UNIVERSITÄT
LEIPZIG

Molecular
BioPhysics

Lecture 7

Soft Matter Physics

Entropy & Free Energy

- Reaction rates and rate laws
- Kinetics of reaction processes
- Transition state model of reaction processes

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Actin filament polymerization as dynamic process

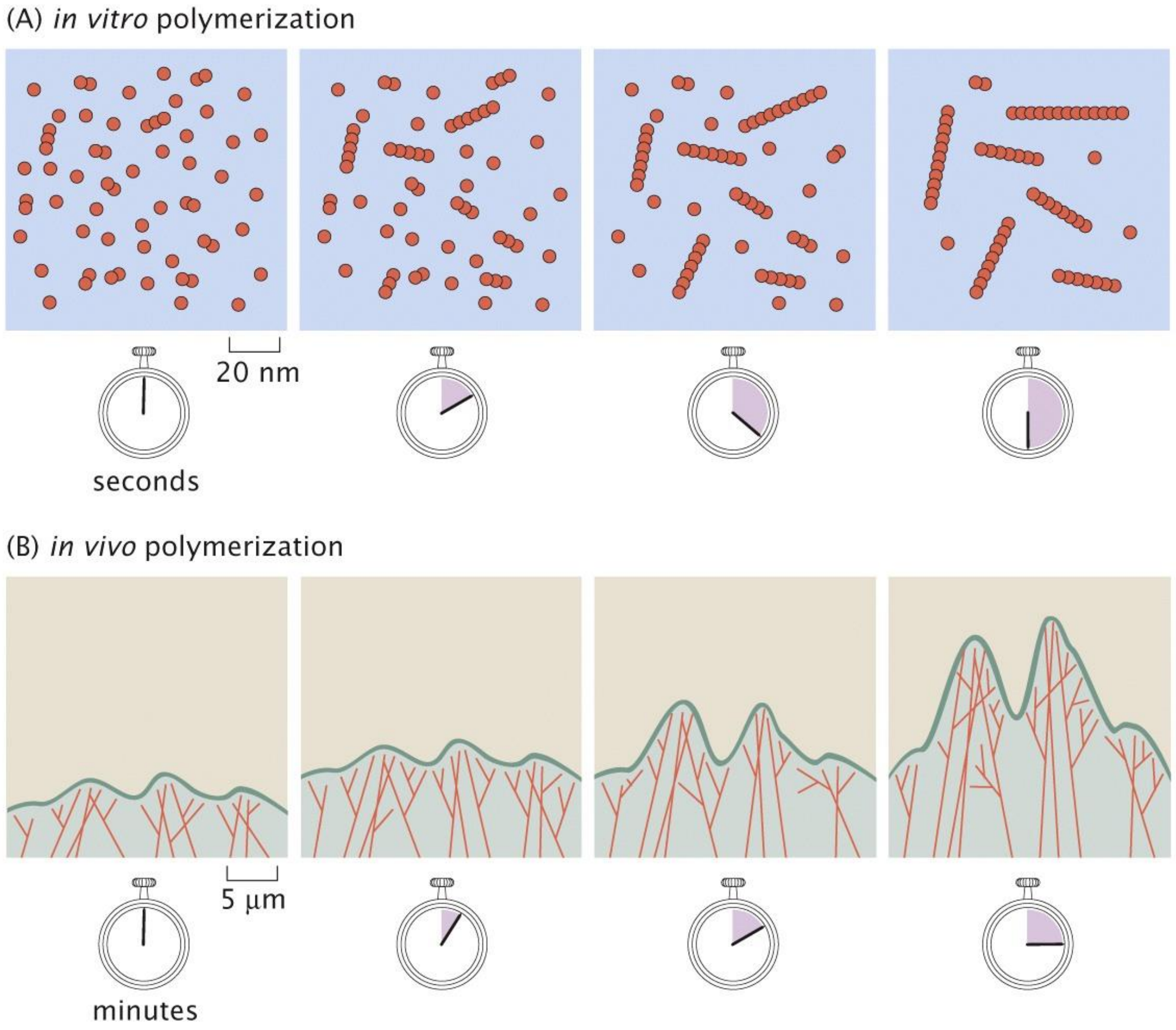


Figure 15.1 Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Hijacking actin polymerization: Listeria

