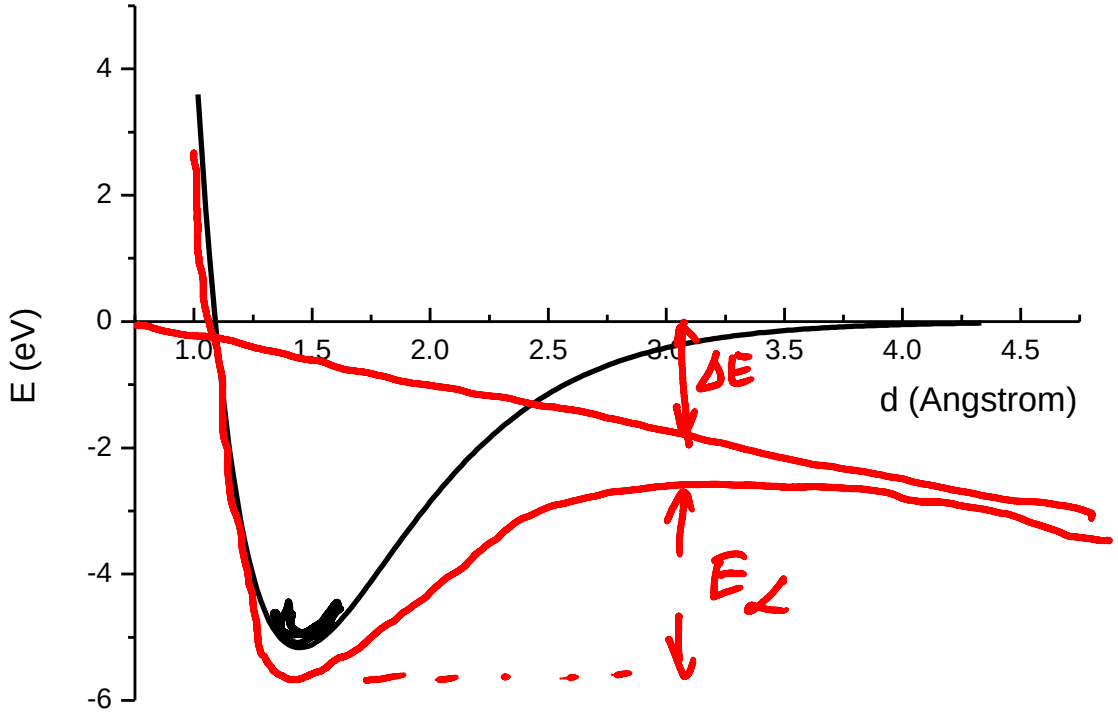
Chapter 01
Atomic interactions and forces

Potential and applied force



$$\Delta E = -\int F\,dx$$

$$= -F \cdot x$$

constant force

metastable state

Off-rate

$$k_{off} = k_0 \exp\left(-\frac{E_\lambda}{kT}\right) = k_0 \exp\left(\frac{-E_B + \Delta E}{kT}\right)$$

Shift of equilibrium position

$$E(r) = E_B + \frac{1}{2}\left.\frac{d^2E}{dr^2}\right|_{r_0}(r-r_0)^2 - F_{ext}\cdot r$$

