Quantum Coherence and Noise in Biology

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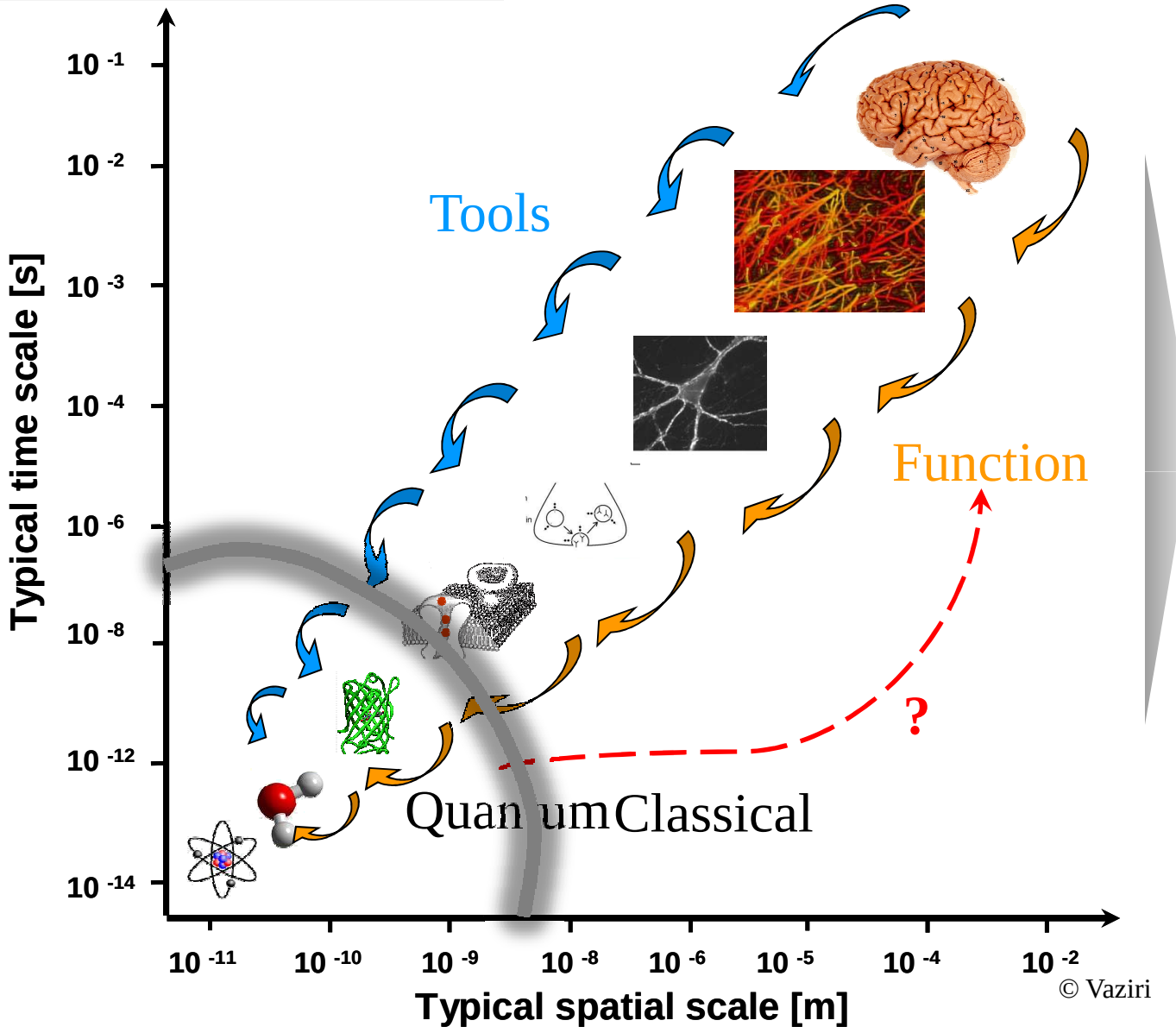
Institut für Theoretische Physik
Universität Ulm

&

Quantum Optics and Laser Science Group
Blackett Laboratory
Imperial College London

Hierarchical structures in biology



Can quantum coherence be relevant for biological function?

Requires tools for studying biological structure and function at unprecedented spatial and temporal resolution

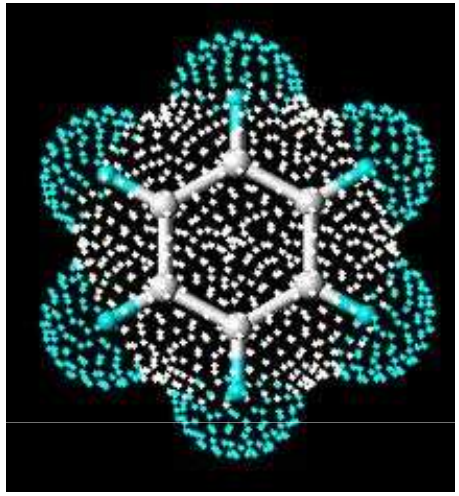
What are we looking for ?

- Quantum coherence certainly exists at the level of chemical bonds

Electrons are delocalized in a coherent superposition

For us this kind of coherence is less interesting !