Listeria movement in cytoplasmic extract

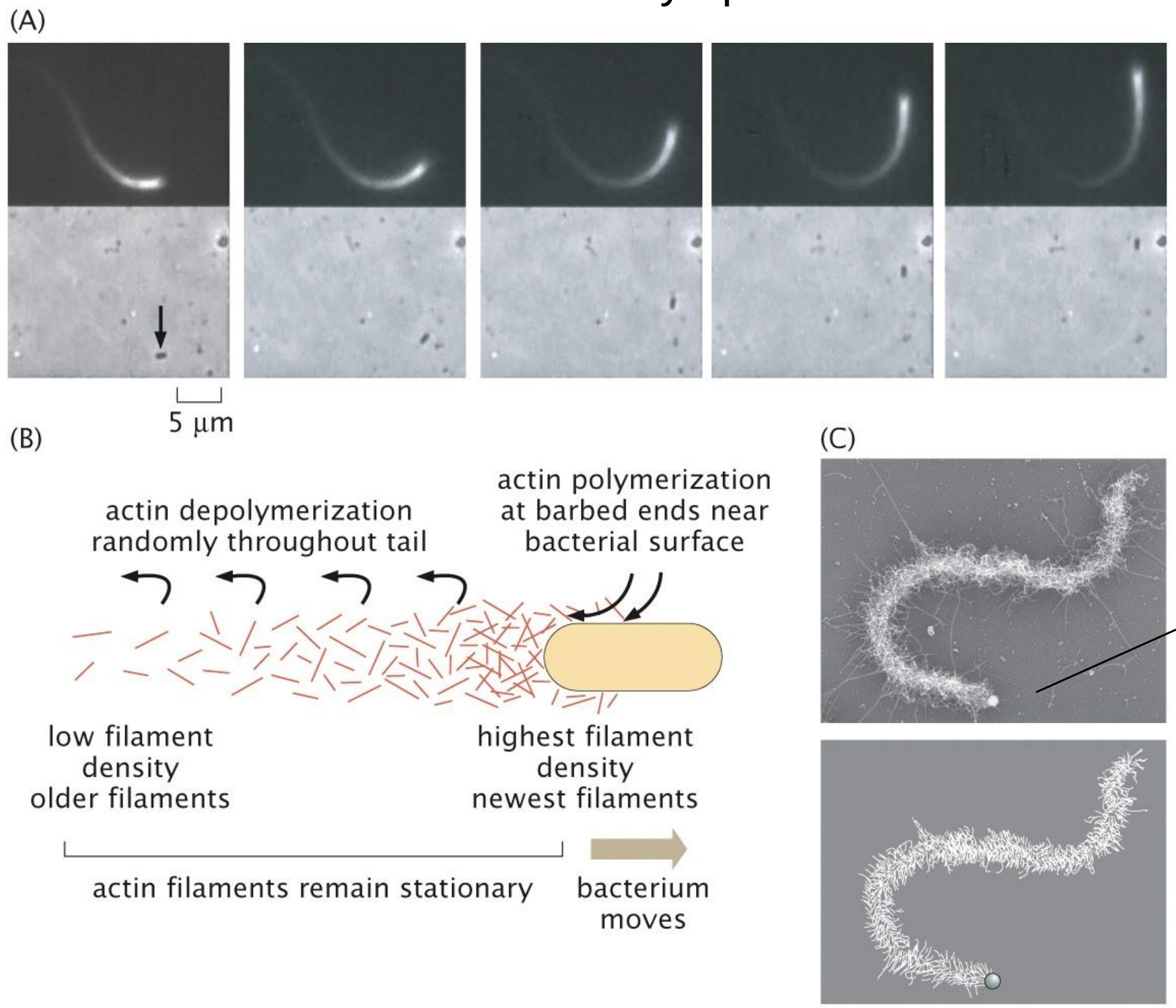


Figure 15.3 Physical Biology of the Cell, 2ed. (© Garland Science 2013)

actin fluorescence

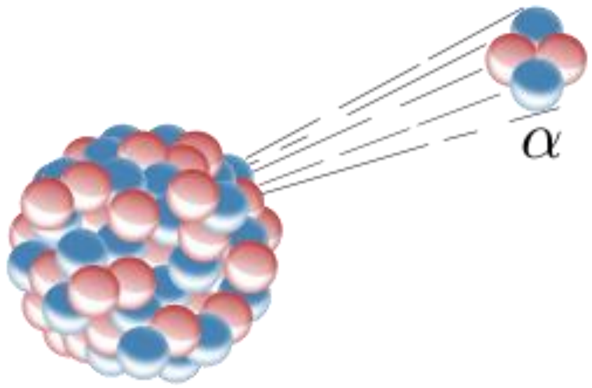
phase contrast

Plastic bead with nucleation protein

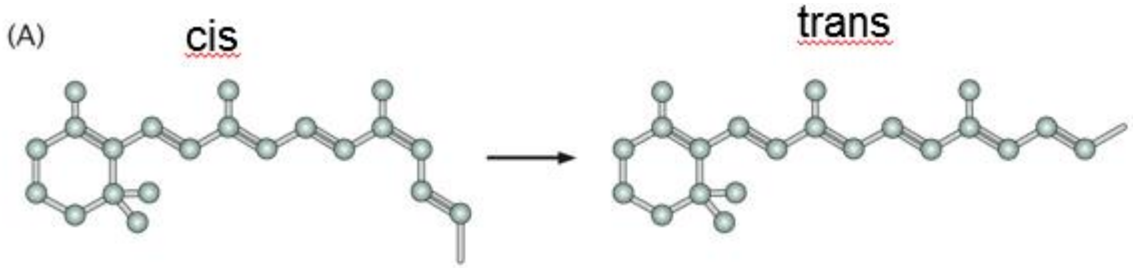
Simple decay reactions

$A \rightarrow B$

Radioactive decay



Molecular isomerization (e.g. after light activation)



Simple decay reaction

Decay of molecular transition:

