Role of organized water in coherence of cellular electrodynamics

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Content

- Oscillator concepts, Q – quality factor, damping
- Bioelectromagnetics problems and protein activity
- Viscoelastic transition of water at interfaces decreases damping
- Small amplitude oscillations – higher Q factor
- Available evidence of molecular resonances (long lifetime vibrations) – coherent dynamics
- *In vivo* microtubule + mitochondria interaction
- Quasicoherent cellular electrodynamic field

Oscillator

$$\ddot{x} + \frac{\omega_0}{Q}\dot{x} + \omega_0^2 x = 0$$

Q - Quality factor

Q > 0.5

underdamped – oscillator "rings"

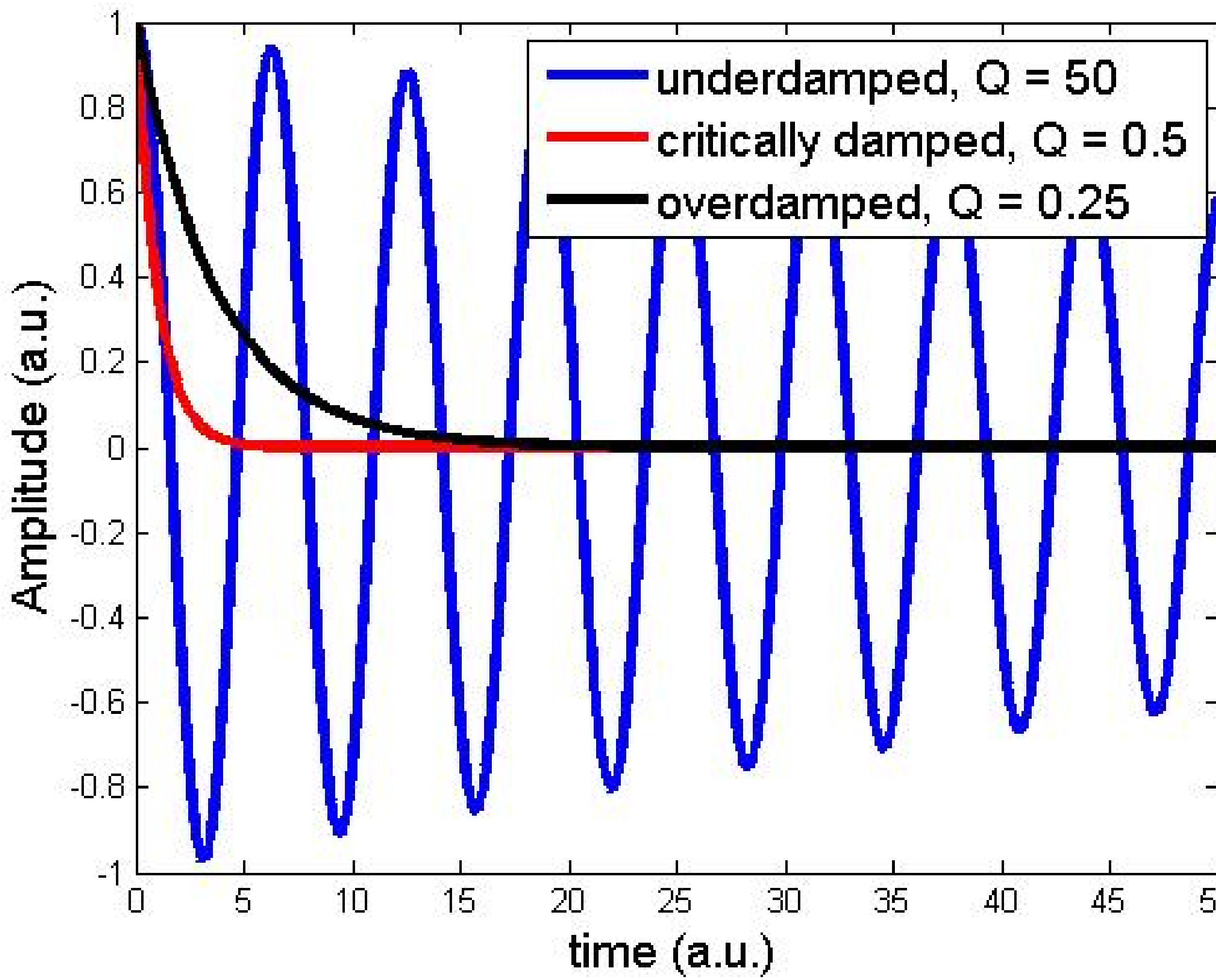
(coherent dynamics)

Q = 0.5

critically damped

Q < 0.5

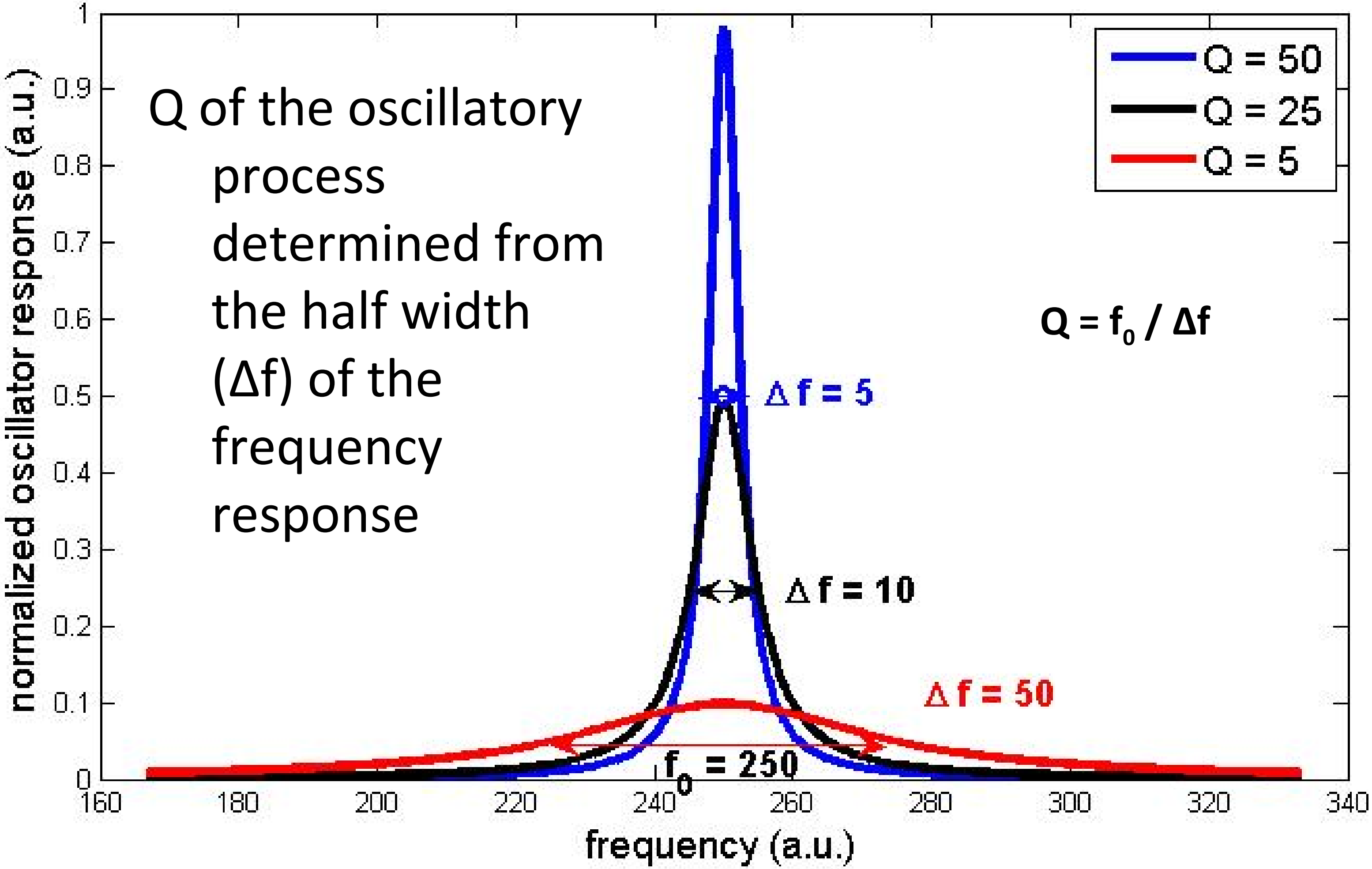
overdamped



Quality factor of the oscillator

$$Q = 2\pi \cdot \frac{\text{Energy stored}}{\text{Power loss}}$$

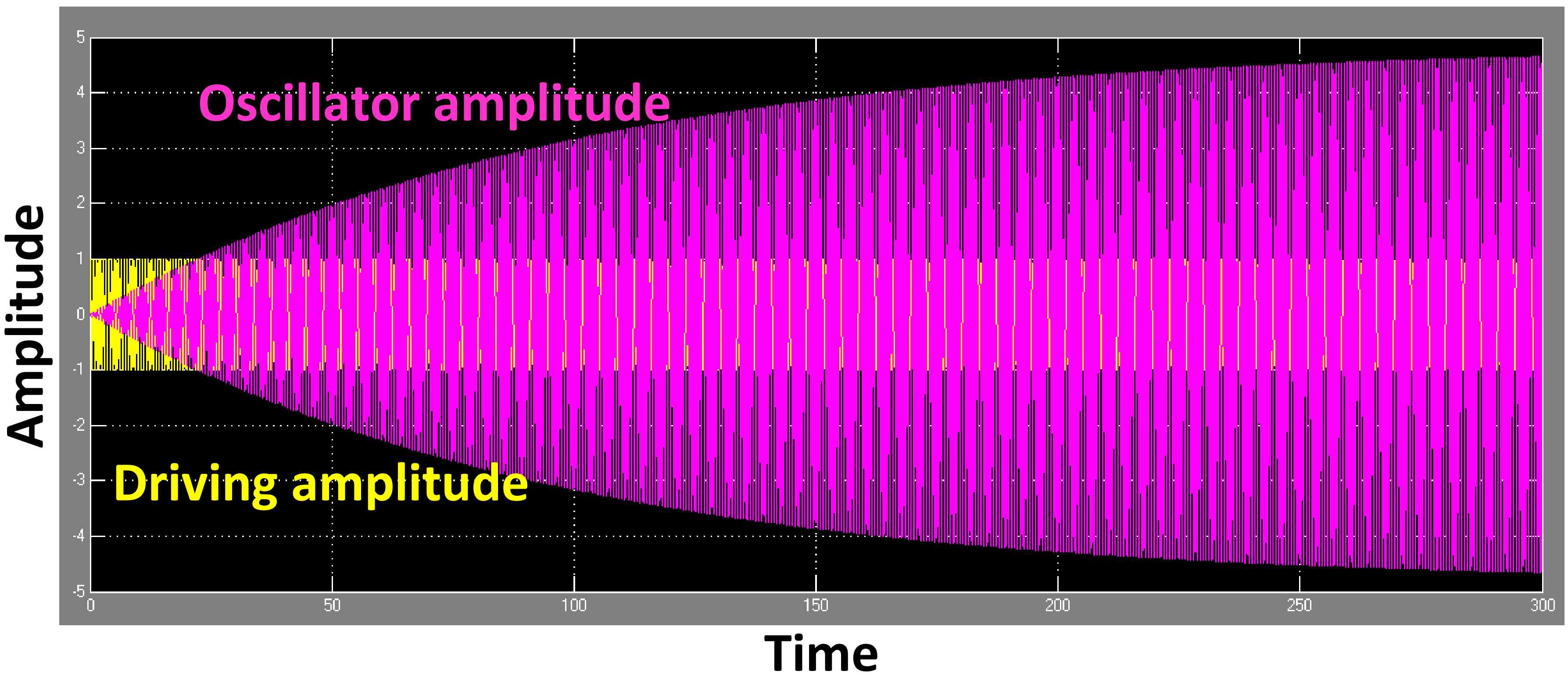
Q of the oscillatory process determined from the half width (Δf) of the frequency response



Quality factor of the oscillator

$$Q = 2\pi \times \frac{\text{Energy stored in oscillator}}{\text{Driving energy per cycle}}$$