Short-ranged, equilibrium, static



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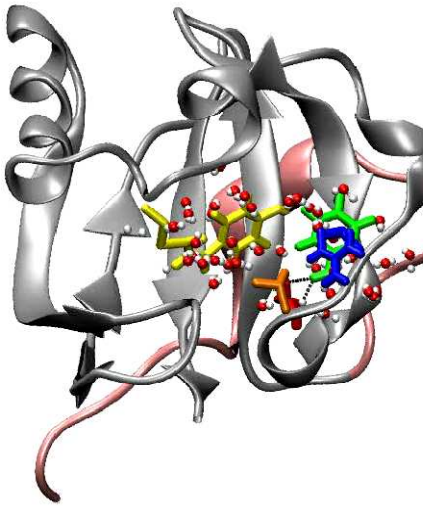
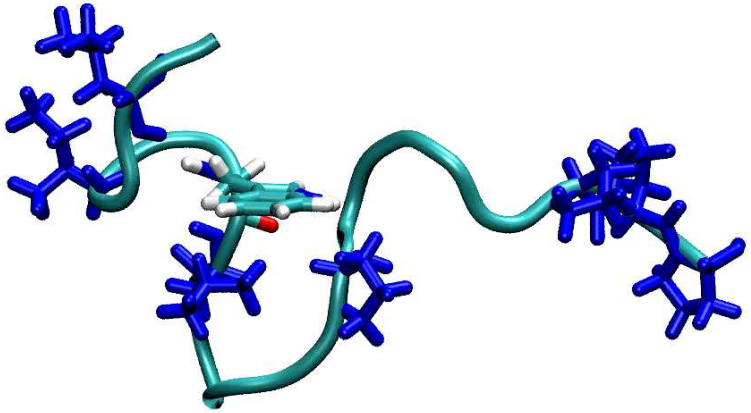
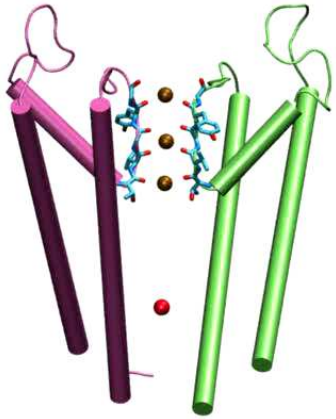
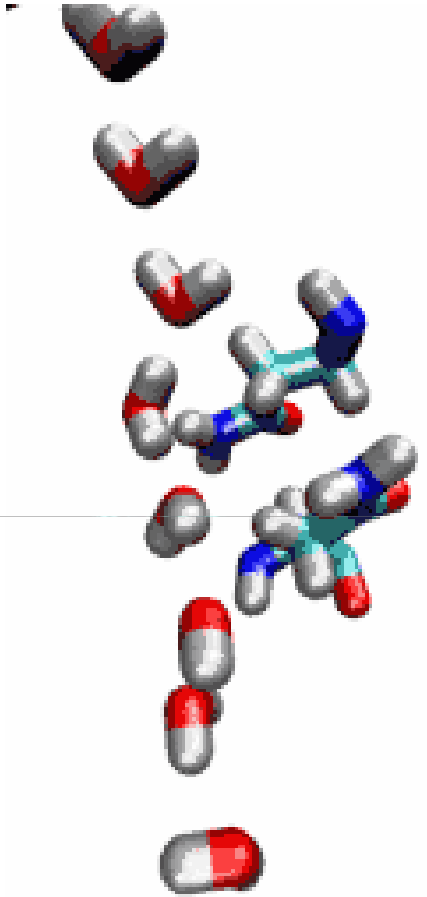


Computational Chemistry
Group, Amsterdam



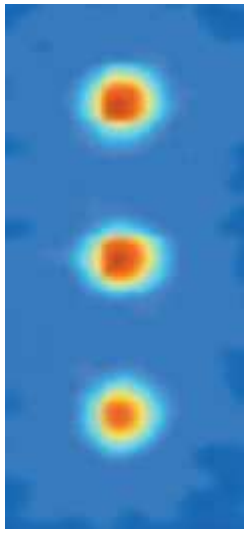


Theoretical and Computational
Biophysics Group, Illinois @ Urbana



Computational Chemistry
Group, Amsterdam

Systems & Environments

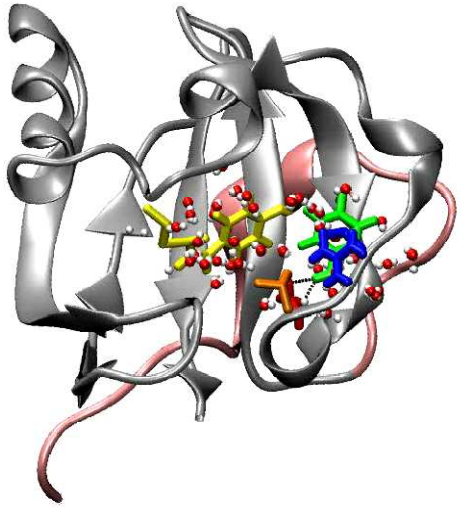


Quantum technologies

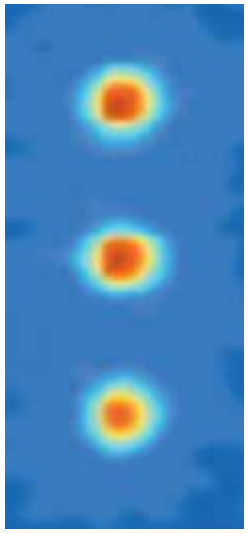
Isolate system to observe & exploit quantum behaviour

Biology

Systems in strong contact with surrounding world



Systems & Environments



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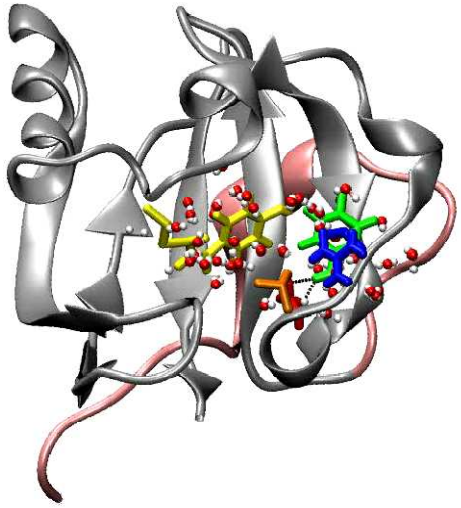
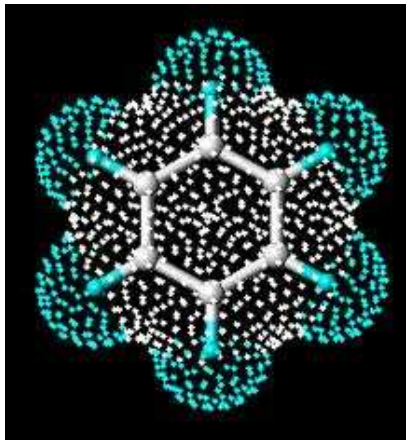
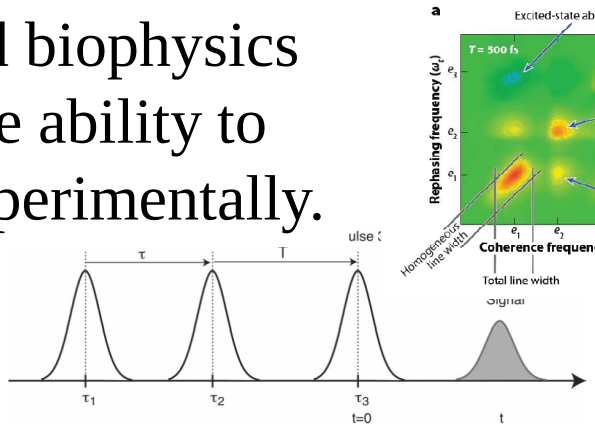


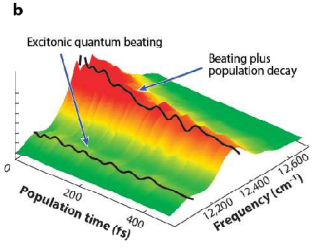
What are we looking for ?