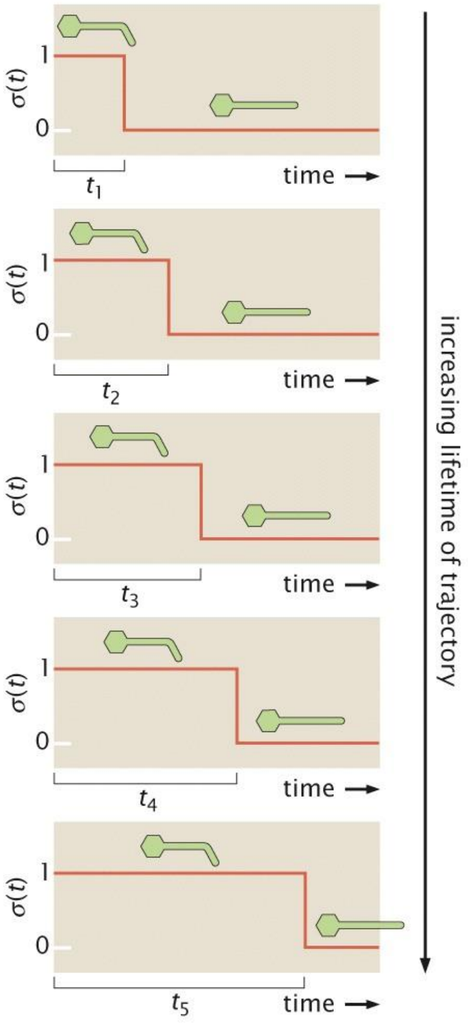
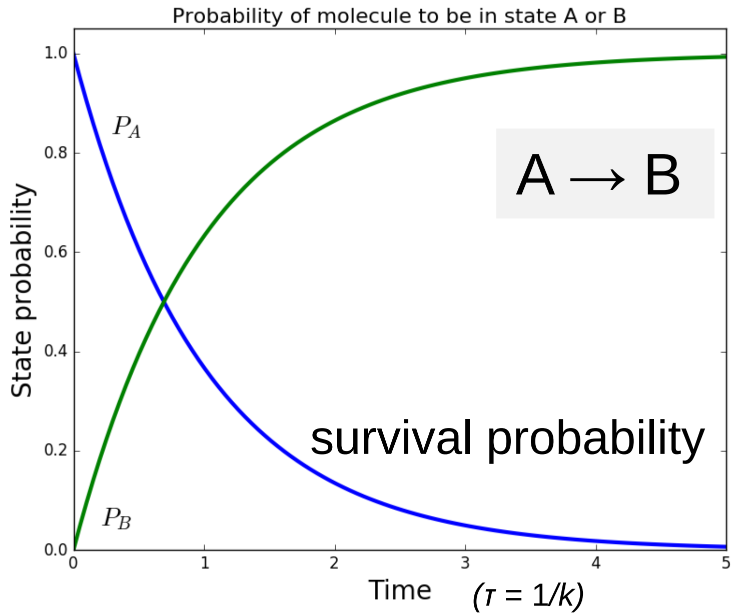
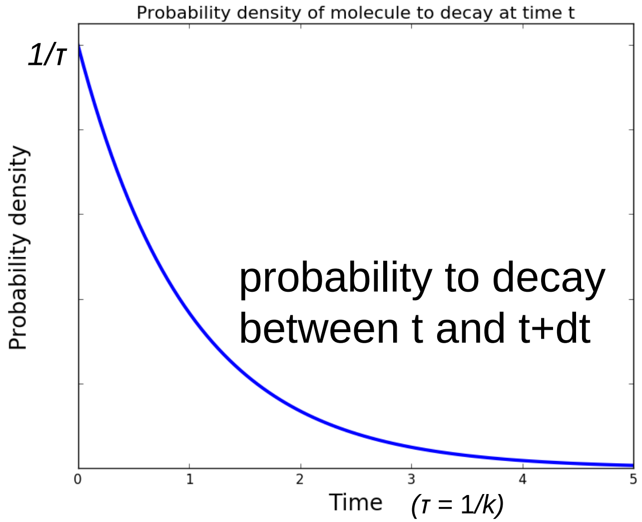


Figure 15.7 Physical Biology of the Cell, 2ed. (© Garland Science 2013)