High Q enables accumulation of energy



Bioelectromagnetics problems and protein function

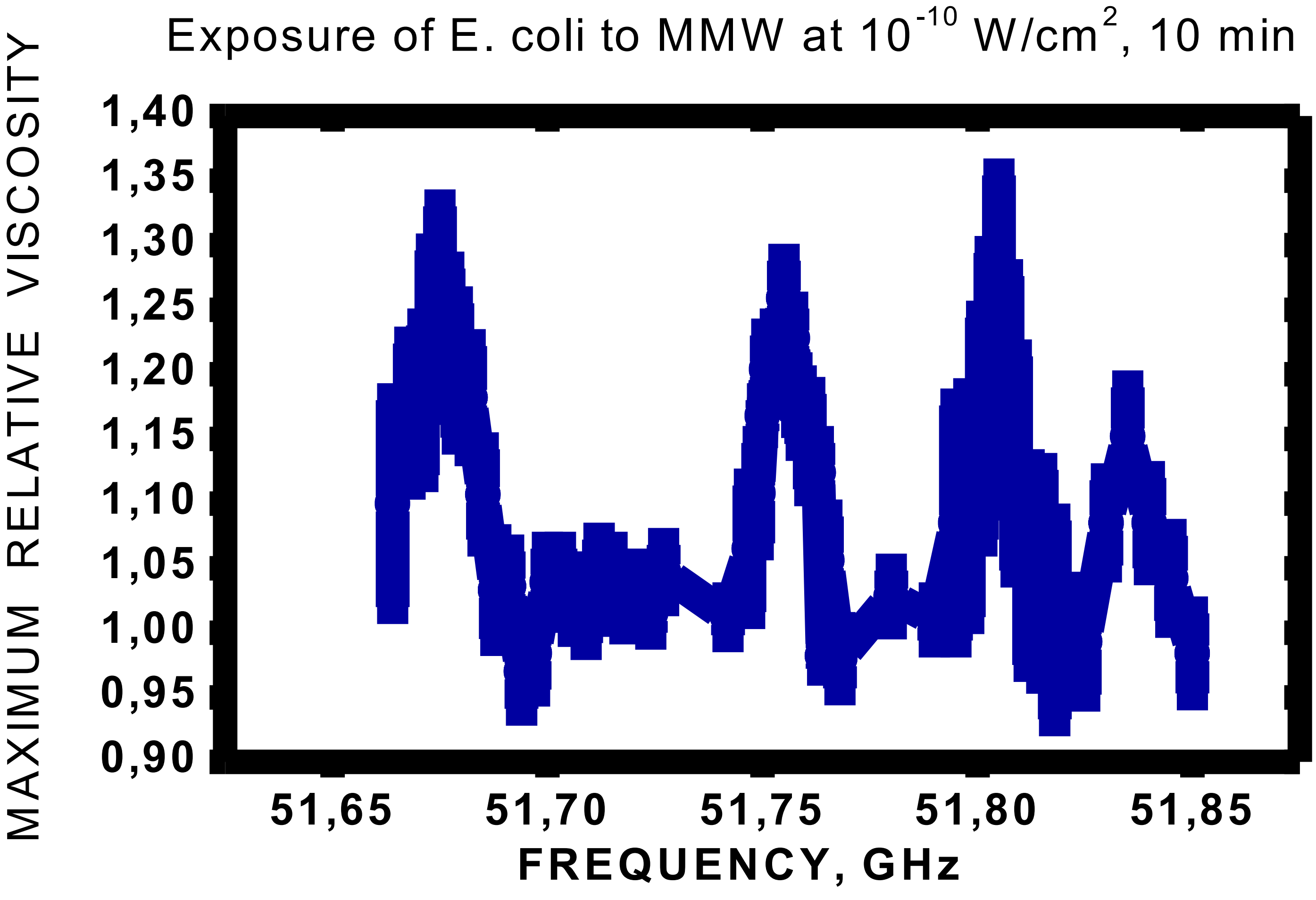
1. Sharp frequency dependent resonance effects of electromagnetic radiation on biological systems

2. Several experimental works suggest that biological systems generate radiofrequency (kHz - GHz) electric oscillations

3. Protein function and reaction kinetics

Bioelectromagnetics problem: Sharp resonant effects

1. Sharp frequency dependent resonance effects on biological systems

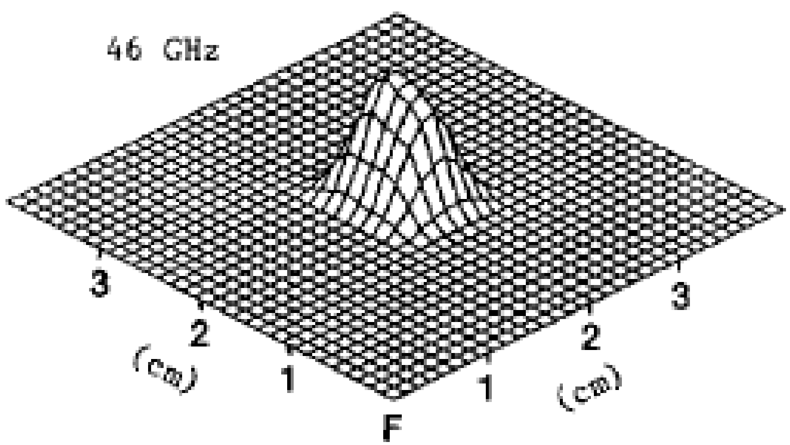


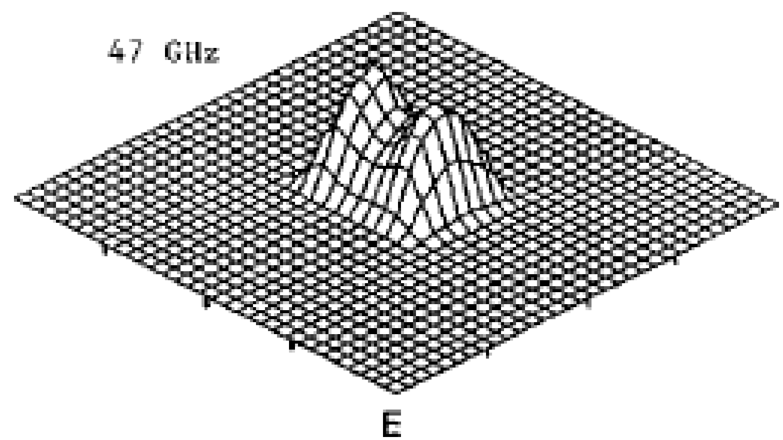
Belyaev et al. 1996

Bioelectromagnetics problem:
Sharp resonant effects

Khizniyak and Ziskin 1994:

absorption pattern of radiofrequency electromagnetic energy depends on frequency for most setups used (horn antennas with dimension much larger than wavelength)

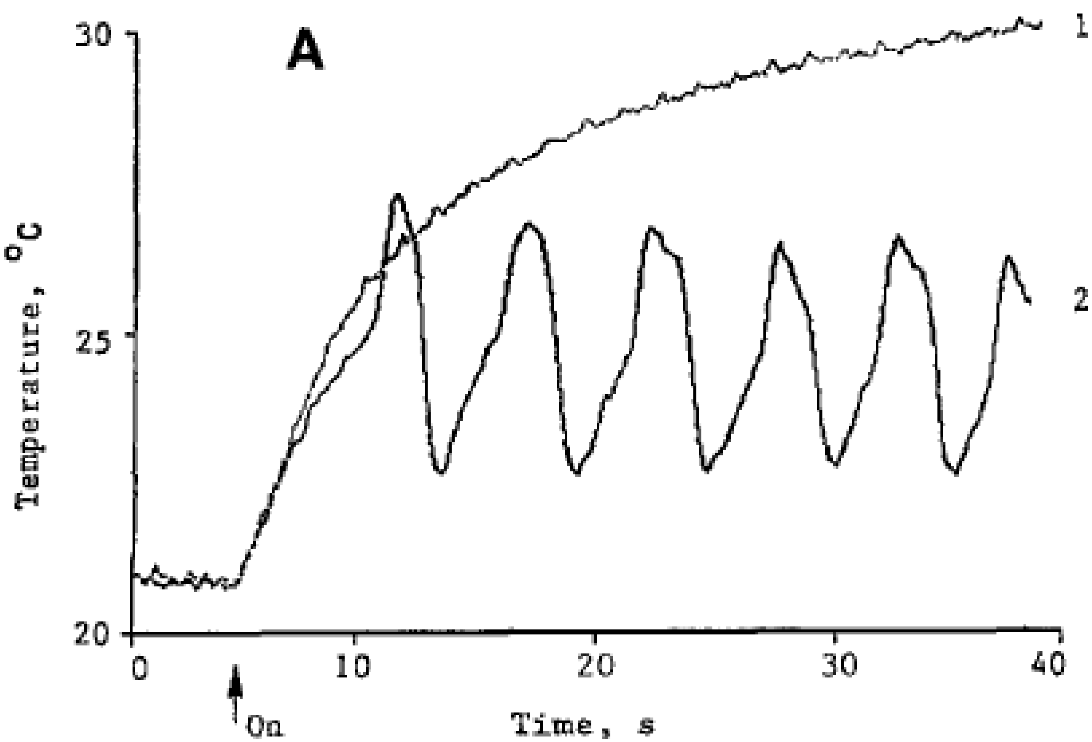




Bioelectromagnetics problem: Sharp resonant effects

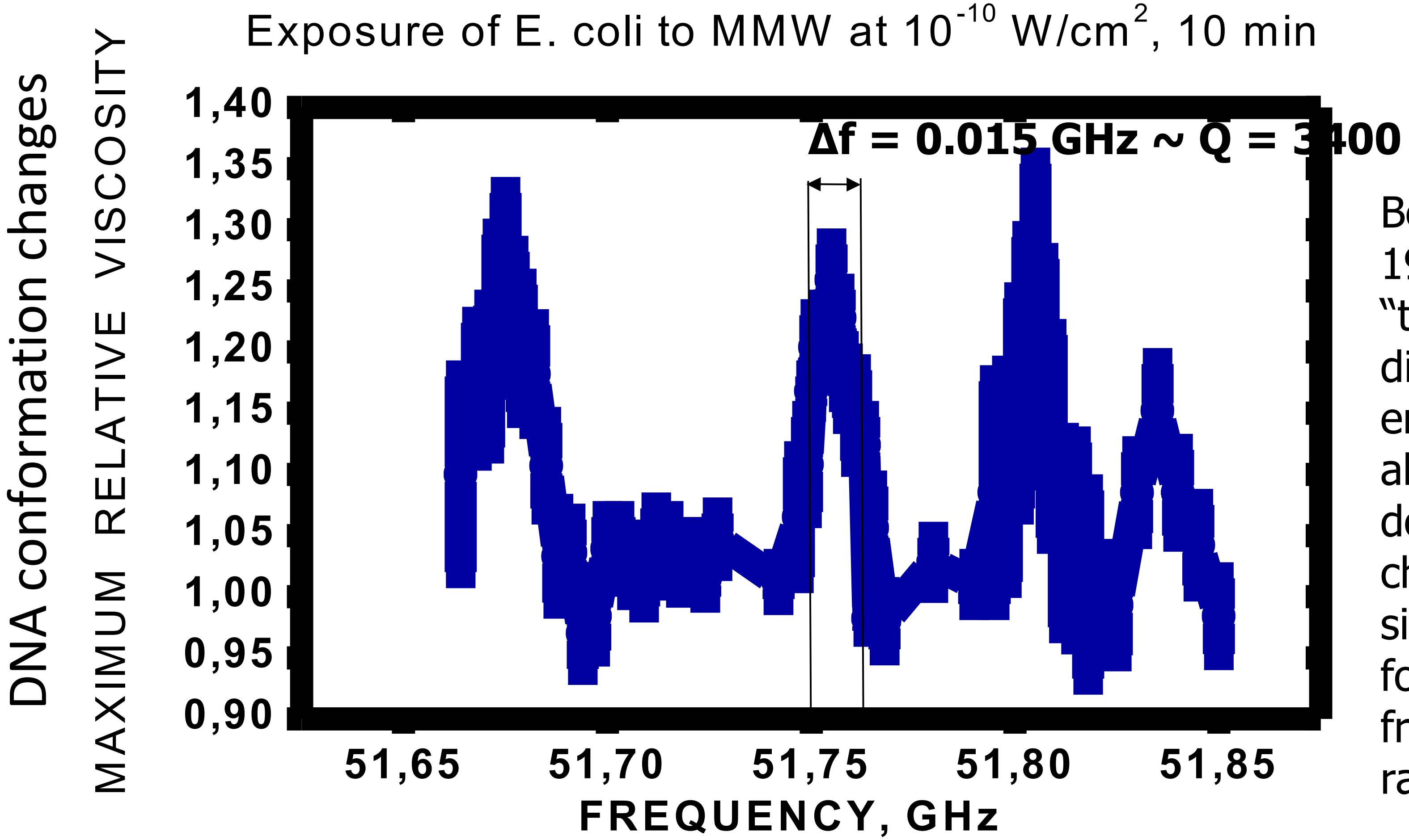
Khizniyak and Ziskin 1996:

spatially inhomogeneous energy absorption in thin liquid media can results in convection due to temperature gradients and temperature oscillations in the liquid



Bioelectromagnetics problem:
1. Sharp resonant effects

Frequencies which give different biological effects are very close to each other.



