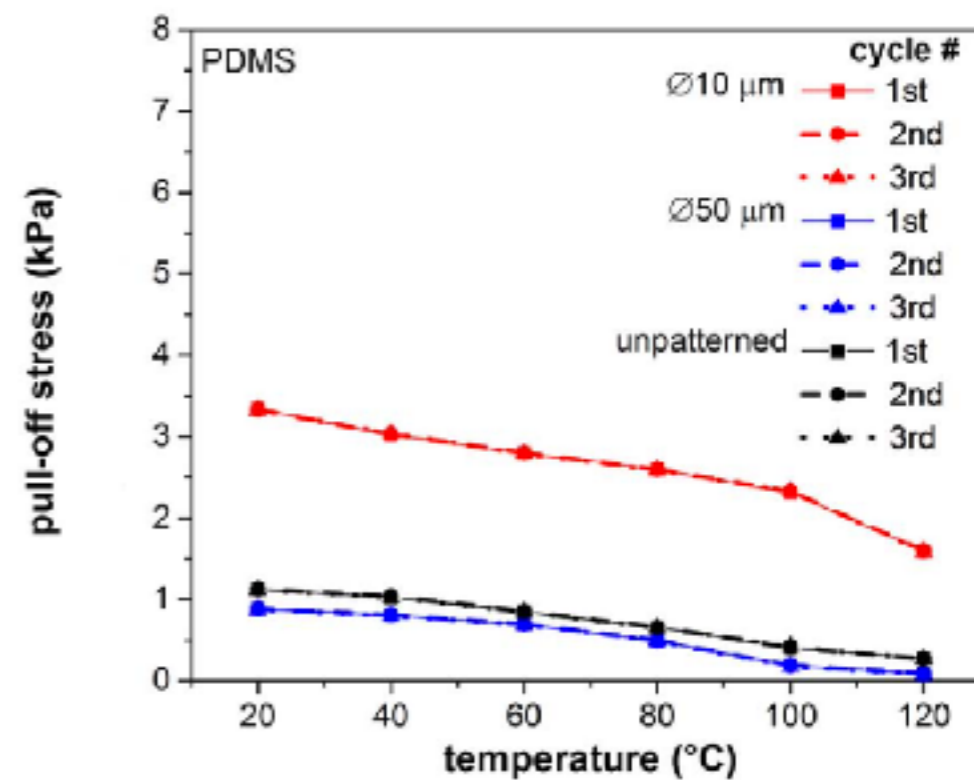
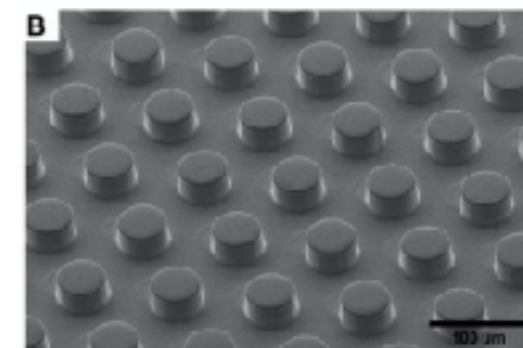
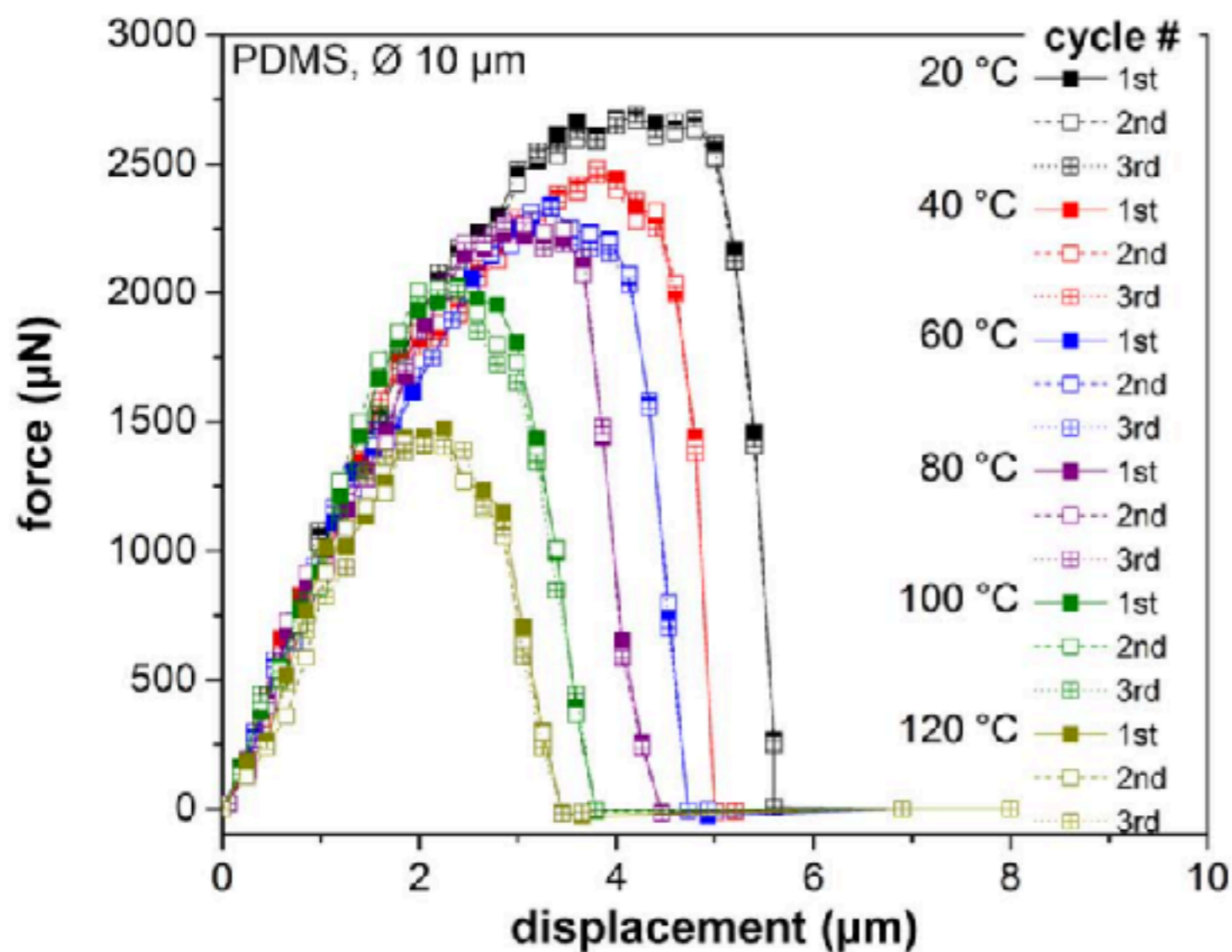
Temperature effects



Felix Rico, *et al.*. Temperature Modulation of Integrin-Mediated Cell Adhesion. *Bioph. J.* **99** 2010 1387–1396



temperature effects



V. Barreau, D. Yua, R. Hensel, E. Arzta, Elevated temperature adhesion of bioinspired polymeric micropatterns to glass. *J. Mechanical Behav. Biomedical Materials*, 76 (2017) 110–118

Extensions / on going works



- rate effects
- DNA denaturation
- multiscale modeling, cerebral damage
- multiwells energy: partial unfolding, dislocations, phase transitions
- non local interactions
- ...

Thank you for your attentions