Simple reversible reaction: Ion channel opening

$$O \underset{k_-}{\overset{k_+}{\rightleftharpoons}} C,$$

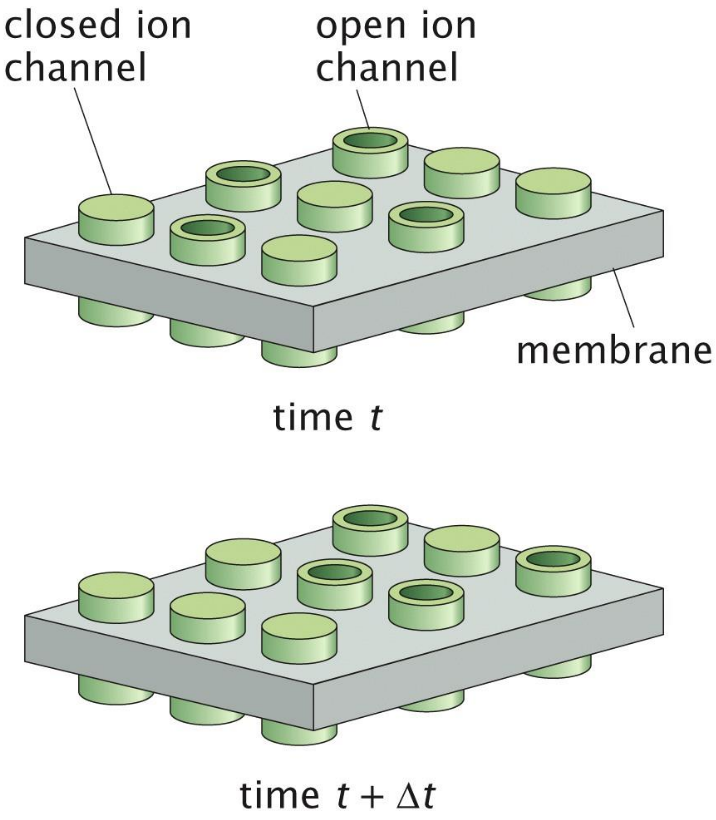
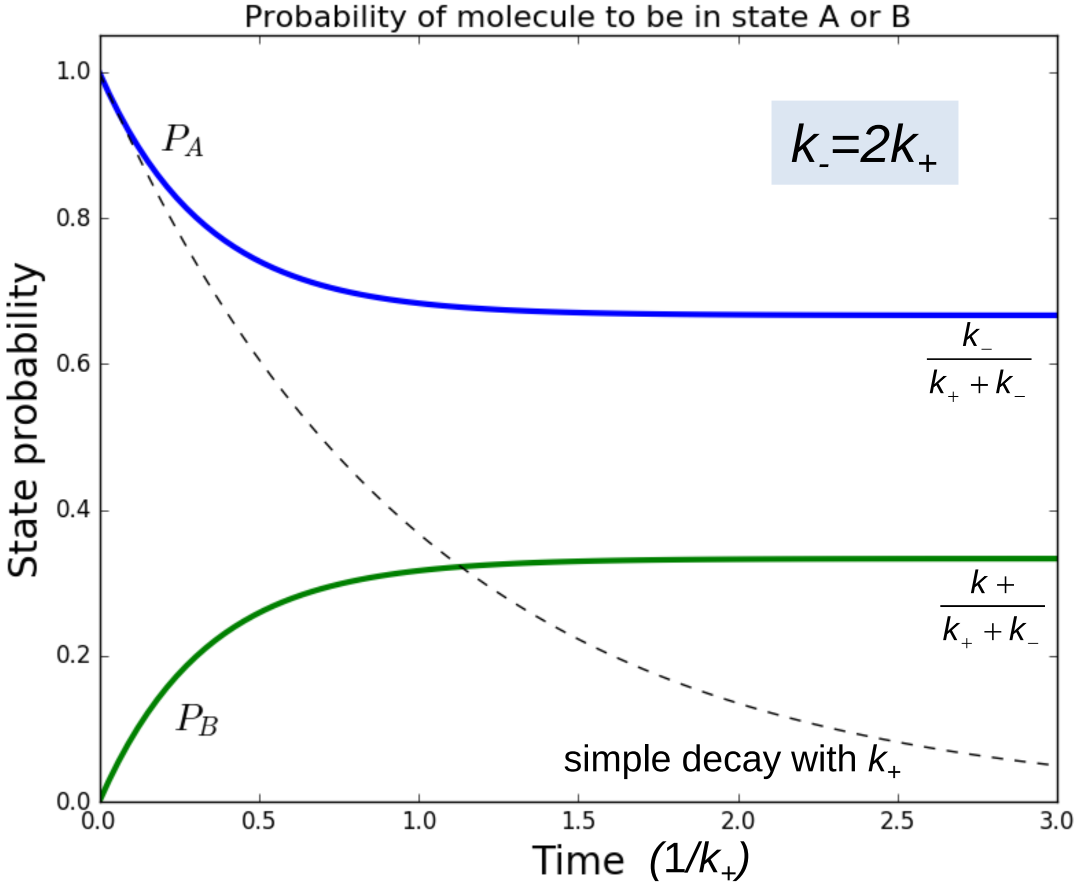
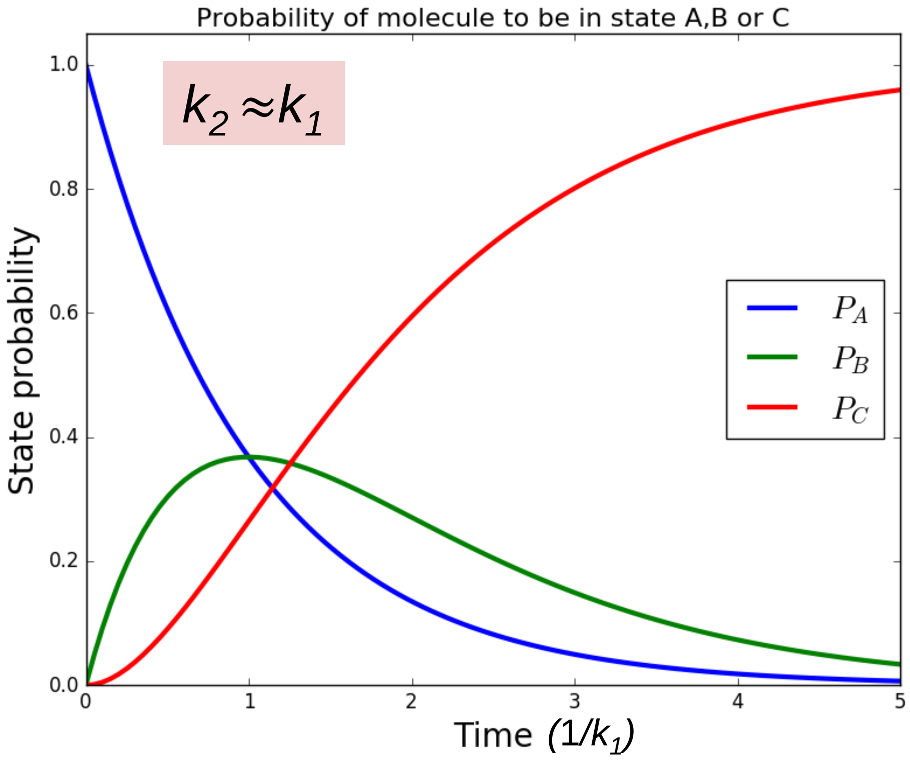


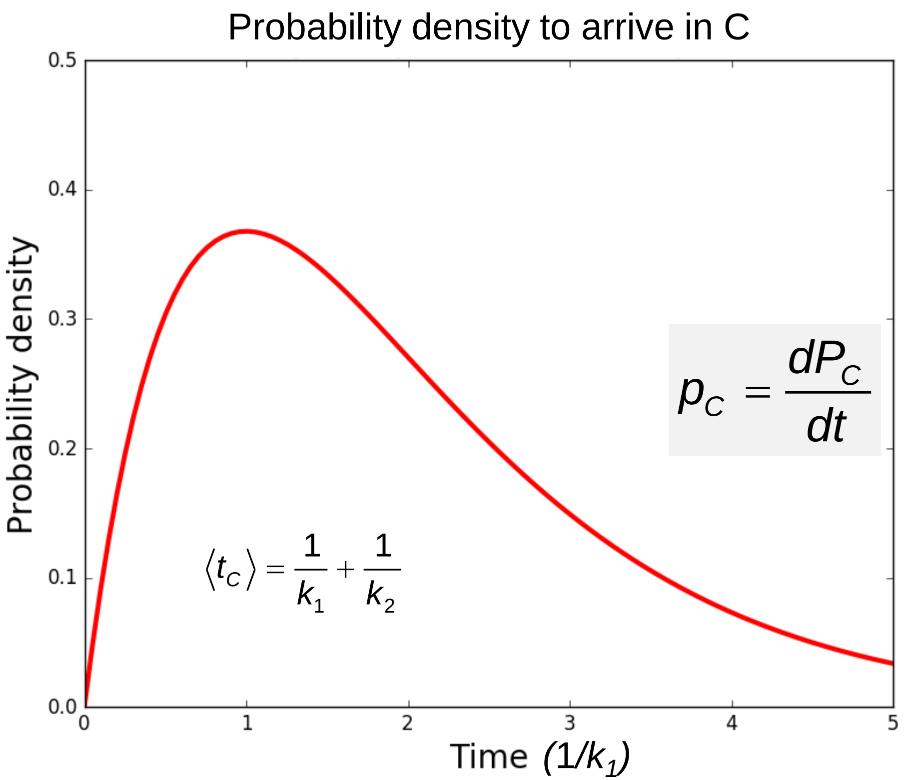
Figure 15.12 Physical Biology of the Cell, 2ed. (© Garland Science 2013)