Belyaev et al. 1996: "the distribution of energy absorption does not change significantly for given frequency range"

Bioelectromagnetics problem: 2. Endogenous electrically polar cellular vibrations

Several experimental works suggest that biological systems generate radiofrequency (kHz - GHz) electric oscillations.

Pokorný et al. 2001: MHz range (*8.085 MHz microtubule resonance*)

Hölzel and Lamprecht: MHz range

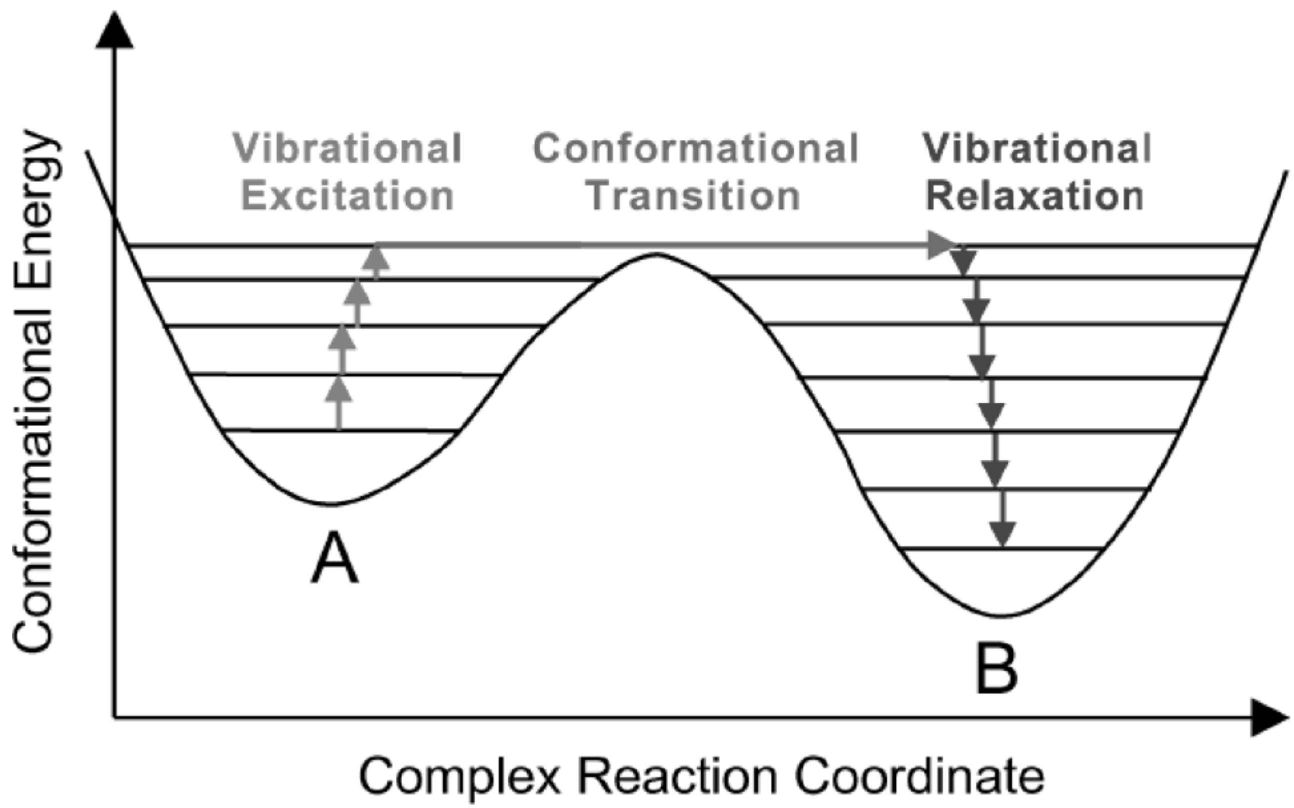
Pohl et al.: attraction of high permittivity dielectric particles to cell membrane (electric oscillations < 1 MHz)

Pelling et al.: kHz mechanical cell membrane vibrations

Theory predicts that this is due to coherent elastoelectric oscillations of electrically polar cellular structures (microtubules, cell membrane) – Fröhlich theory

3. Protein activity

A. Vibrational dynamics important for **protein conformation changes**. To make a conformational transition from one structure to another the corresponding collective modes must be excited up the vibrational ladder in order to cross the transitional energy barrier.



3. Protein activity

B. **Chemical reactivity of the molecular systems**

Chemical reaction kinetics (e.g. standard models described by the Arrhenius equation and transition-state theory) is based on Planck thermal distribution of energy which will not hold if vibration mode responsible for chemical activity is excited above thermal level

Activation energy

Pre-exponential factor

$$k = A \cdot e^{-\frac{E_a}{k_B T}}$$

Rate constant

Boltzmann constant

~~**Temperature**~~

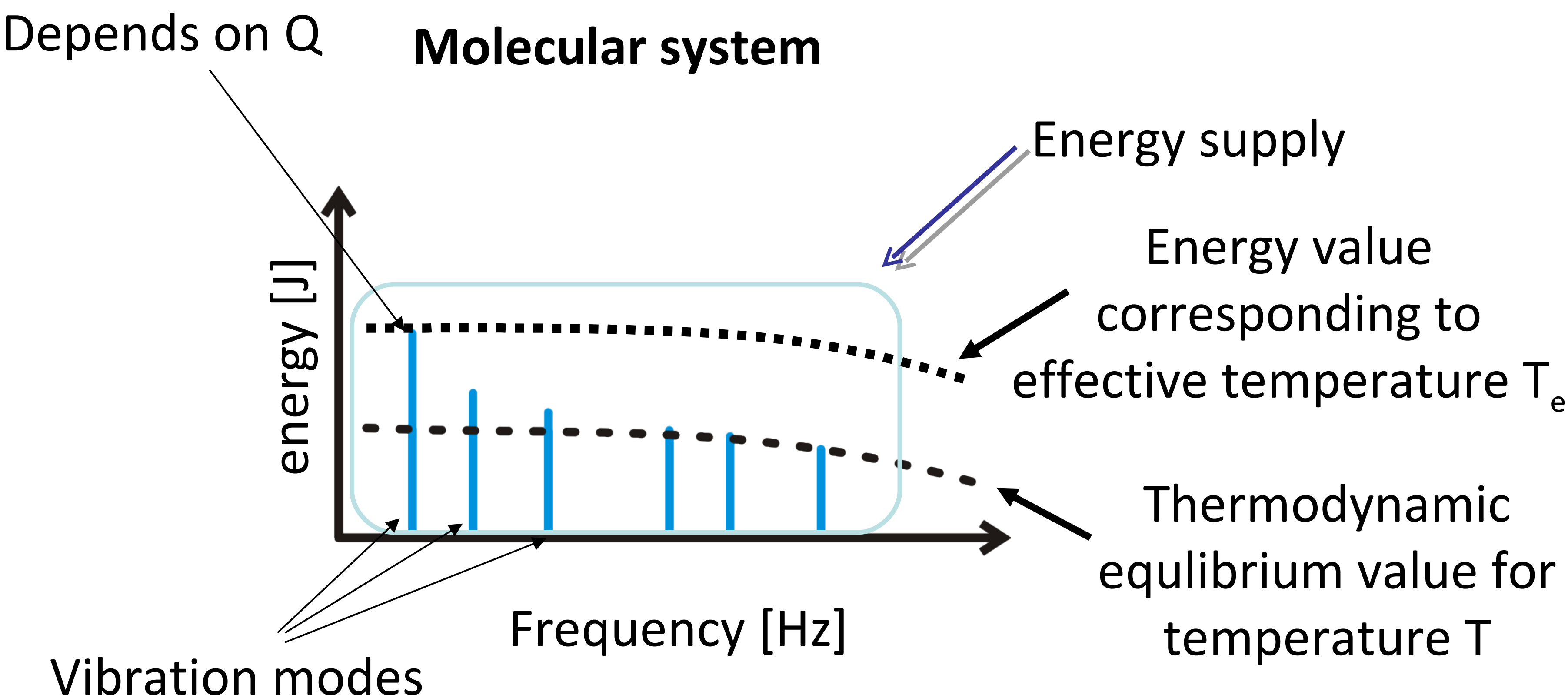
Effective temperature

$$T_e > T$$

3. Protein activity

B. **Chemical reactivity of the molecular system**

Molecular system



Biomolecular vibrations

Currently accepted view: overdamped

Reviews of Adair (2002) and Prohofsky (2004) on possibility of biomolecular resonant interactions with EM field: not significant because of overdamped vibrational dynamics

Reasoning is based on the assumption that water overdamps any oscillatory molecular motion

Underdamped ?

1. Viscoelastic transition of water (increased hydration) increases Q factor of oscillations

2. Small amplitude molecular oscillations are less damped

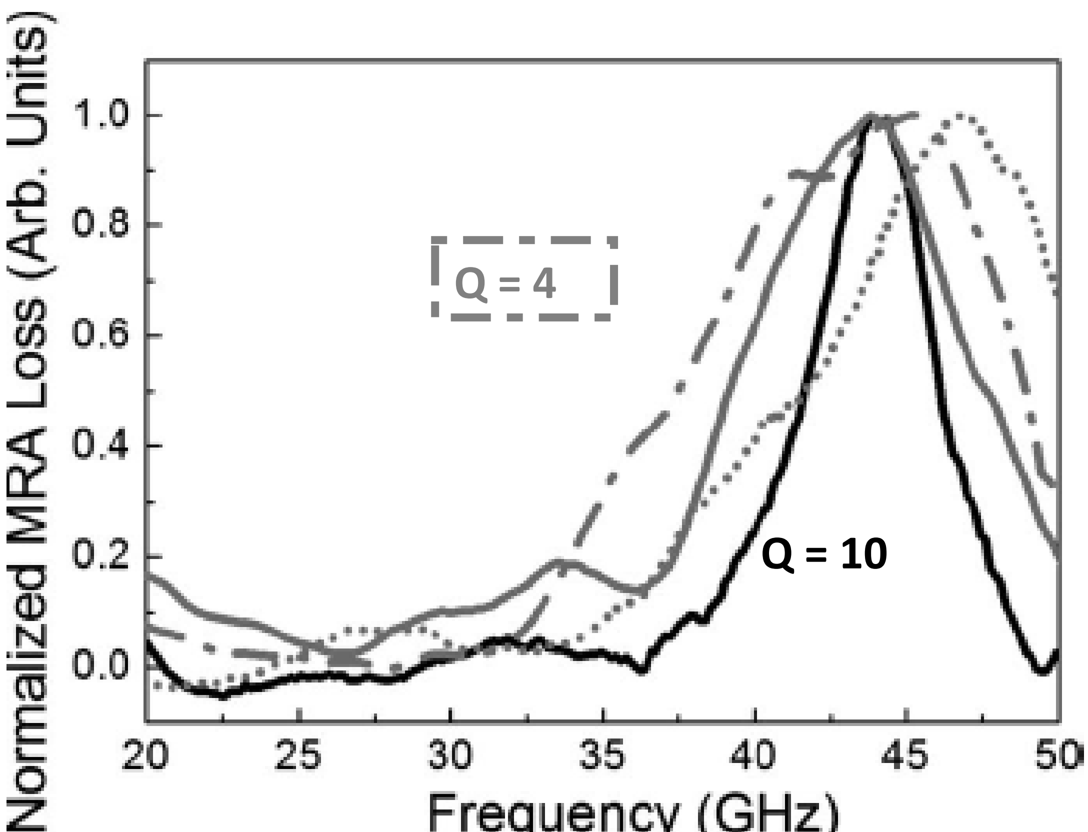
3. *In vivo* cellular situation: water strongly organized due to many interfaces

Microtubule - mitochondria interaction

1. Viscoelastic transition

Van Zandt 1986-1989: above certain frequency (in GHz region), water which hydrates biomolecules starts to change its behavior from viscous to elastic – damping decreases