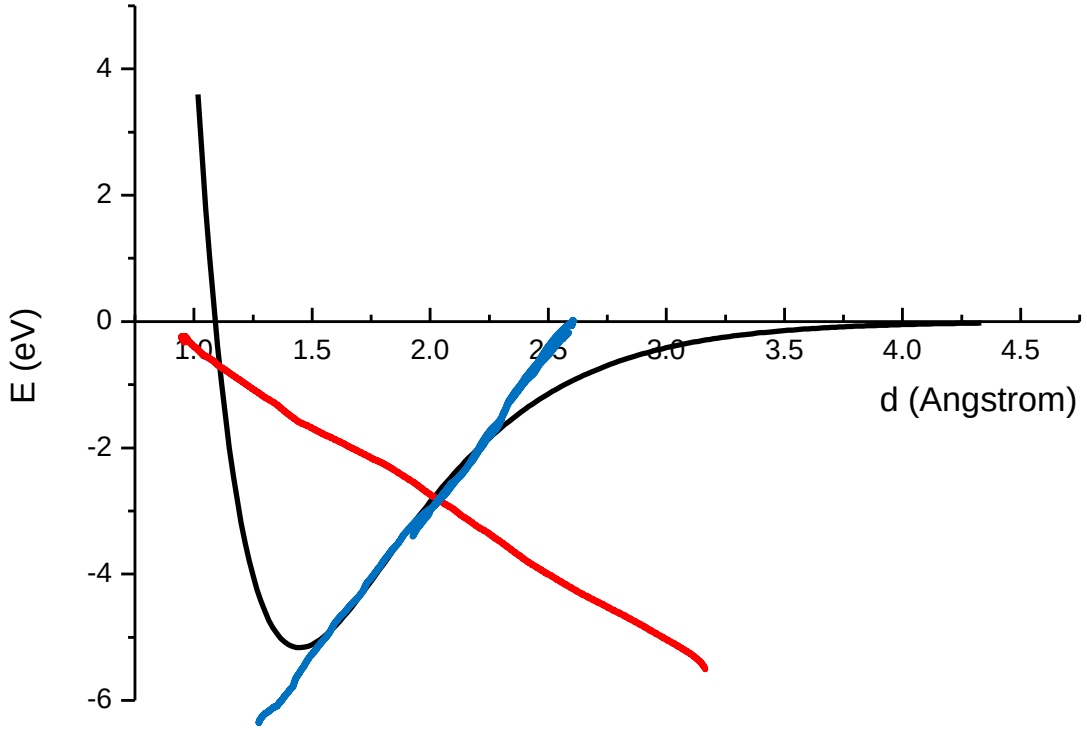
$$\frac{dE}{dr} = 0 \quad \Rightarrow \quad \left.\frac{d^2E}{dr^2}\right|_{r_0}(r-r_0) - F_{ext} = 0$$

$$r = r_0 + \frac{F_{ext}}{\left.\frac{d^2E}{dr^2}\right|_{r_0}} = r_0 + \frac{F_{ext}}{k}$$

Atomic spring with spring constant

$$k = \left.\frac{d^2E}{dr^2}\right|_{r_0}$$

Rupture force



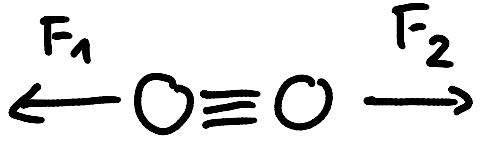
$$F_{rupture} = \frac{6\,eV}{1.3\,Å}$$

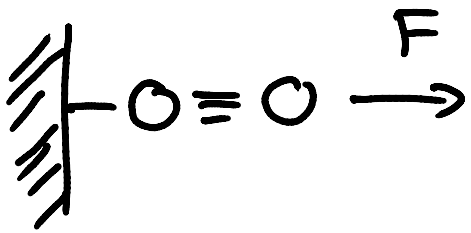
$$= \frac{6\,eV \cdot 1{,}6 \times 10^{-19}\,J}{1.3 \times 10^{-10}\,m}$$