Two-step reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

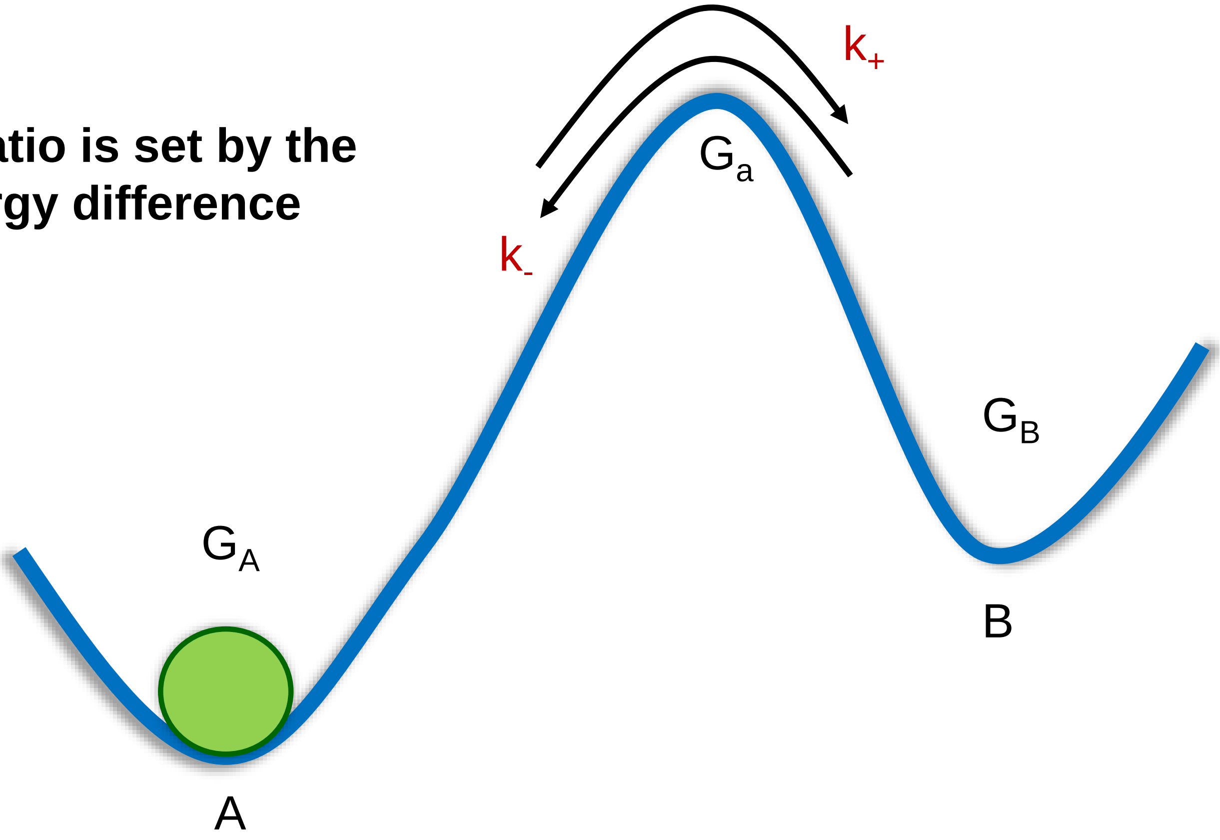




The intermediate state B needs to be filled before C starts to get occupied

Detailed balance: connecting energies & rates

Rate ratio is set by the energy difference



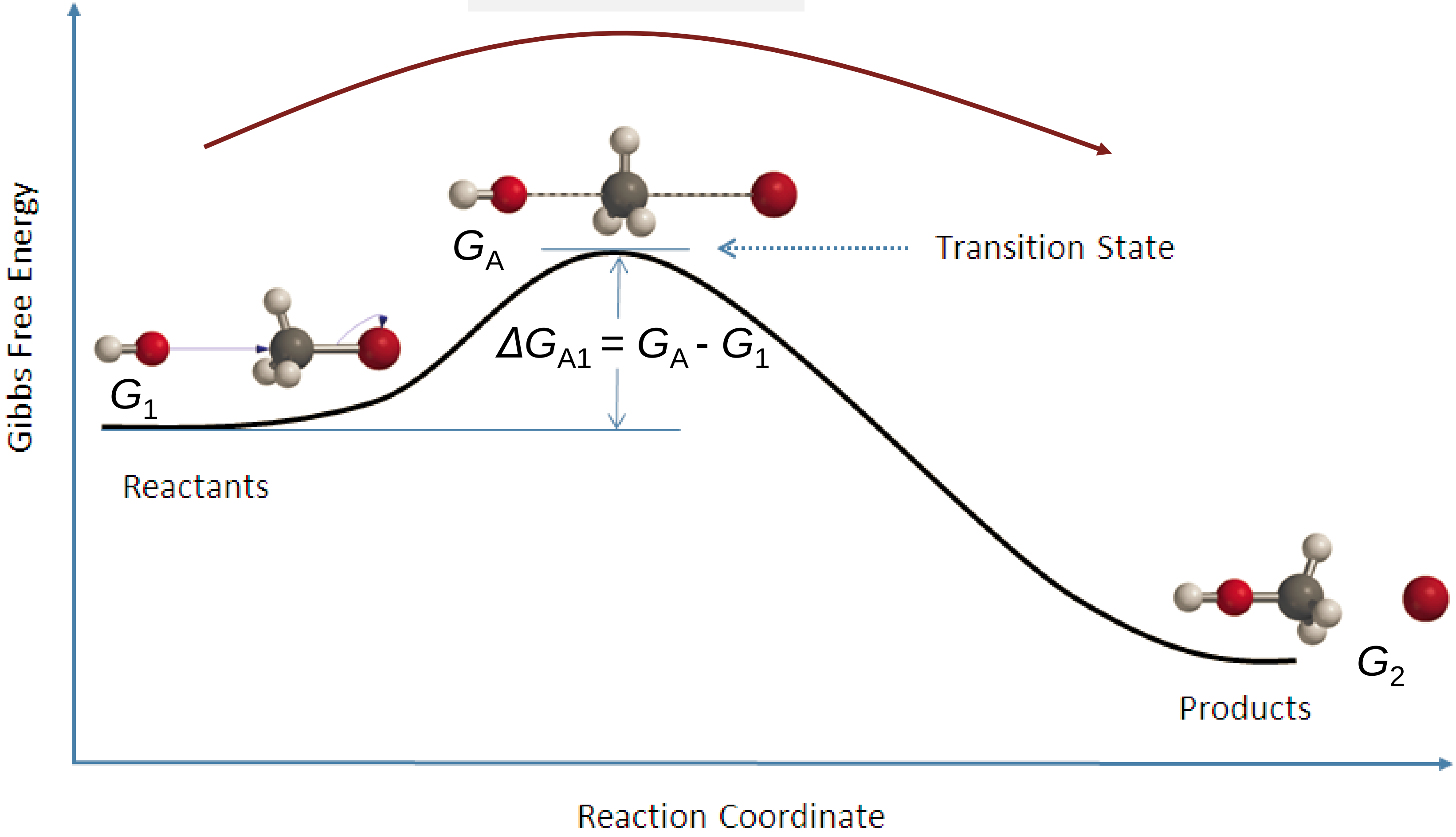
Detailed balance at equilibrium: each elementary process is equilibrated by reverse

$$0 = \frac{dP_B}{dt} = k_+ P_A - k_- P_B$$

$$\Rightarrow \frac{k_+}{k_-} = e^{-\overbrace{(G_B - G_A)}^{\Delta_r G^\circ}/k_B T} = K_{eq}$$