- Questions:
  - Length and time scales of quantum coherence
  - Role of coherence
  - Role of the environmental noise
  - Theory of strong network-environment interaction
  - Identify principles of noisy quantum network dynamics
  - Experimental verification of theoretical hypotheses

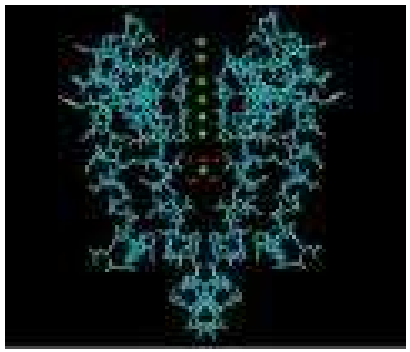


Convergence of optics and biophysics techniques have led to the ability to explore these questions experimentally.



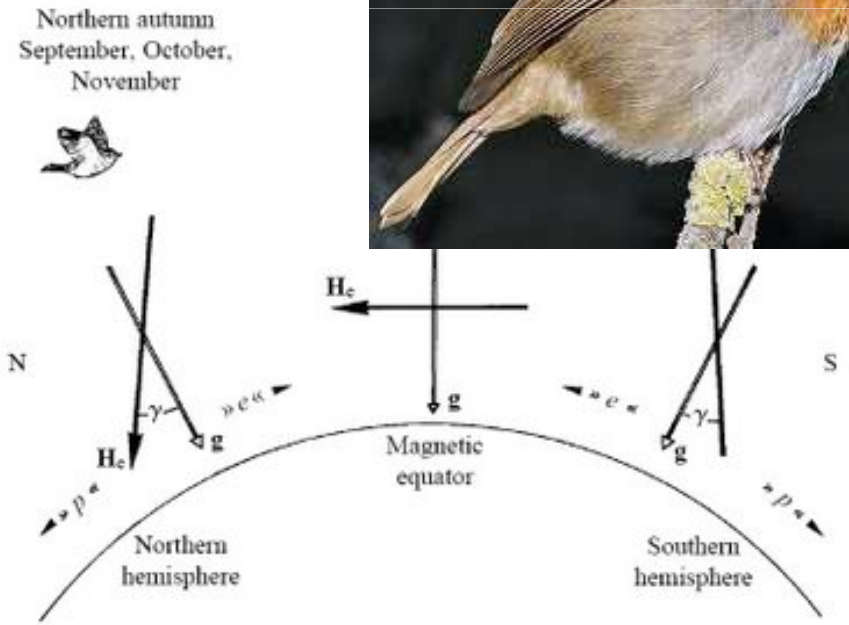


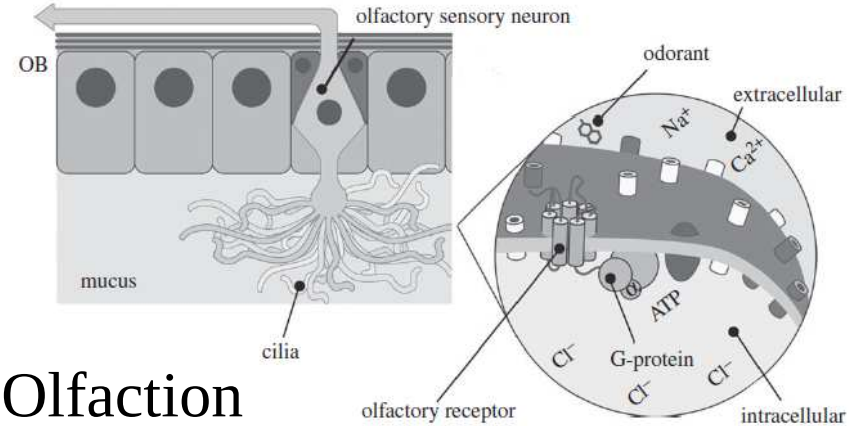
Photosynthesis



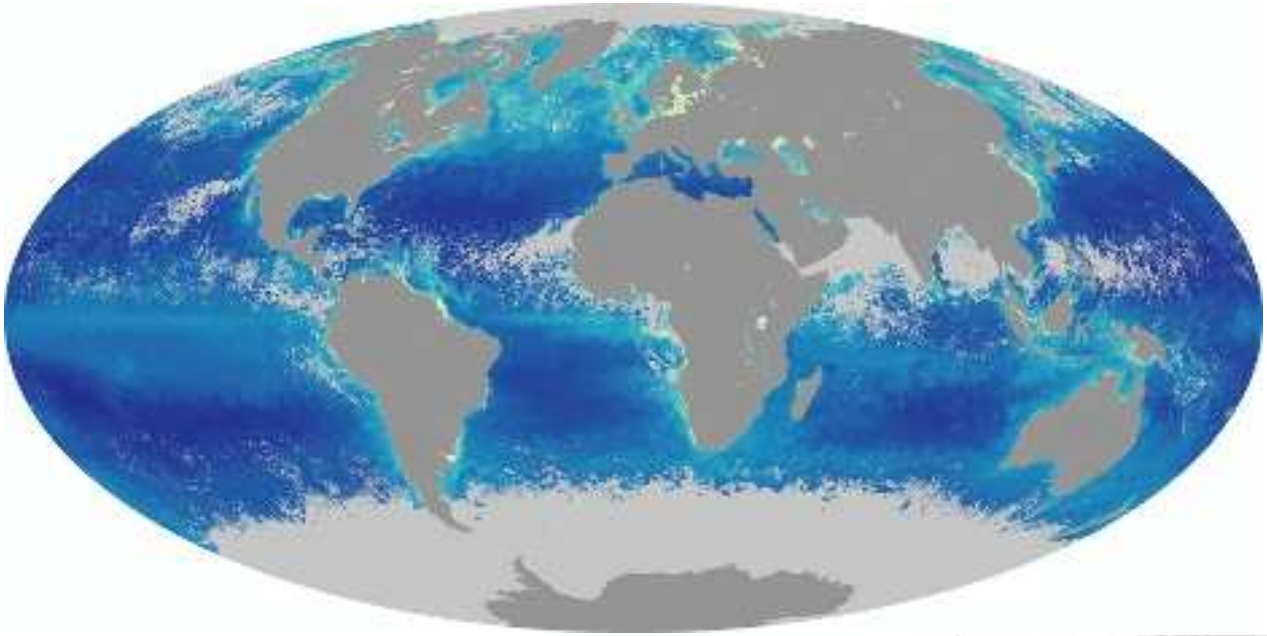
Ion channels

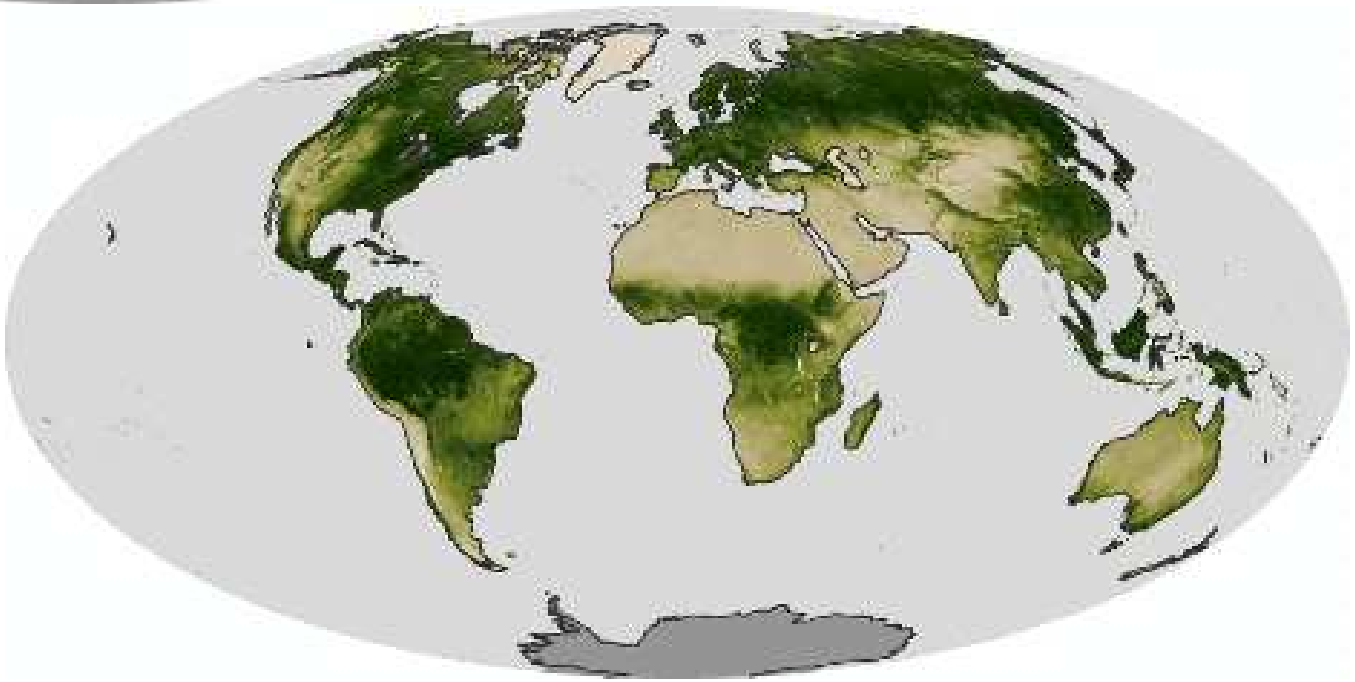
Magnetic Vision

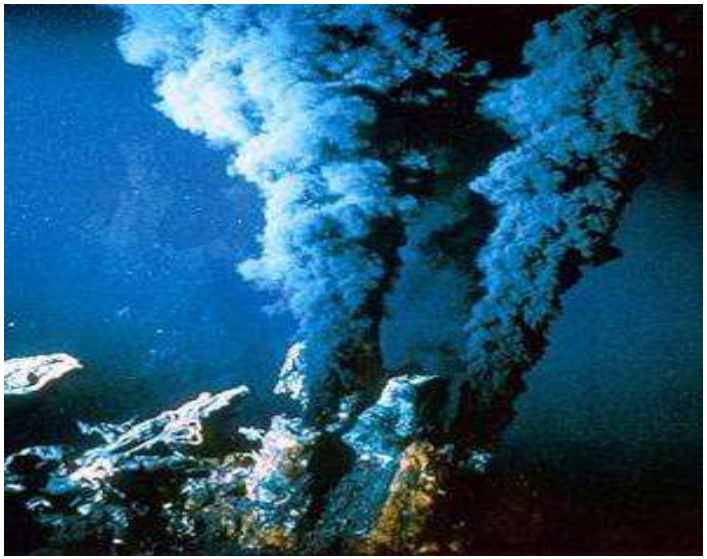


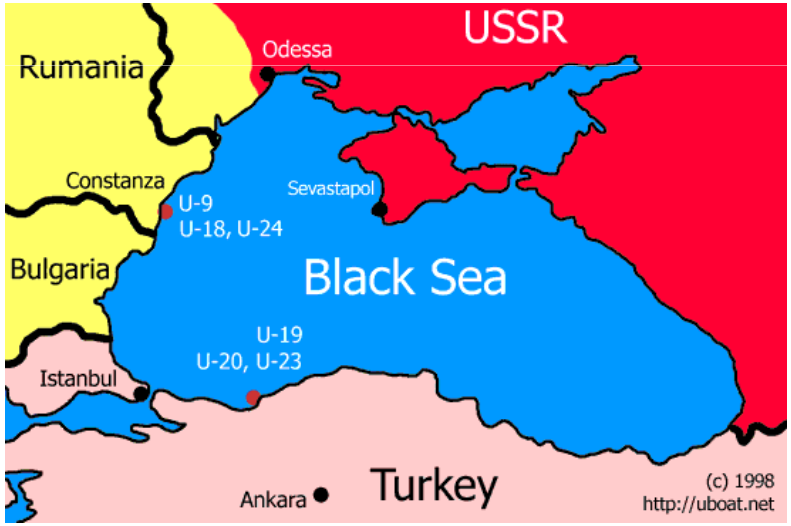


Olfaction