Liu et al. 2009: **microwave absorption (Q factor) by virus particles increased** when **hydrophilicity of virus surface is increased** by changing the pH of suspension – viscoelastic transition of hydration shell



1. Viscoelastic transition

Increased hydration (organization of water) at biomolecular surface

↓

lower damping of biomolecular oscillations

2. Small amplitude oscillations

Small amplitude biomolecular oscillations (less than size of damping medium units – water molecules or water clusters) are less damped

Romanovski et al. 2003, 2006: “Stokes theory cannot be used for estimating the damping of micromolecular systems since it is applicable only for macrosystems for which water environment is represented as continuous viscous medium”

MD calculations:

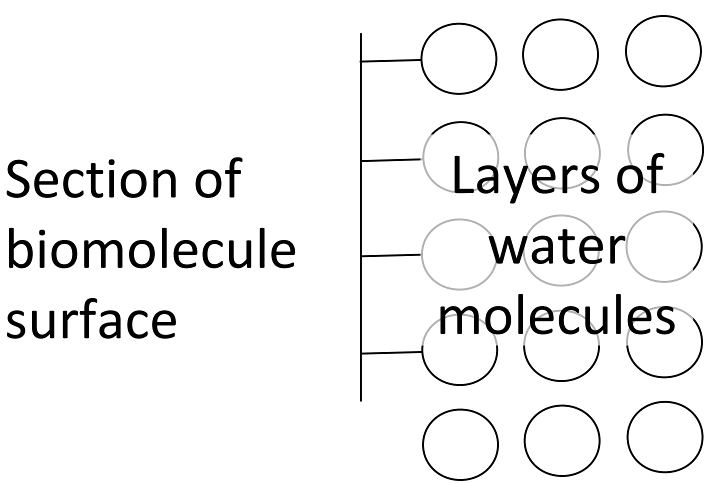
<= 0.1 nm amplitudes of small atomic groups vibrations – Q factor 10-400

2. Small amplitude oscillations

Layer-organized water reduces damping of vibrations, especially parallel longitudinal vibrations

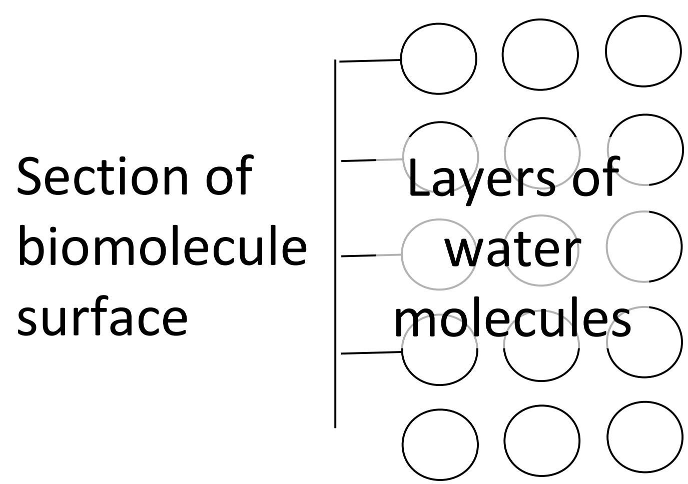
Amplitude < $A_{threshold}$

Elastic



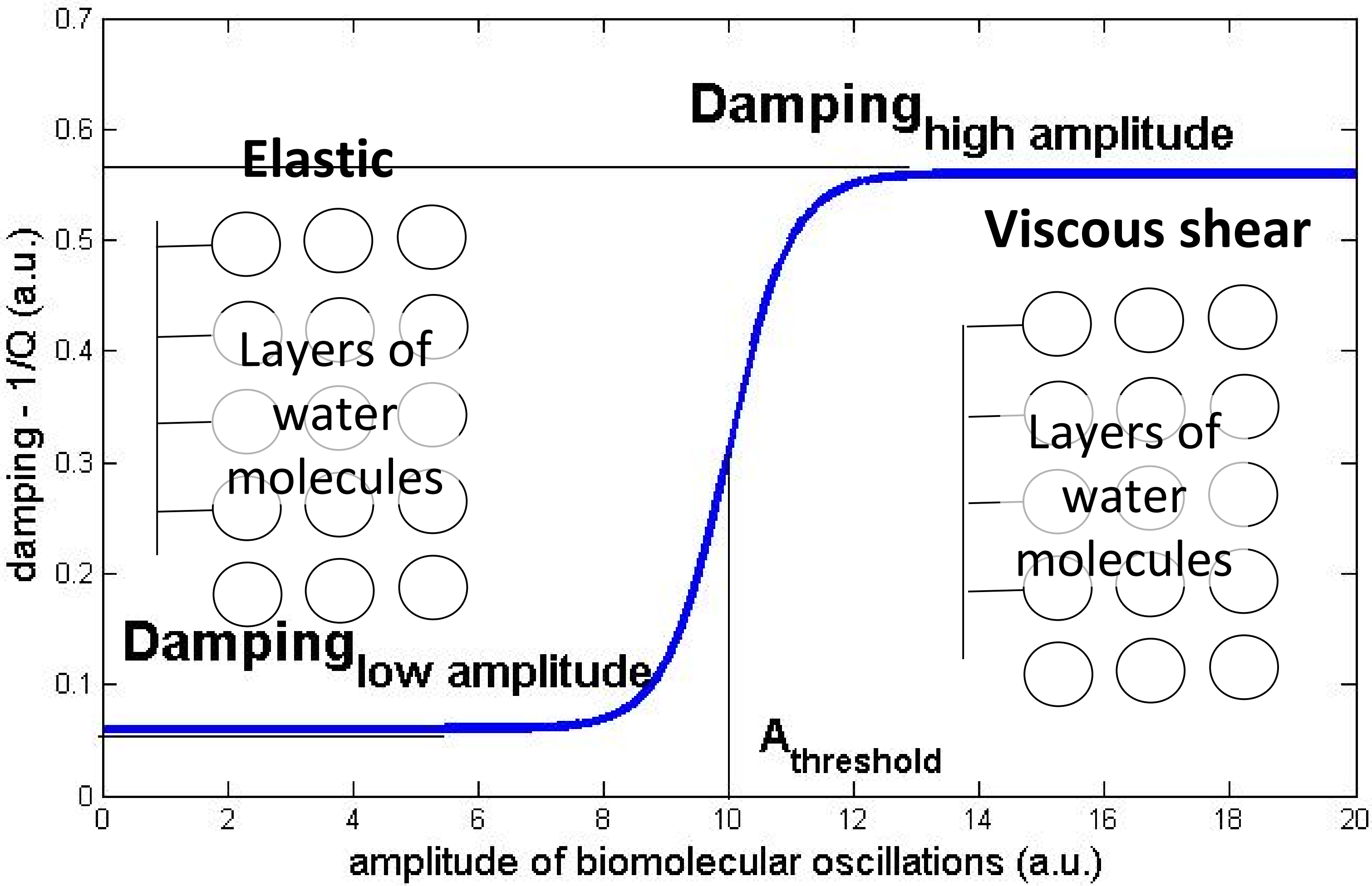
Amplitude > $A_{threshold}$

Viscous shear



2. Small amplitude oscillations

$$\ddot{x} + \frac{\omega_0}{Q}\dot{x} + \omega_0^2 x = F(t)$$



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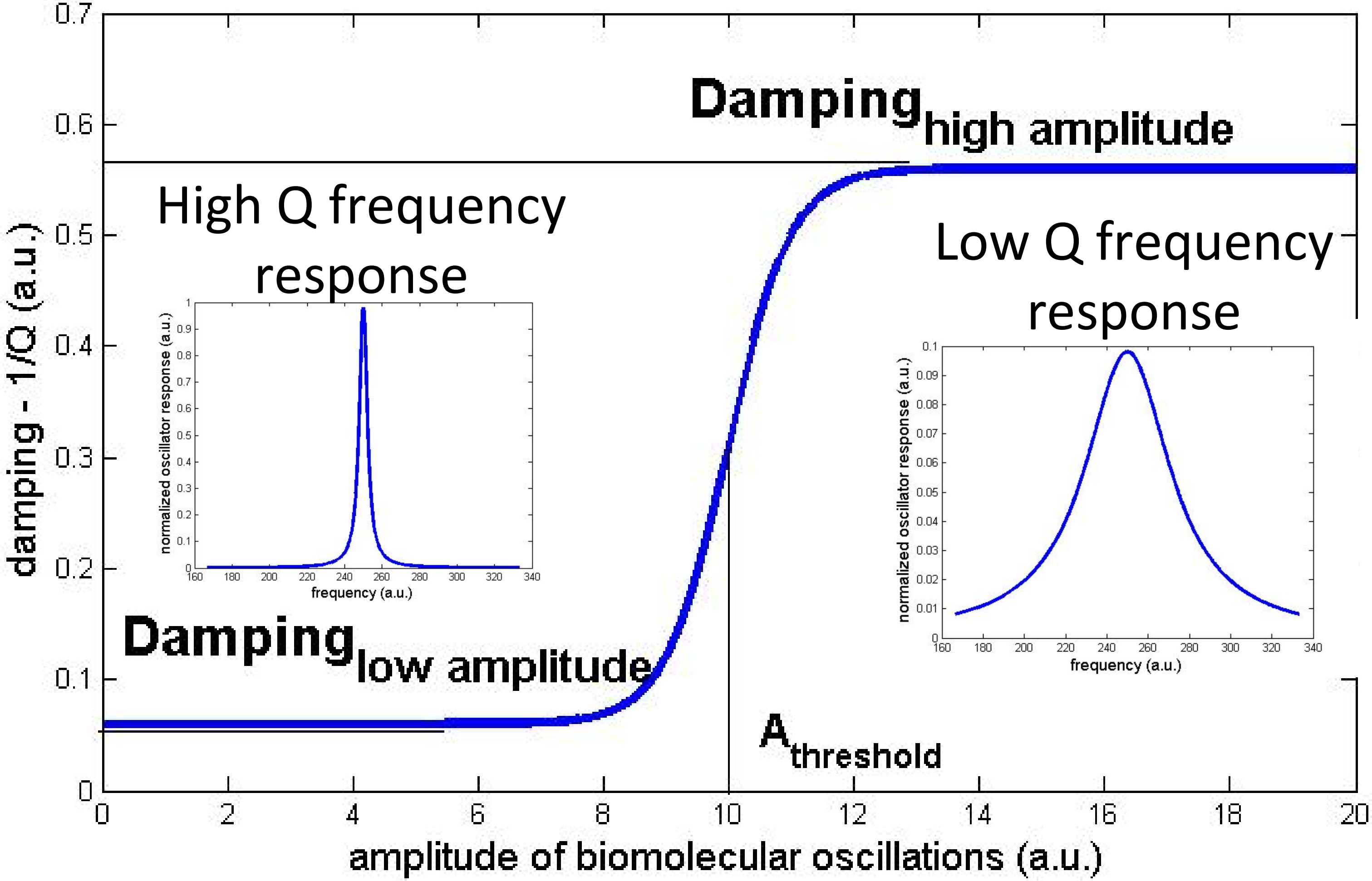
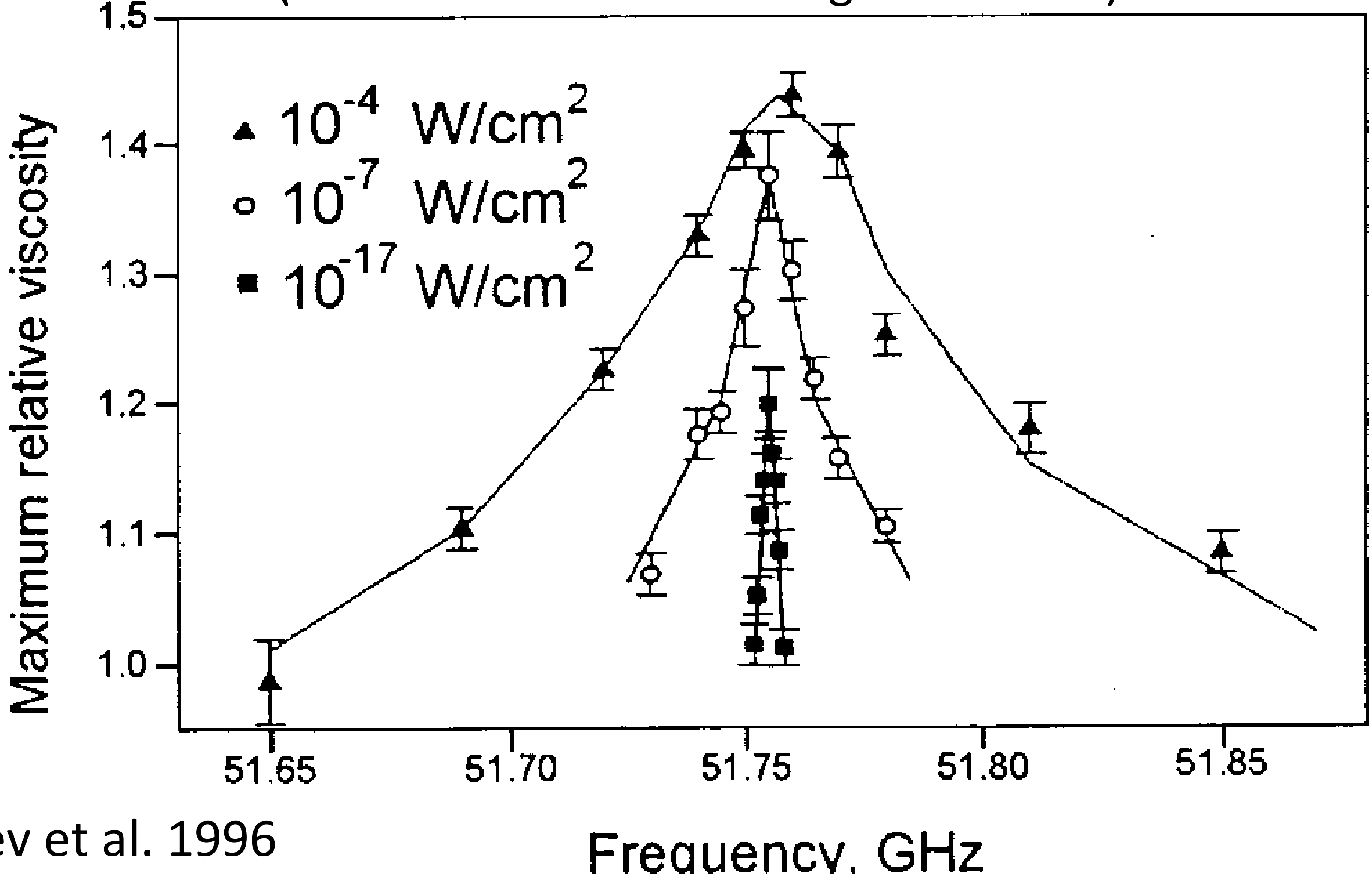