$$= 7.39 \times 10^{-9}\,\frac{J}{m}$$

$$= 7.39\,nN$$

Force pair vs. anchored molecule



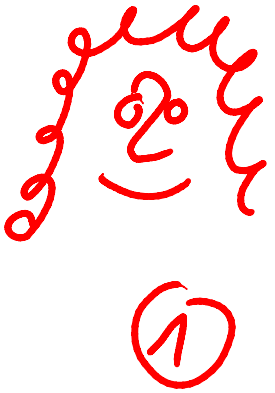


$F_1 = -F_2$

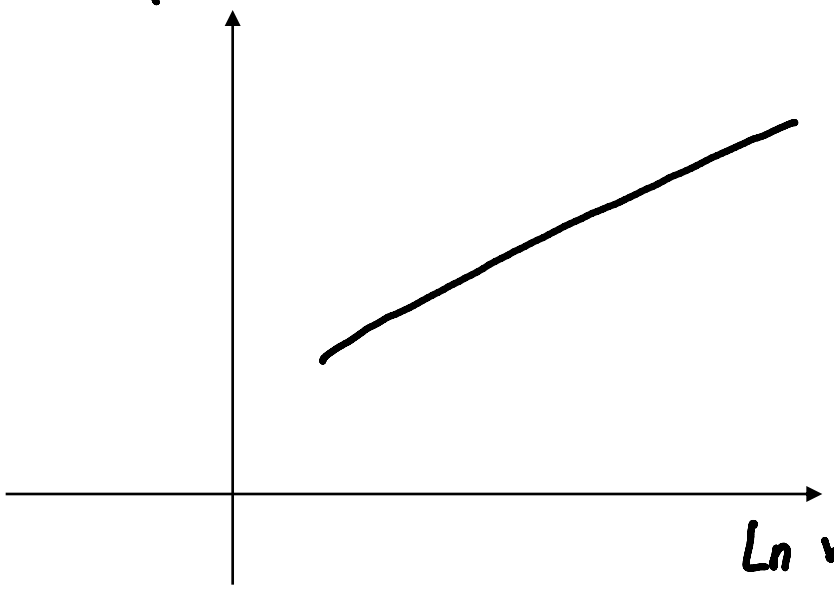
For the same experiment:

$F = \frac{1}{2} F_2$? $F = F_2$? $F = 2F_2$?

$F = F_2$



Rate dependence of rupture force



$$F^* = F_\beta \cdot \ln\left(\frac{t_o}{F_\beta} \cdot r\right)$$

$$F_\beta = \frac{kT}{\Delta x}$$

Δx activation length

Book
"Nanobiomechanics"

$$F^* = \frac{kT}{\Delta x} \ln r + \frac{kT}{\Delta x}\left(\ln t_o - \ln F_\beta\right)$$