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Rumania
Odessa
Constanza
U-9
U-18, U-24
Sevastapol
Bulgaria
Black Sea
U-19
U-20, U-23
Istanbul
Ankara
Turkey
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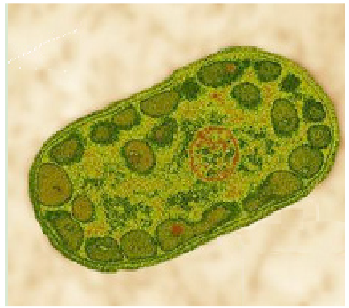
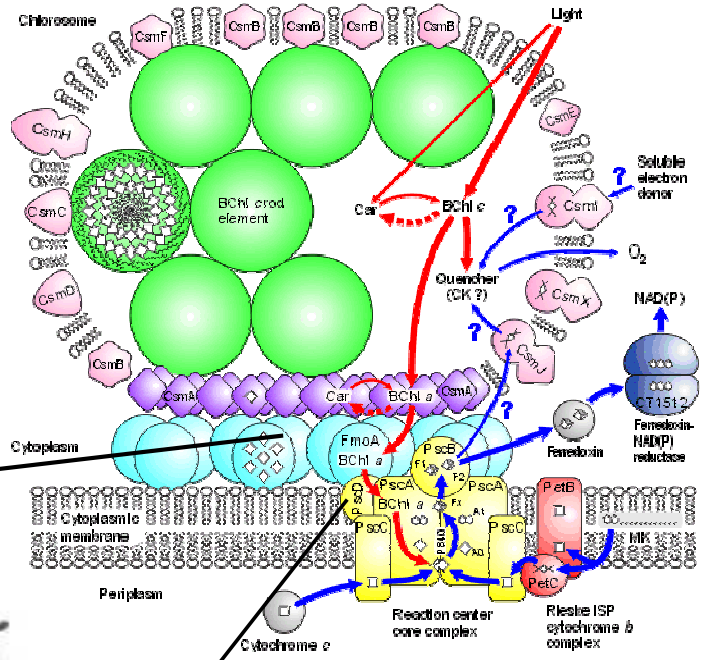
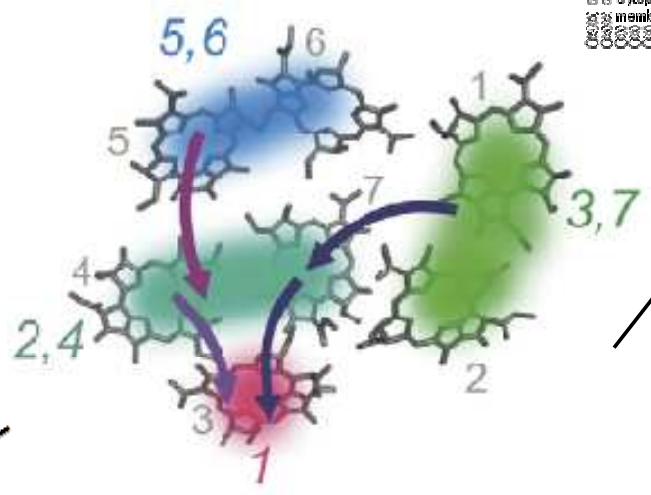
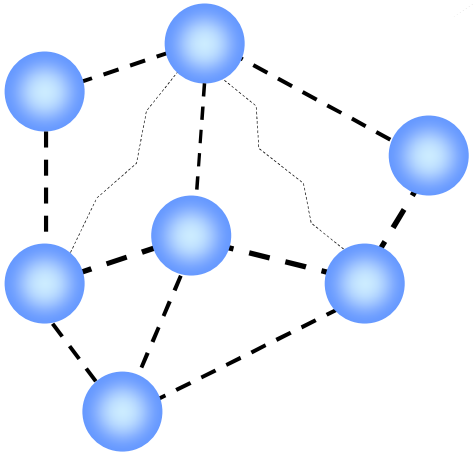
Deconstructing the dynamics