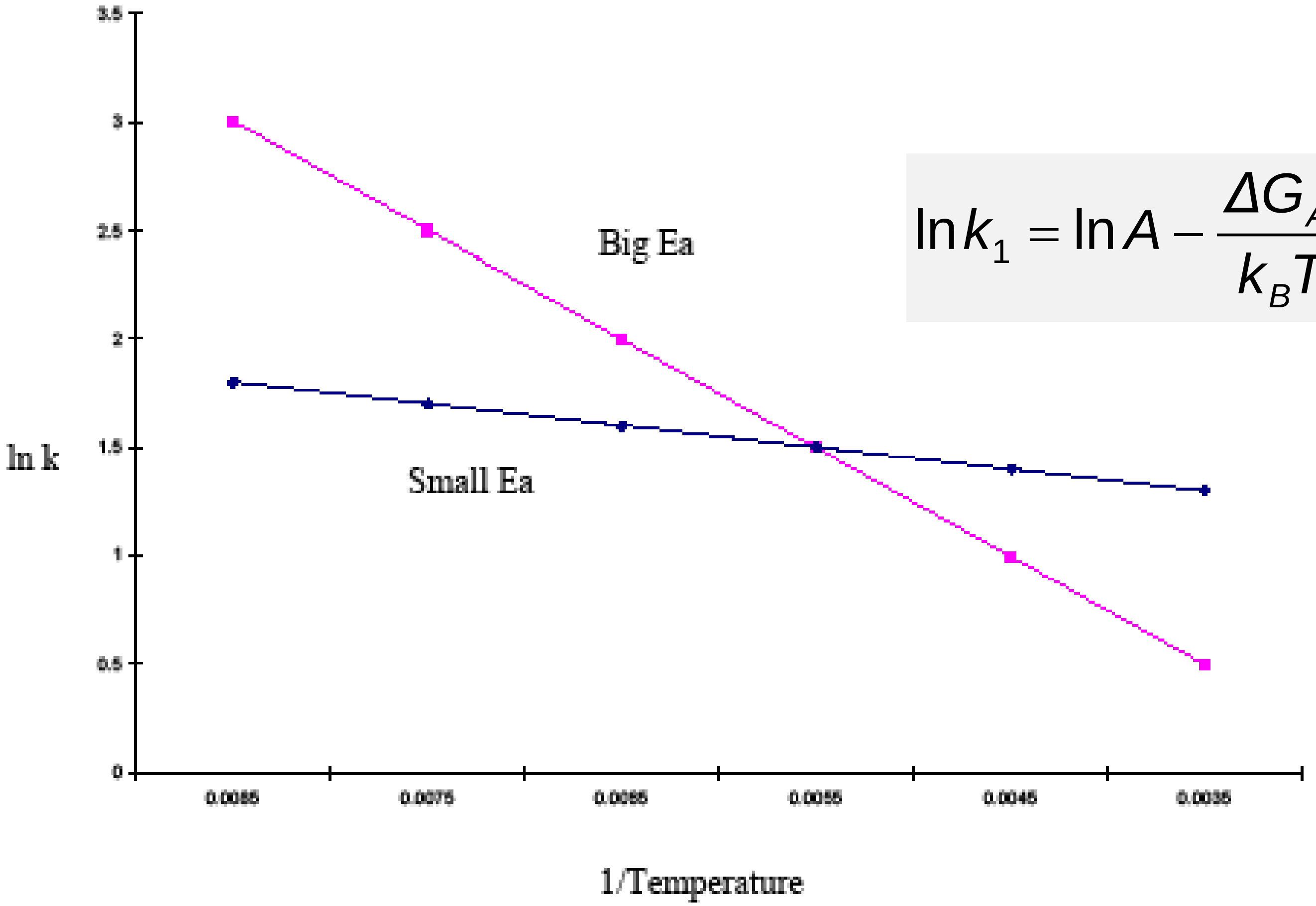
Transition state model

$$k_1 = A \cdot e^{-\Delta G_{A1}/k_B T}$$ **Arrhenius law**



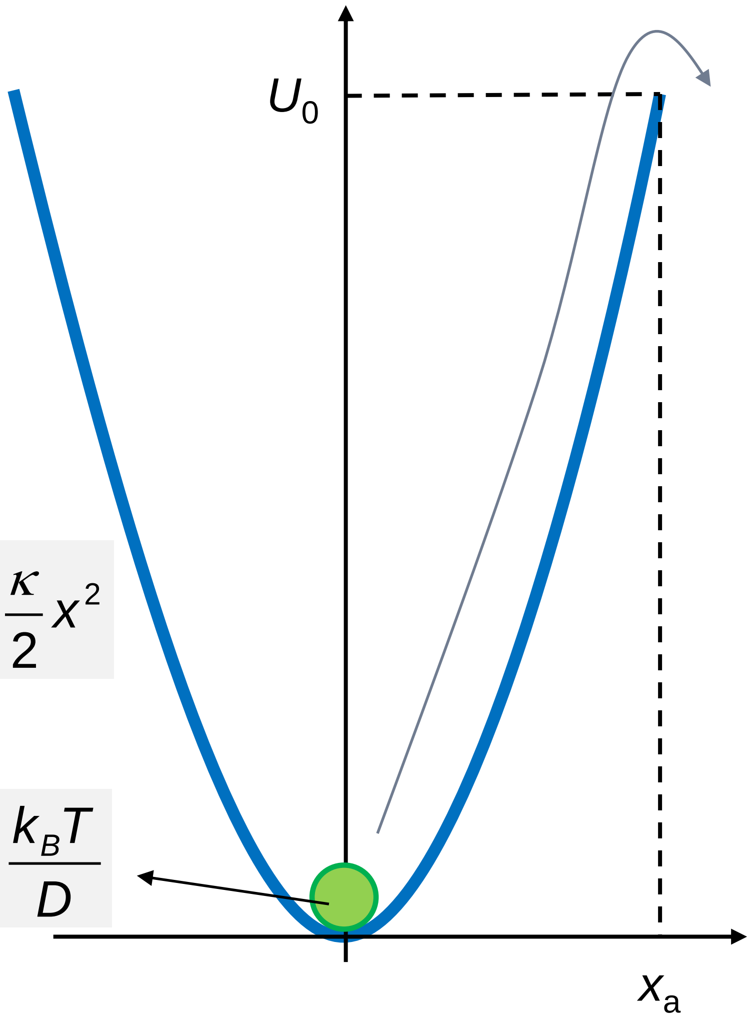
Reaction: $HO^- + CH_3Br \rightarrow [HO\text{---}CH_3\text{---}Br]^{\ddagger} \rightarrow CH_3OH + Br^-$

Arrhenius plot



$$\ln k_1 = \ln A - \frac{\Delta G_{A1}}{k_B T}$$