Off-rate under applied force

$$k_0 = A \exp\left(-\frac{E}{k_B T}\right) = \frac{1}{t_0}$$

How does E decrease, when we apply a force F.
Linear, to 1st order

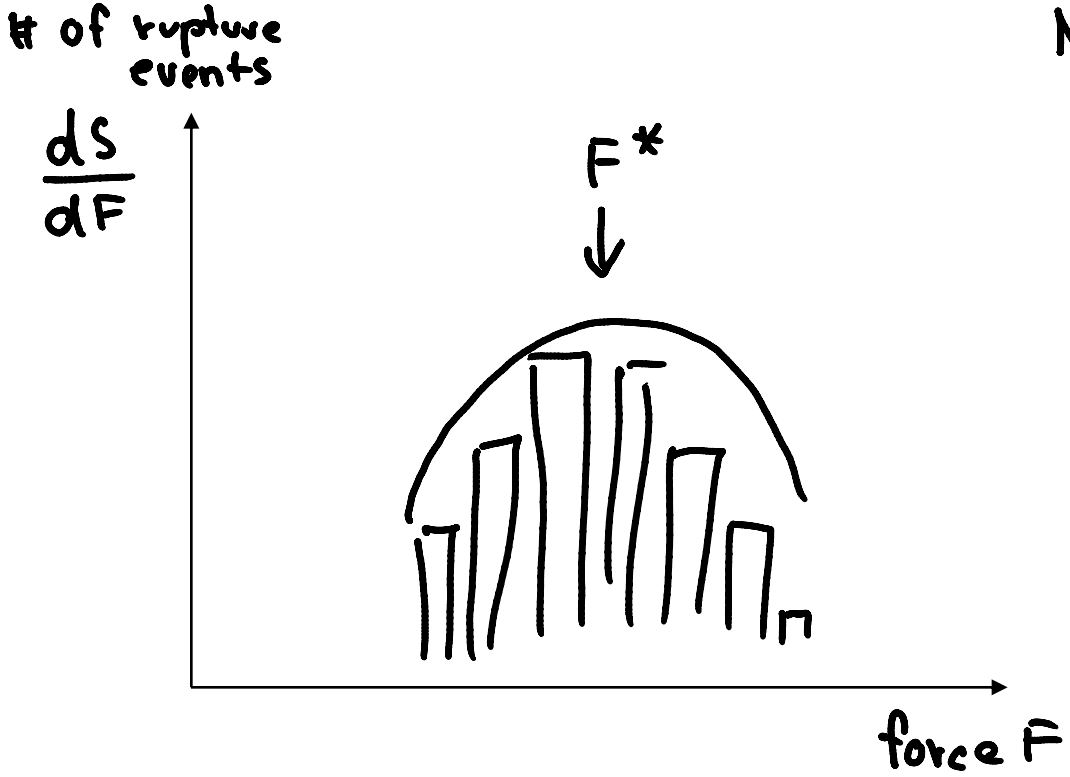
$$F_\beta = \frac{kT}{\Delta x}$$

$$k_D = A \exp\left(-\frac{E - F \cdot \Delta x}{kT}\right)$$

$$= A \exp\left(-\frac{E}{kT}\right) \exp\left(F \frac{\Delta x}{kT}\right) = k_0 \exp\left(\frac{F}{F_\beta}\right)$$

Number of breaking bonds – histogram presentation

Histogram analysis of repeated experiments



Number of remaining bonds

$S(t)$

$$\frac{dS}{dt} = -k_D S(t)$$

$$S(t) = S(0)\, e^{-k_D \cdot t}$$

Determine F^* (mean force)

as $\left.\frac{d^2S}{dF^2}\right|_{F^*} = 0$

Evans' formula

$$\frac{dS}{dt} = \frac{dS}{dF} \cdot \frac{dF}{dt} = \frac{dS}{dF} \cdot r = -k_D S \qquad \frac{dS}{dF} = -\frac{k_D}{r} \cdot S$$

$$\frac{d^2S}{dF^2} = -\frac{1}{r}\left(\frac{dk_D}{dF} \cdot S + k_D \frac{dS}{dF}\right) \overset{!}{=} 0 \qquad \frac{dk_D}{dF} = \frac{d}{dF}\left(A \exp\left(-\frac{E - F \cdot \Delta x}{kT}\right)\right)$$

$$\frac{d^2S}{dF^2} = -\frac{1}{r}\left(\frac{k_D}{F_\beta} \cdot S + k_D\left(-\frac{k_D}{r} \cdot S\right)\right) = 0 \qquad = \frac{\Delta x}{kT} k_D = \frac{k_D}{F_\beta}$$

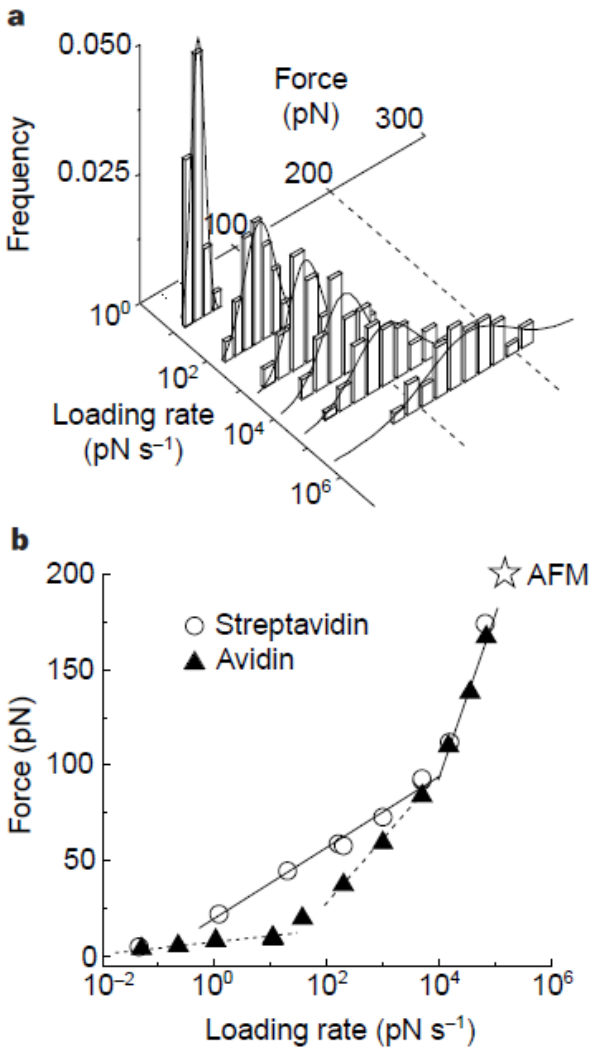
$$\frac{k_D}{F_\beta} - \frac{k_D^2}{r} = 0 \qquad k_D = \frac{r}{F_\beta}$$