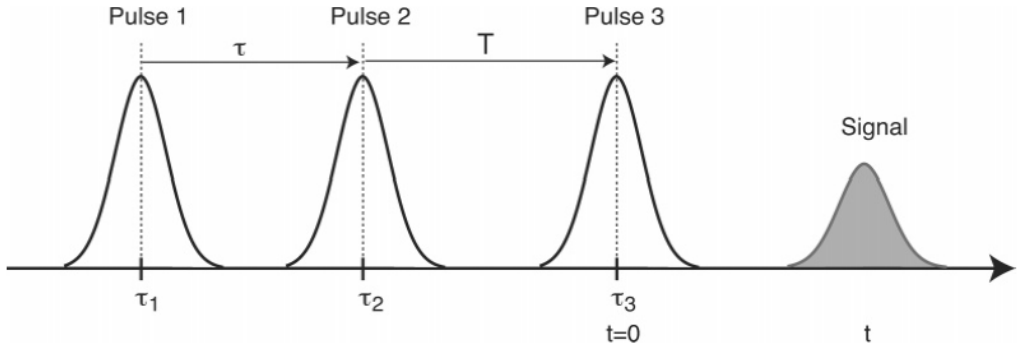
Deconstructing the dynamics

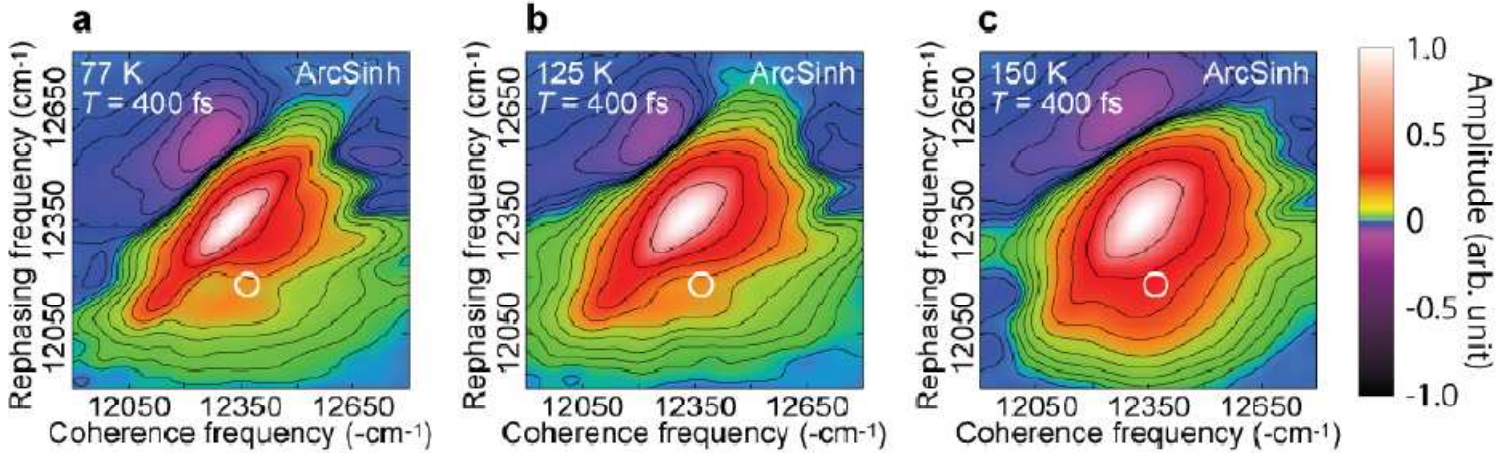


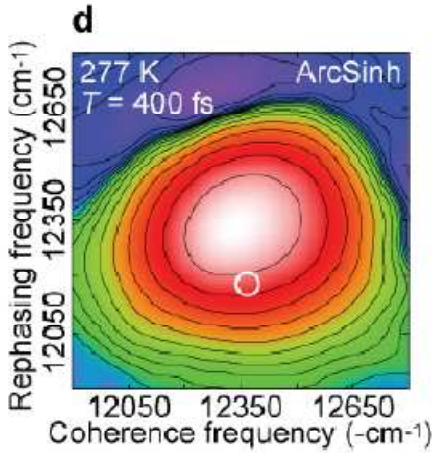


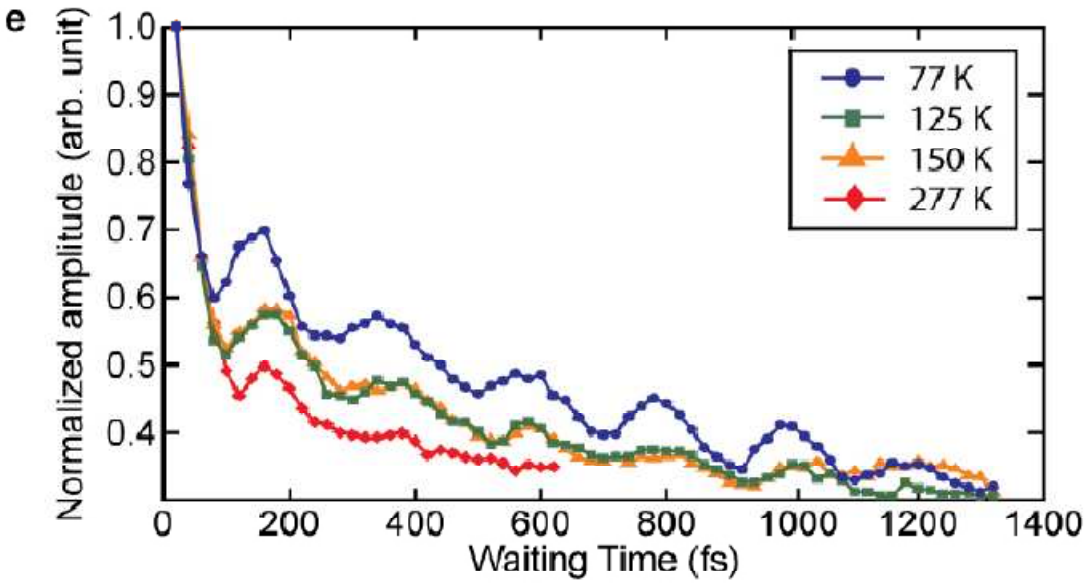












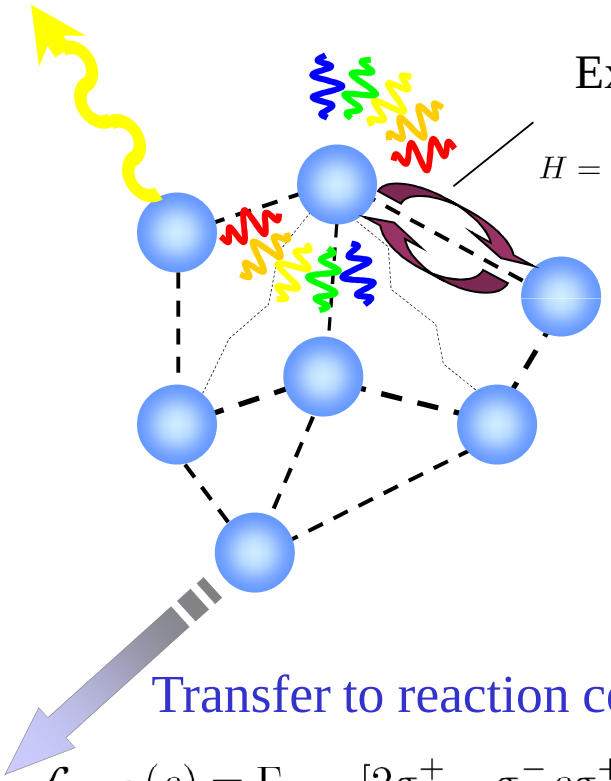
Engel et al, Science 2007
Panitchayangkoon et al, PNAS 2010

Coherent excitation transport

$$\mathcal{L}_{diss}(\rho) = \sum_{j=1}^{N} \Gamma_j [-\{\sigma_j^+ \sigma_j^-, \rho\} + 2\sigma_j^- \rho \sigma_j^+]$$

Loss of excitation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \mathcal{L}$$



Exchange of excitation

$$H = \sum_{j=1}^{N} \hbar\omega_j \sigma_j^+ \sigma_j^- + \sum_{j \neq l} \hbar v_{j,l} (\sigma_j^- \sigma_l^+ + \sigma_j^+ \sigma_l^-)$$

Transfer to reaction centre

$$\mathcal{L}_{sink}(\rho) = \Gamma_{N+1}[2\sigma_{N+1}^+ \sigma_k^- \rho \sigma_k^+ \sigma_{N+1}^- - \{\sigma_k^+ \sigma_{N+1}^- \sigma_{N+1}^+ \sigma_k^-, \rho\}]$$