2. Small amplitude oscillations

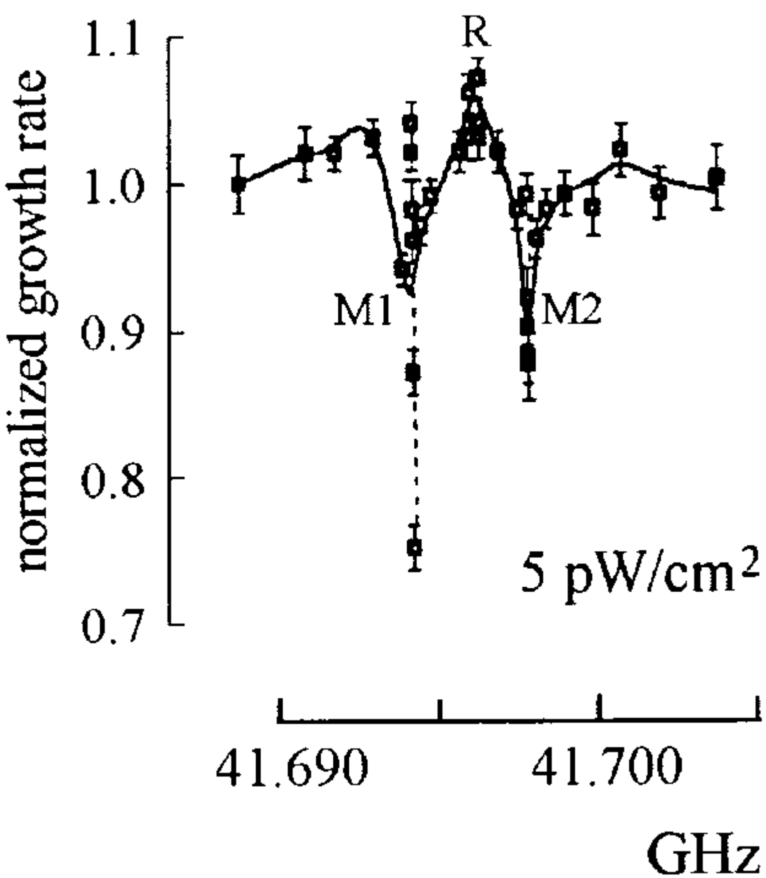
Biological effect of electromagnetic radiation
(DNA conformation changes in *E. Coli*)

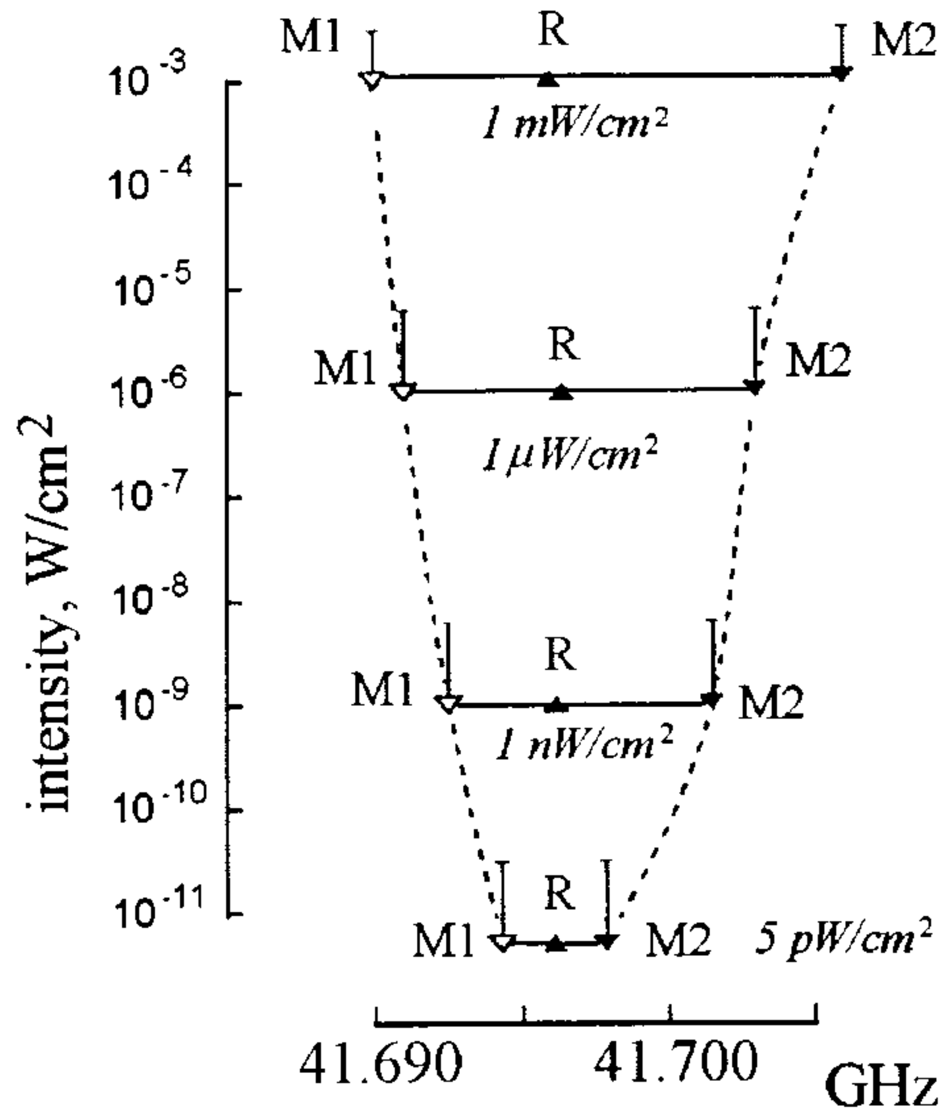


Belyaev et al. 1996

2. Small amplitude oscillations

Grundler and Kaiser 1992





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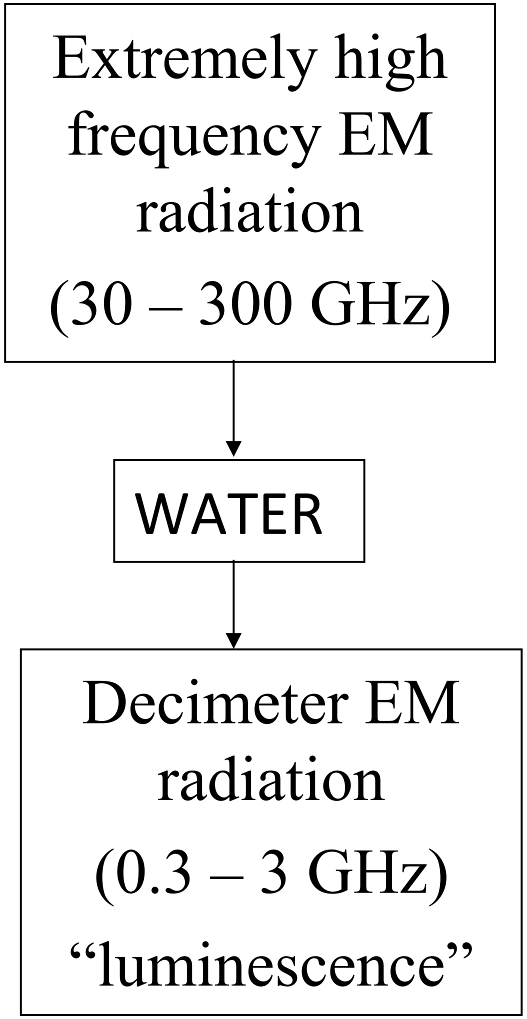
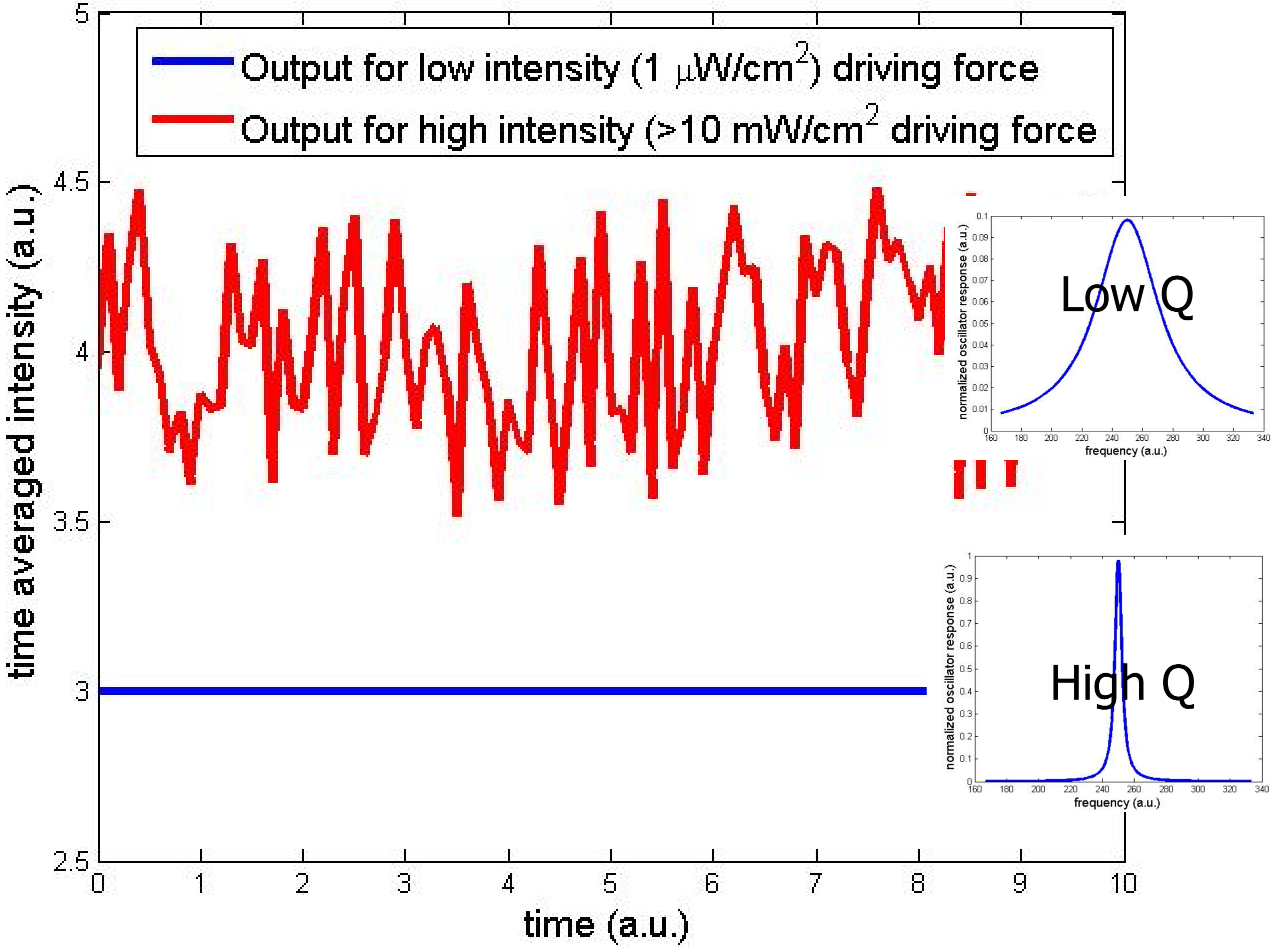


Sinitsyn et al. 2000



Interpretation: Luminescence of hexagonal water clusters

2. Small amplitude oscillations

Small amplitude biomolecular oscillations (amplitude < $A_{threshold}$) are able to oscillate with less damping, i.e. with higher Q factor.