Kramers rate theory



$$U = \frac{\kappa}{2} x^2$$

$$\gamma = \frac{k_B T}{D}$$

Drag coefficient

Kramers time:
Time to diffuse out of a harmonic potential

$$t_k = \underbrace{\frac{\gamma}{\kappa}}_{\tau} \frac{\sqrt{\pi}}{2} \sqrt{\frac{k_B T}{U_0}} e^{U_0 / k_B T}$$

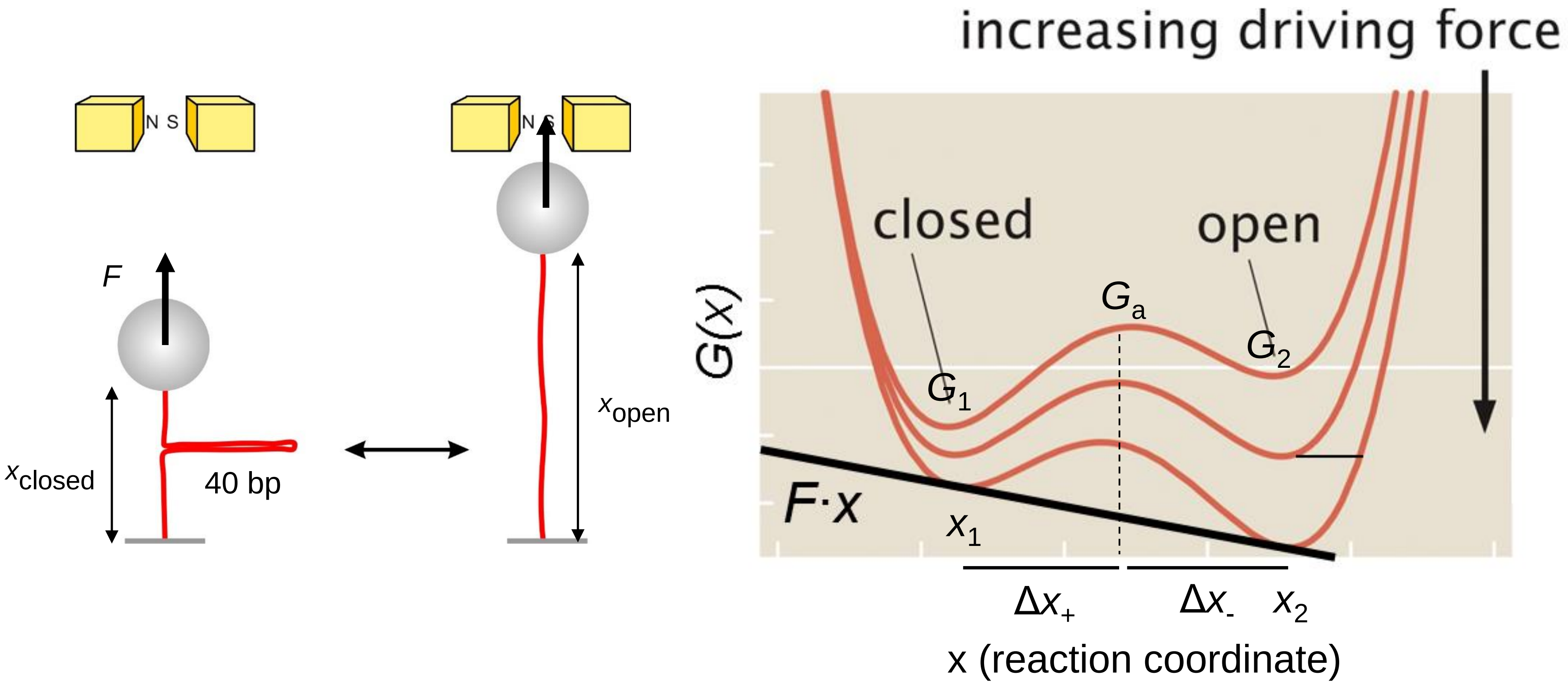
relaxation time of strongly overdamped oscillator