Plenio & Huelga, New J. Phys. 2008
Caruso, Chin, Datta, Huelga, Plenio, J. Chem. Phys. 2009
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Mohseni, Rebentrost, Lloyd, Aspuru-Guzik, J. Phys. Chem. 2008
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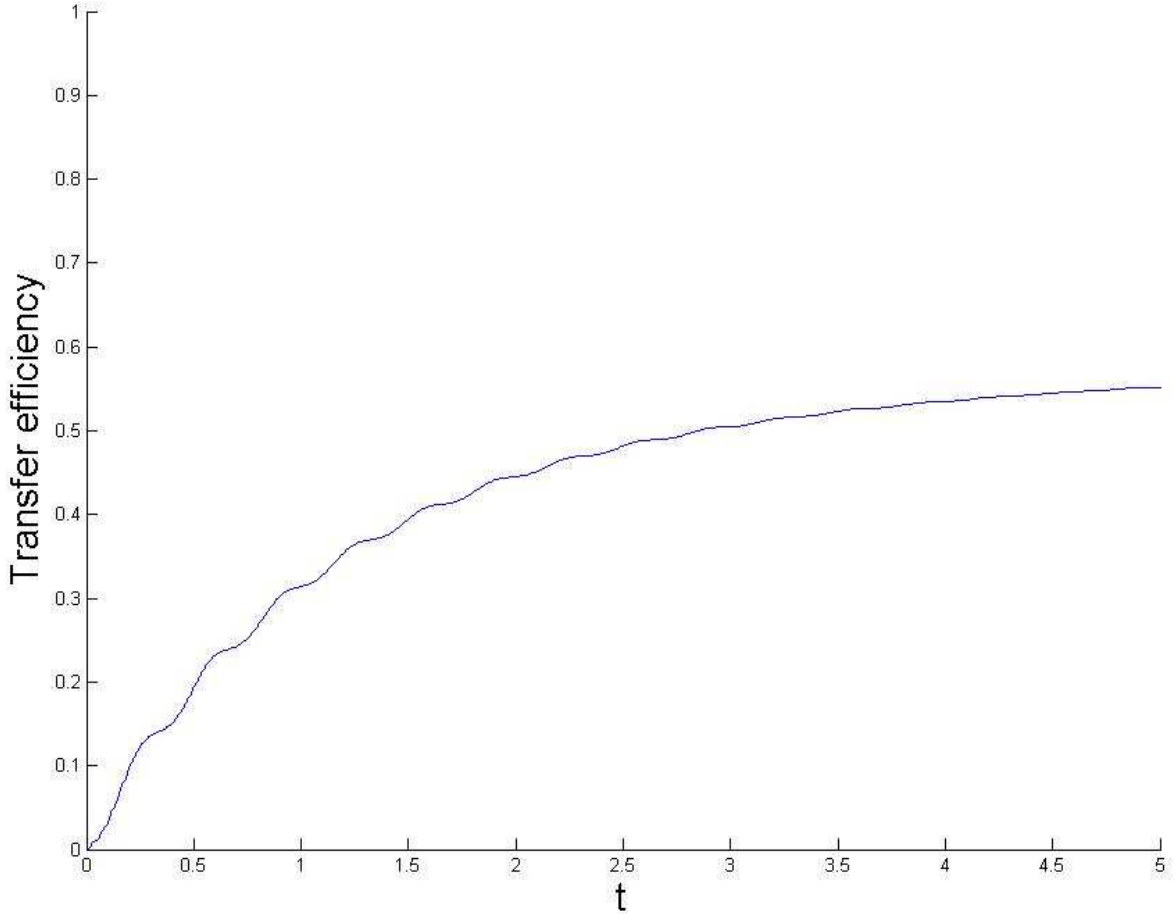
Coherent excitation transport



ge of excitation

$$\sigma_j^- + \sum_{j \neq l} \hbar v_{j,l} (\sigma_j^- \sigma_l^+ + \sigma_j^+ \sigma_l^-)$$

$$- \{\sigma_k^+ \sigma_{N+1}^- \sigma_{N+1}^+ \sigma_k^-, \rho\}]$$

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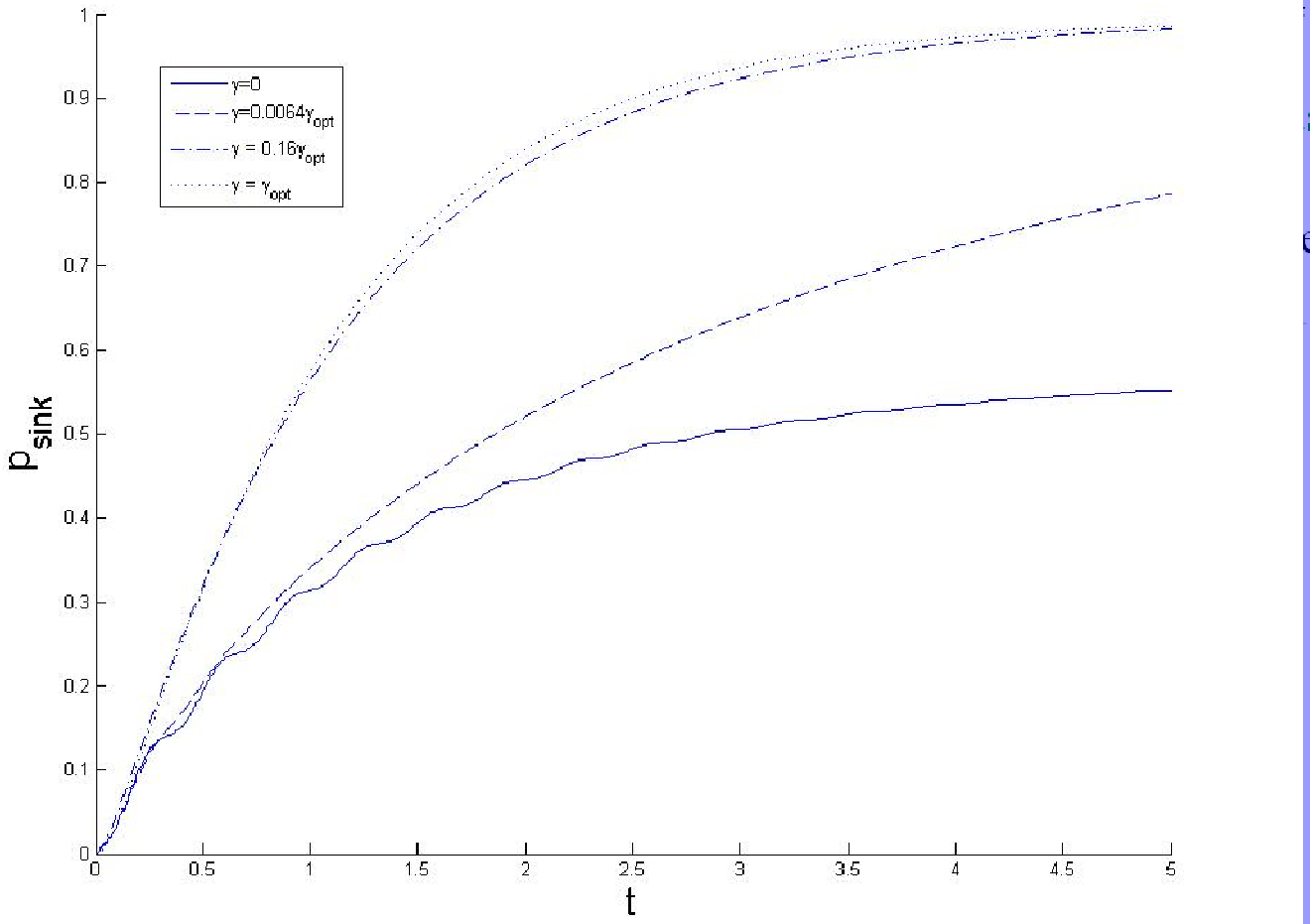
Coherence and noise for optimal transport