Small amplitude molecular oscillations are more likely to sustain coherence

Spectral peak width

Why don’t we usually observe sharp (high Q) peaks in spectroscopy of biomolecules ?

A. Most (absorption) spectroscopy techniques need to use high input power to obtain detectable signal – high driving power -> lower Q factor

B. Brandt et al. 2008 – broadening of the spectral peak not necessarily due to damping, but due to the inhomogeneous broadening, variations in relative intensities, anharmonicity

Evidence of underdamped protein vibrations/oscillations

Coherent protein collective low frequency (1 - 3 THz) vibrations, femtosecond coherence spectroscopy:

Gruia et al. 2008: 10 types of ferric heme proteins (metMb, cyt c,...)

Cimei et al. 2004: azurin - blue copper protein

$Q = 4 \div 20$

Vos et al. 1990-2000, Engel et al. 2007, room temperature quantum coherence, vibrations of photosynthetics centers, $Q = 4 \div 10$

Evidence of underdamped protein vibrations

Xie et al. 2002 – bacteriorhodopsin 2 THz collective vibration, time-resolved picosecond far infrared pump/probe spectroscopy:

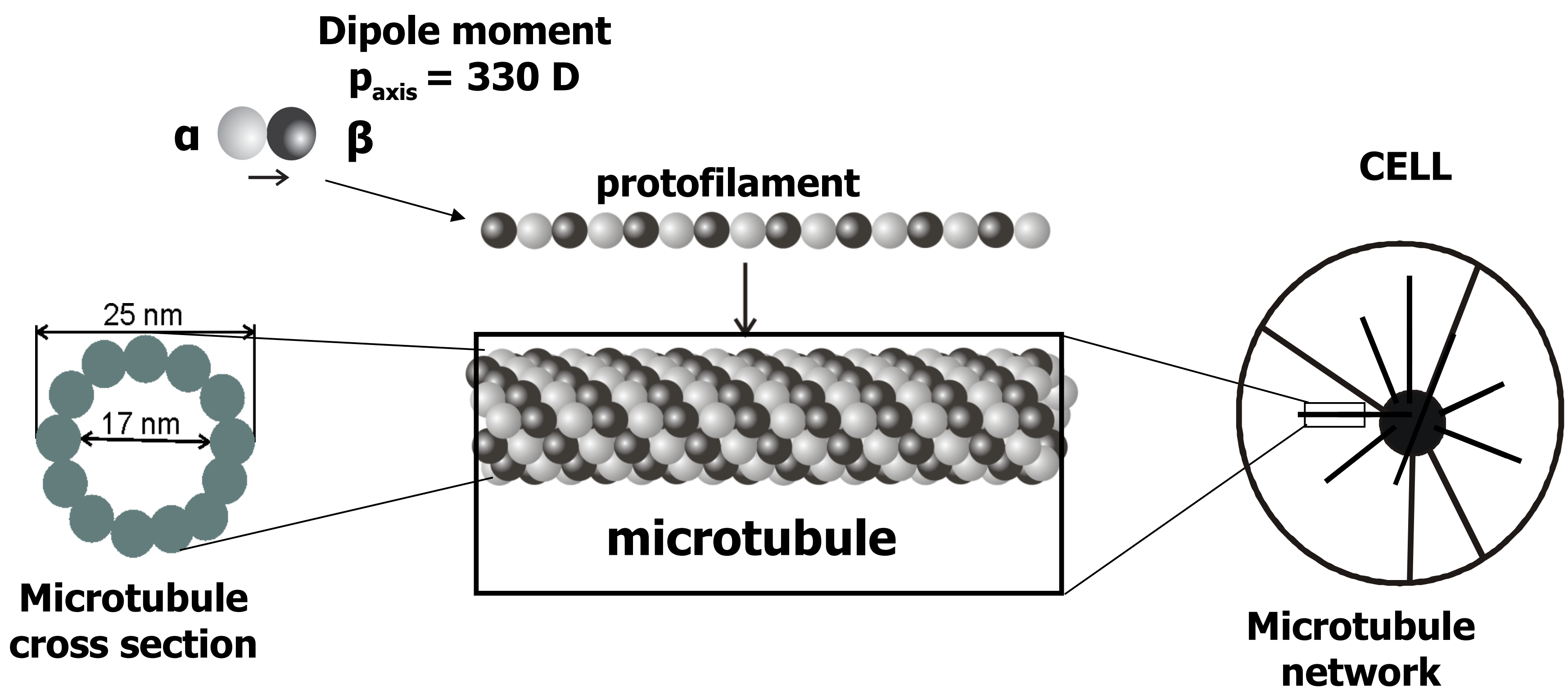
Q = 1500

"…results indicate coupling strength of the collective modes to the solvent is relatively weak and the homogenous modes within the heterogenous envelope are relatively underdamped…"