$$\frac{1}{t_0} \exp\left(\frac{F^*}{F_\beta}\right) = \frac{r}{F_\beta}$$

$$F^* = F_\beta \ln\left(\frac{t_0}{F_\beta} \cdot r\right)$$

Evans et al. Biophysical Journal 72 (1997) 1541

Evans' results for biotin-streptavidin



Merkel et al. Nature 397 (1999) 50

Eduard-Martin Preis 2017

Gekühlt wird hier per Muskelkraft

Die Universität des Saarlandes verleiht den Eduard-Martin-Preis an zwölf ihrer Doktoranden.

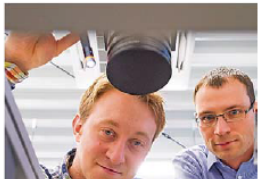
SAARBRÜCKEN (lec) Wie lässt sich ein Kühlschrank oder eine Klimaanlage ohne großen Energieaufwand betreiben? Die überraschende Antwort könnte lauten: mit Muskelkraft. Aber nicht mit menschlicher, sondern mit künstlicher. Die Idee dazu entwickelte der Mechatroniker Marvin Schmidt in seiner Doktorarbeit. Dafür erhält er jetzt als ei von zwölf Doktoranden der Sa Uni aus unterschiedlichen Fa richtung den Eduard-Martin-Pr der Universitätsgesellschaft.

„Wir setzen Formgedächtnis-M terialien ein, sogenannte künstlic Muskeln, um Wärme zu transport ren", erläutert Schmidt sein Kc zept. „Werden diese verformt, n men sie anschließend die alte Fo wieder an. Hierdurch können sie Muskeln an- und entspannen. I bei nehmen sie Wärme auf und

ben sie wieder ab. Das nutzen wir zum Kühlen." Ein ensprechender Prototyp zu Luftkühlung werde gerade gebaut.

Einer anderen Form von künstlichen Muskeln widmet sich die Doktorarbeit der Sportsoziologin Monika Frenger, die ebenfalls einen Eduard-Martin-Preis erhält.

Die weiteren Preisträger sind Alexandra Windsberger (Jura), Hannelore Lisa Fell (Medizin), Madhurima Dhara (Medizin), Petr Kellnhofer (Informatik), Tobias Mai (Mathematik), Johanna Blass (Biochemie), Lina Schiffer (Biochemie), Caroline Schäfer (Betriebswirtschaftslehre), Annemarie Friedrich (Compu-



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Single-molecule force spectroscopy of fast reversible bonds

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In single-molecule force spectroscopy, the unbinding force is often used to quantify the interaction strength of single molecular bonds. We analyze force spectroscopy of fast reversible bonds probed in thermodynamic equilibrium by considering the dynamics of force probe and molecular linker. The effect of cantilever and linker dynamics is systematically addressed by measuring the unbinding force of single cyclodextrin inclusion complexes by atomic force spectroscopy for a variety of molecular linkers and varying force probe stiffness. The unbinding force of individual bonds probed in thermodynamic equilibrium is not unique for the molecular system but scales with $\sqrt{k_{\mathrm{cl}}}$, the square root of the force probe stiffness, and is largely independent of the molecular linker stiffness. The observations are explained by an effective potential resulting from fast linker fluctuations and fast rebinding kinetics which is probed by an AFM cantilever. The slow cantilever dynamics in the kHz range act as mechanical low pass filter, allowing for fast rebinding kinetics of the molecular complex in the order of 10^6 kHz. The binding energy of the complex can be estimated from the unbinding force as a function of cantilever stiffness, however with some uncertainty arising from lack of a model in three dimensions.