Kramers rate law:
In case of full coupling to solvent

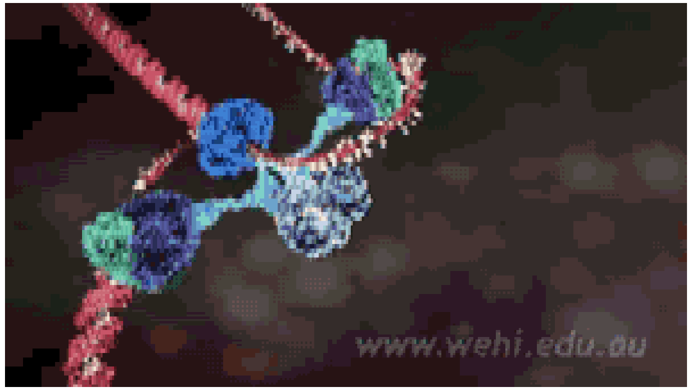
$$k_1 = \frac{\varepsilon_1}{2 t_k} = \frac{\varepsilon_1}{\sqrt{\pi}} \frac{\kappa}{\gamma} \sqrt{\frac{\Delta G_{a1}}{k_B T}} e^{-\Delta G_{a1} / k_B T}$$

Force dependence of reaction rates

For external driving force, e.g. a mechanical force

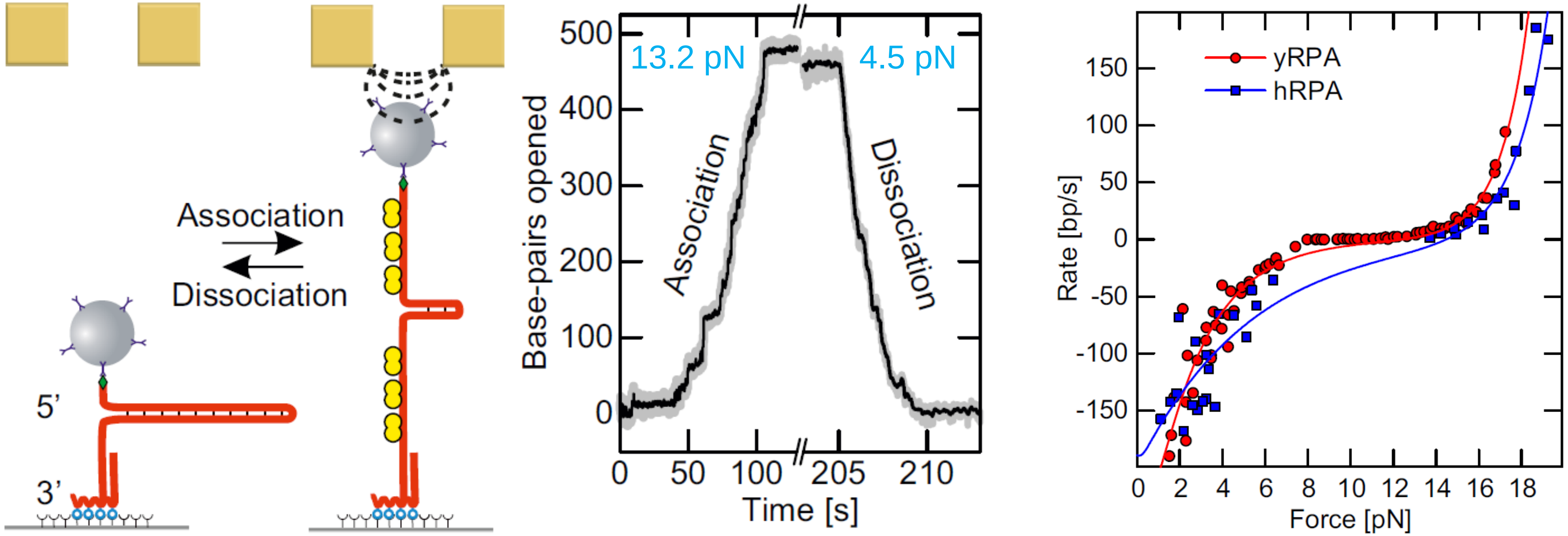


Force-regulated binding of RPA protein at a DNA fork



RPA (replication protein A) binds all single-stranded DNA that is produced in the cell

Monitore binding on a DNA hairpin under force



Kemmerich et al. Nucleic Acids Res. (2016)