In vivo situation:
microtubules + mitochondria case

…from underdamped vibrations to
coherent cellular electrodynamics

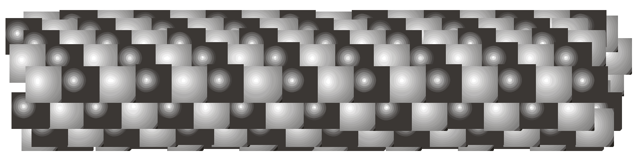
Microtubules



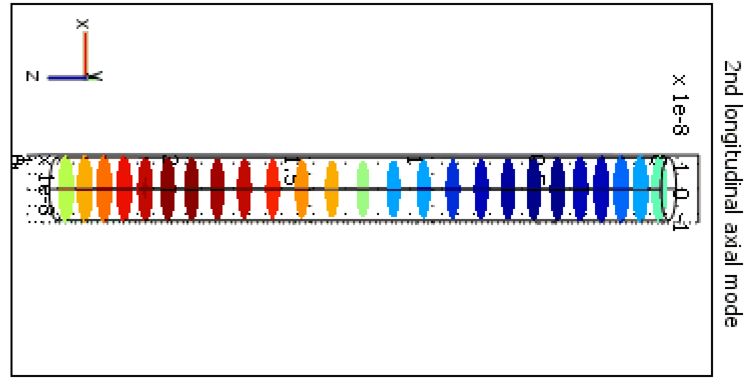
Vibration states of microtubules

- Frequency of microtubule elastic vibrations: kHz - GHz

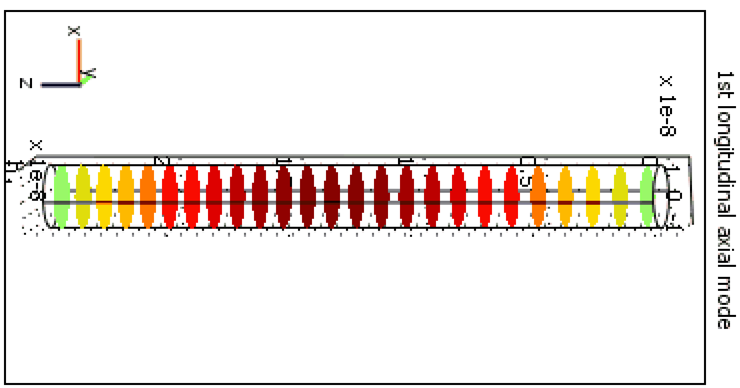
Microtubule



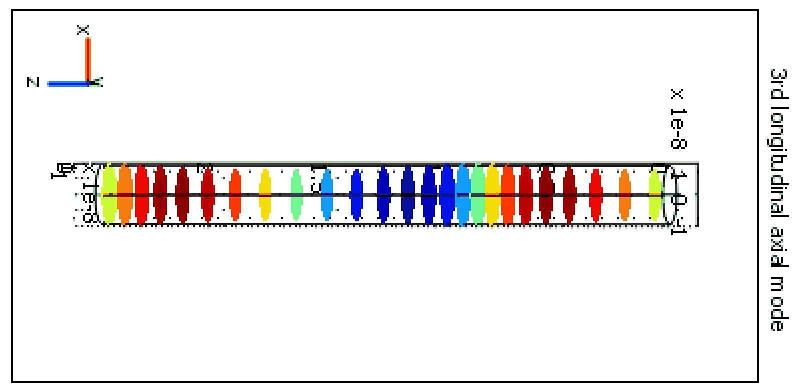
2nd longitudinal mode



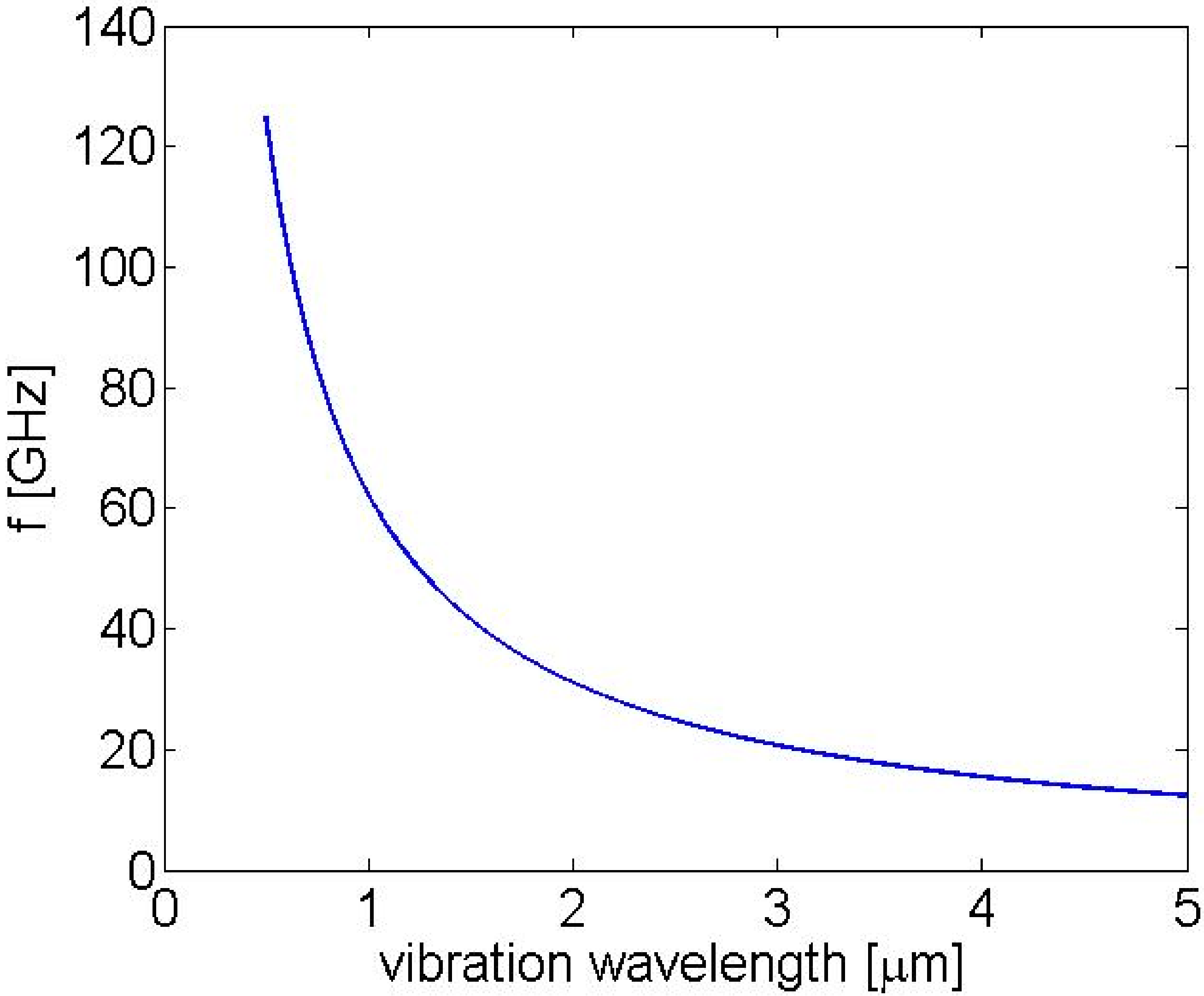
1st longitudinal mode



3rd longitudinal mode

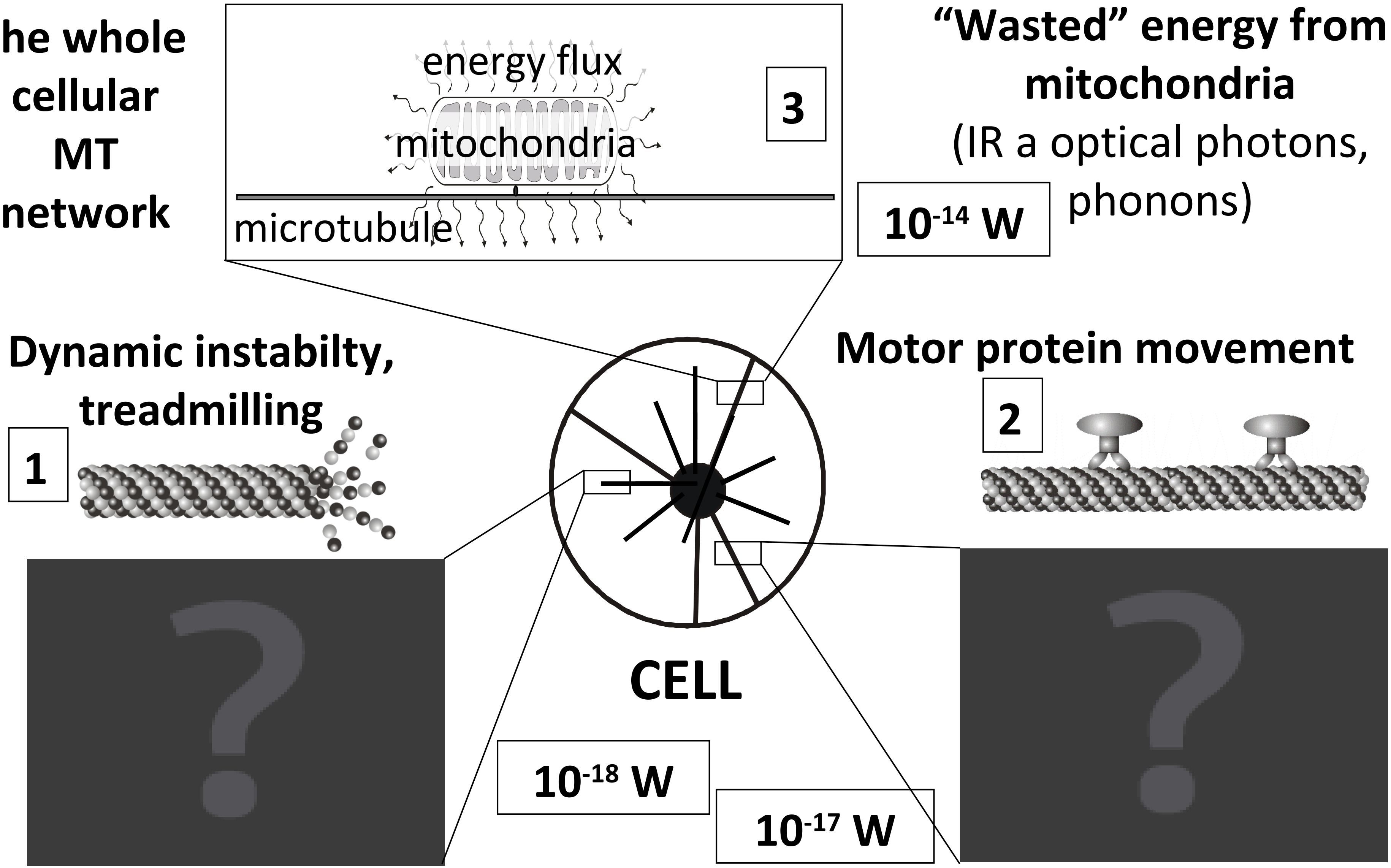


Longitudinal axial microtubule vibrations



Energy supply to microtubule

Power rates for the whole cellular MT network

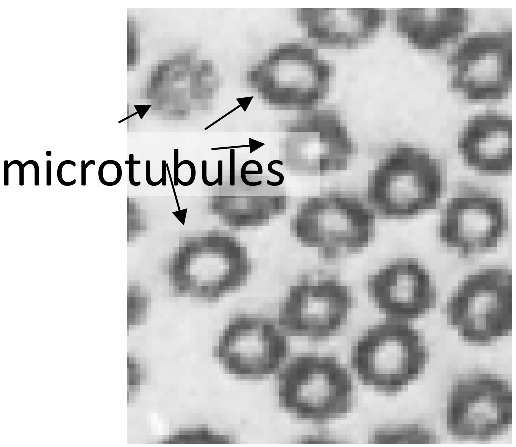


Water and damping of microtubule vibrations

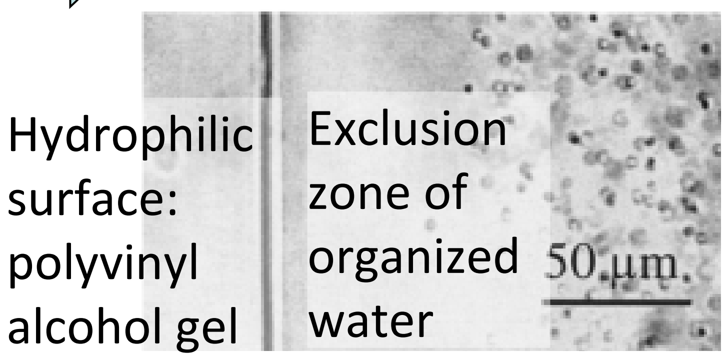
There are “clear zones” around microtubules (Stebbings &Hunt 1982)

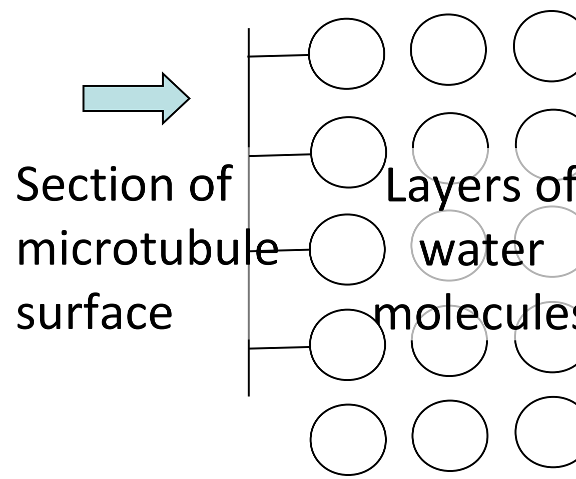
Microtubules have hydrophilic sites. Such surfaces can organize water into layers – form exclusion zones

Layer-organized water reduces damping of vibrations

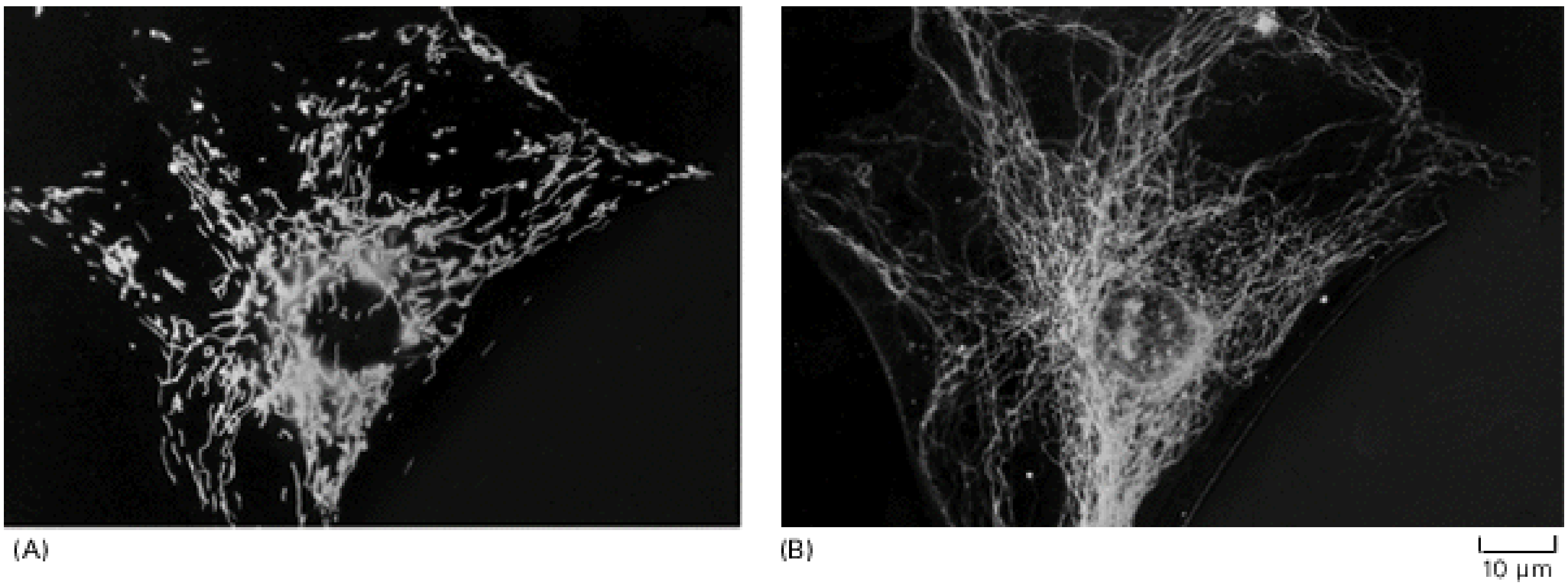


Cryo electron microscopy: microtubule cross section





Mitochondria are located near microtubules



Morphological relationship between mitochondria and microtubules. Immuno-fluorescence images (Alberts et al 2008)

LEFT: Mitochondria, RIGHT: Microtubules

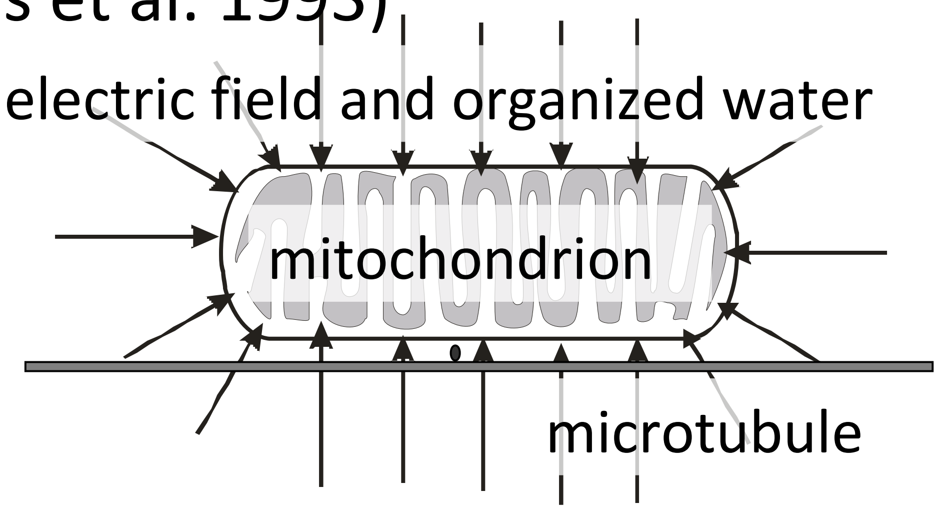
Extra water organization by nearby mitochondria

Strong electric field (3 MV/m) near functional mitochondria (Tyner et al. 2007)

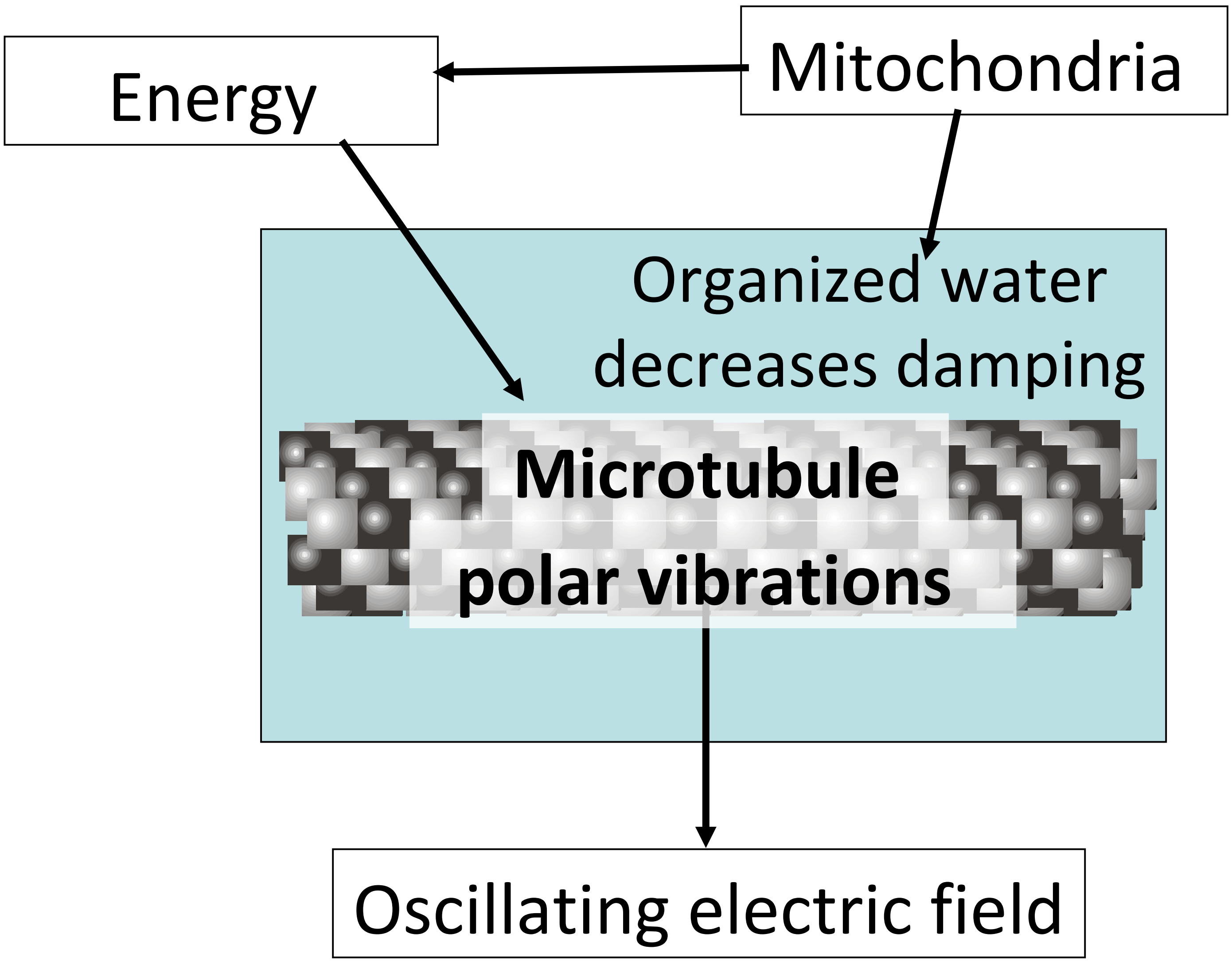
Functional mitochondria are necessarily source of IR radiation due to production of heat.

IR also promotes organization of water (Chai et al. 2009)

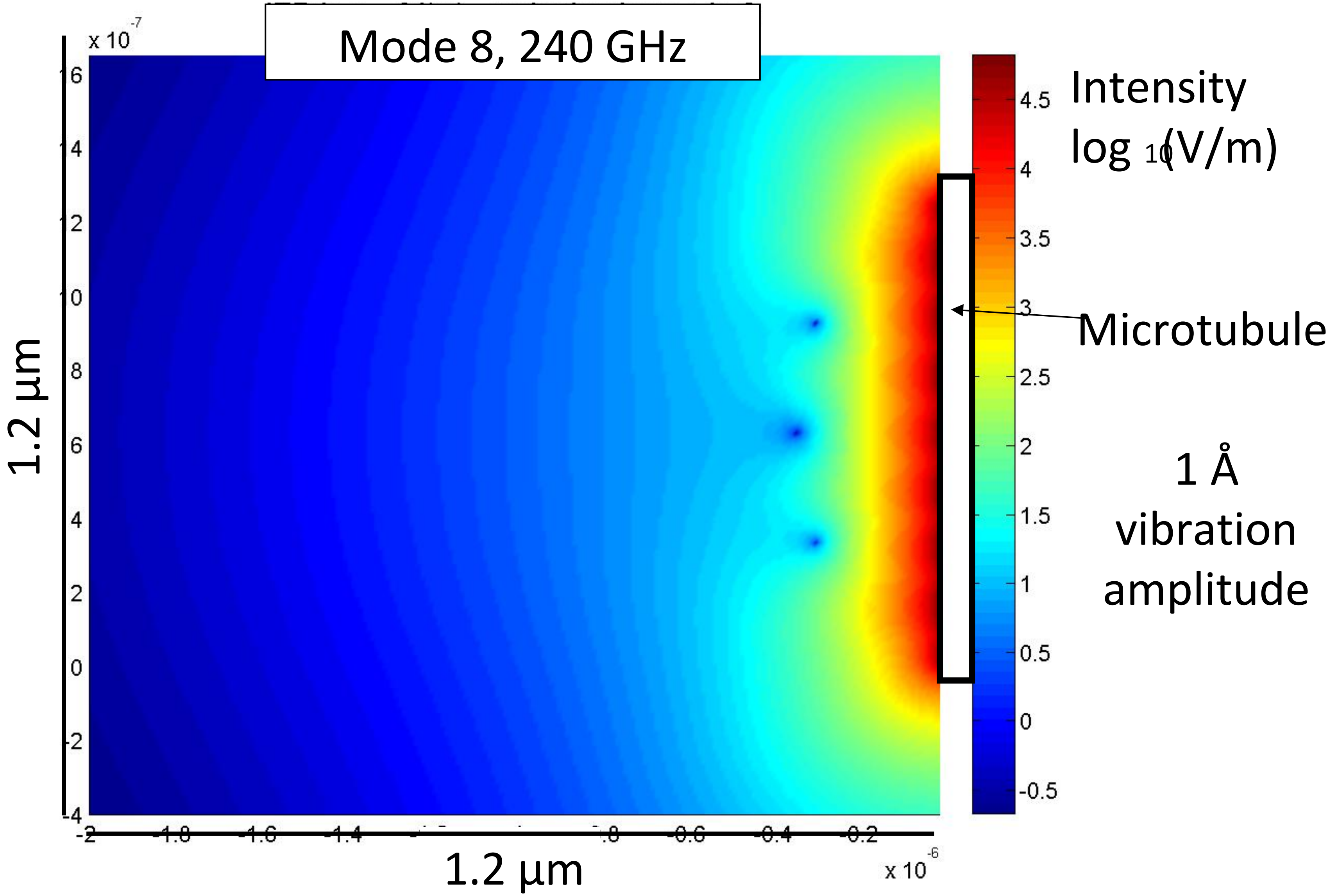
Organized water (exclusion zones) near mitochondria (Trombitas et al. 1993)



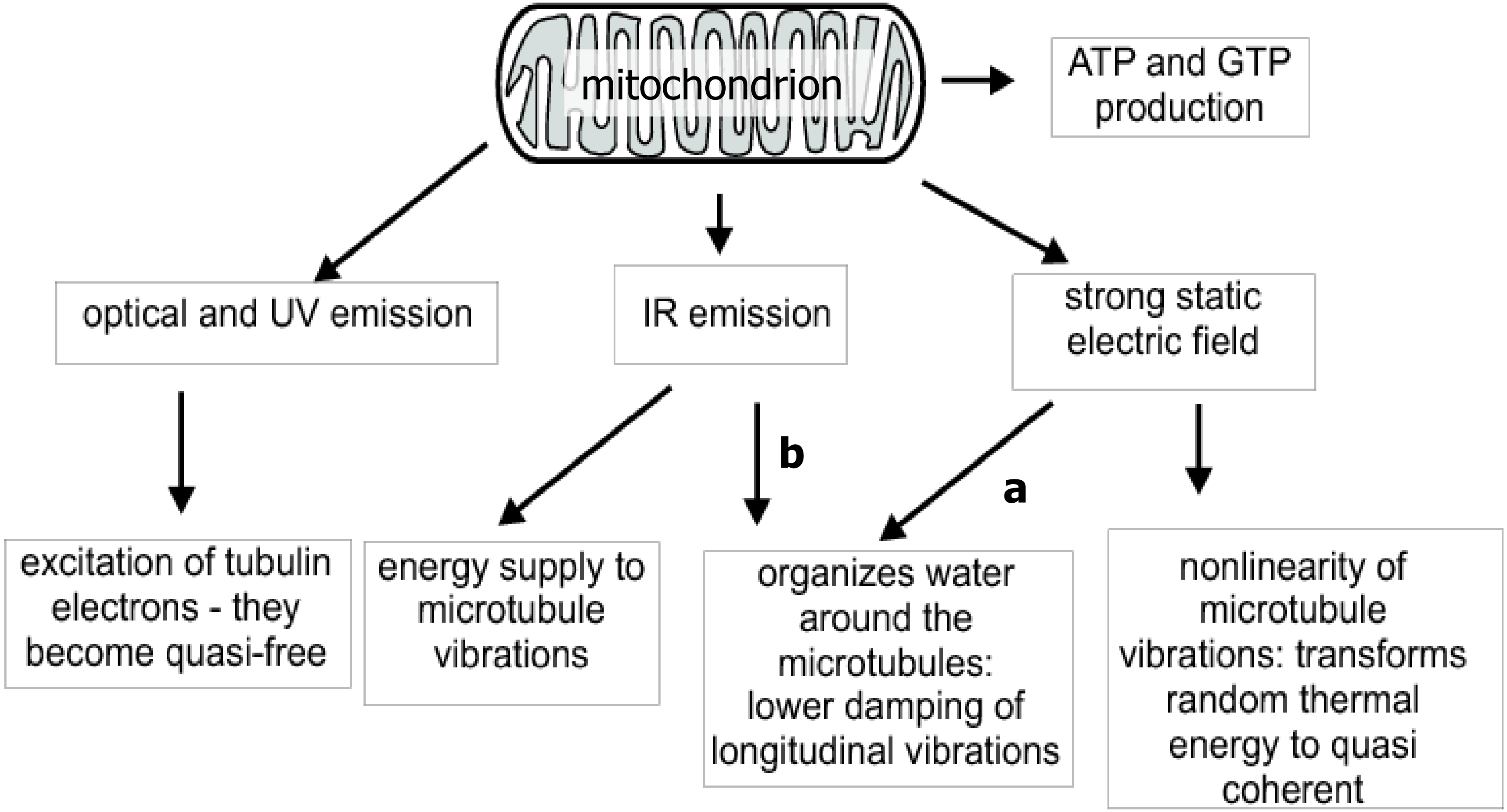
Microtubule + mitochondria



Calculated oscillating electric field around microtubule: an example



Multiple roles of mitochondria



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a - Fuchs E C, Woisetschläger J, Gatterer K, Maier E, Pecnik R, Holler G and Eisenkölbl H, **The floating water bridge**, *J. Phys. D Appl. Phys.* 2007, 40, 6112-14

b - Chai B, Yoo H and Pollack G H, **Effect of radiant energy on near-surface water,** *J. Phys. Chem. B,* 2009, 42, 13953-8

Conclusions

Organization of water at the biomolecular interface

→

Viscoelastic transition of water

→

decreased damping of polar biomolecular oscillations with amplitude $A < A_{threshold}$

↓

(quasi)coherent polar biomolecular oscillations

→

Electrodynamic field organizing cellular processes

Organized water enables/gives rise to coherent biomolecular behavior

Thank you for attention !

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