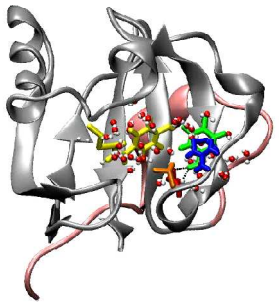


$, \rho\} + 2\sigma_j^+\sigma_j^-\rho\sigma_j^+\sigma_j^-]$

sing

e of excitation

$\sigma_j^- + \sum_{j\neq l}\hbar v_{j,l}(\sigma_j^-\sigma_l^+ + \sigma_j^+\sigma_l^-)$



$- \{\sigma_k^+\sigma_{N+1}^-\sigma_{N+1}^+\sigma_k^-, \rho\}]$

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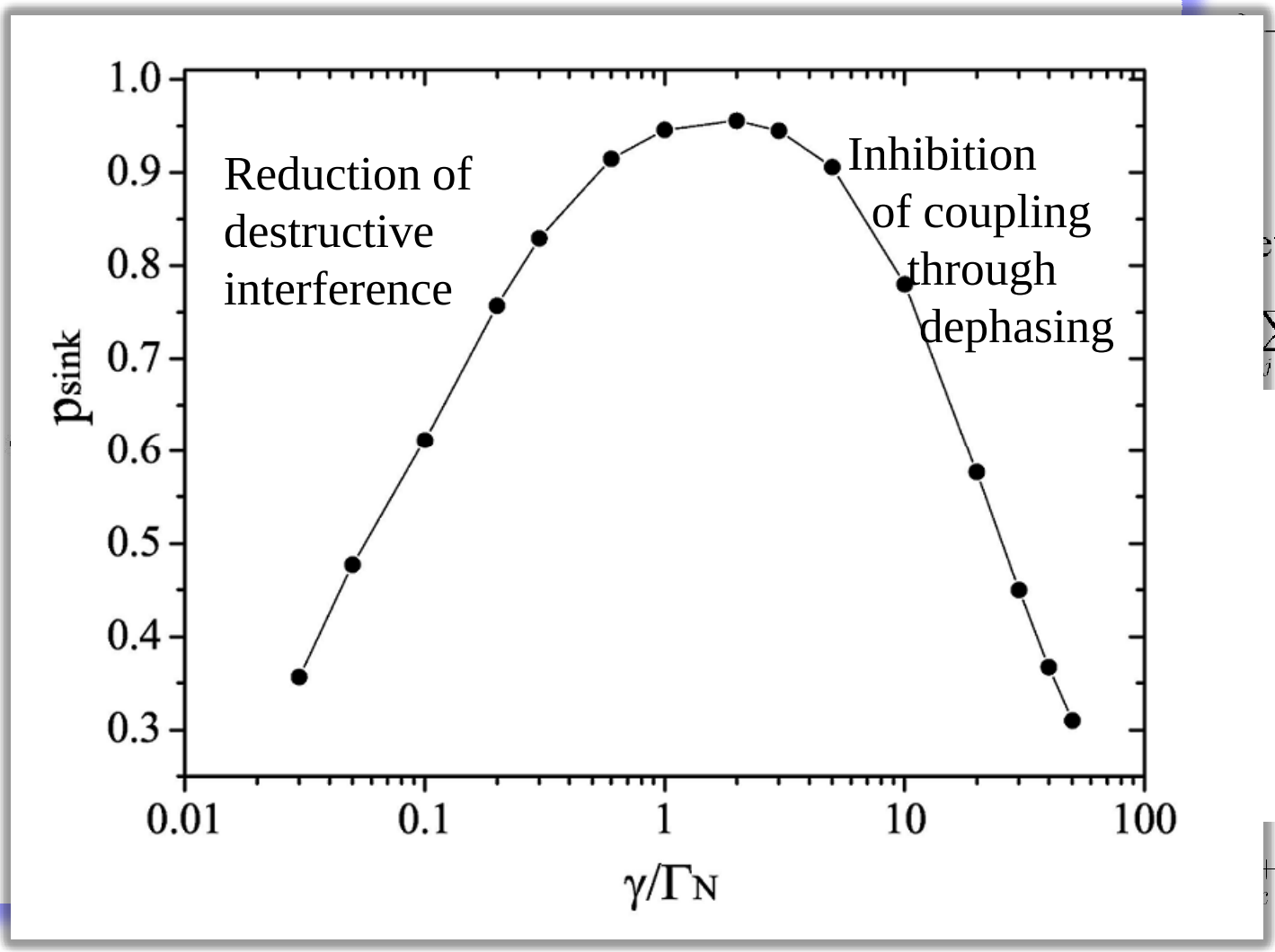
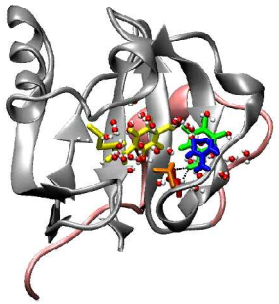


$+ 2\sigma_j^+\sigma_j^-\rho\sigma_j^+\sigma_j^-]$

excitation

$\sum_{j\neq l} \hbar v_{j,l}(\sigma_j^-\sigma_l^+ + \sigma_j^+\sigma_l^-)$



$\sigma_{N+1}^-\sigma_{N+1}^+\sigma_k^-, \rho\}]$

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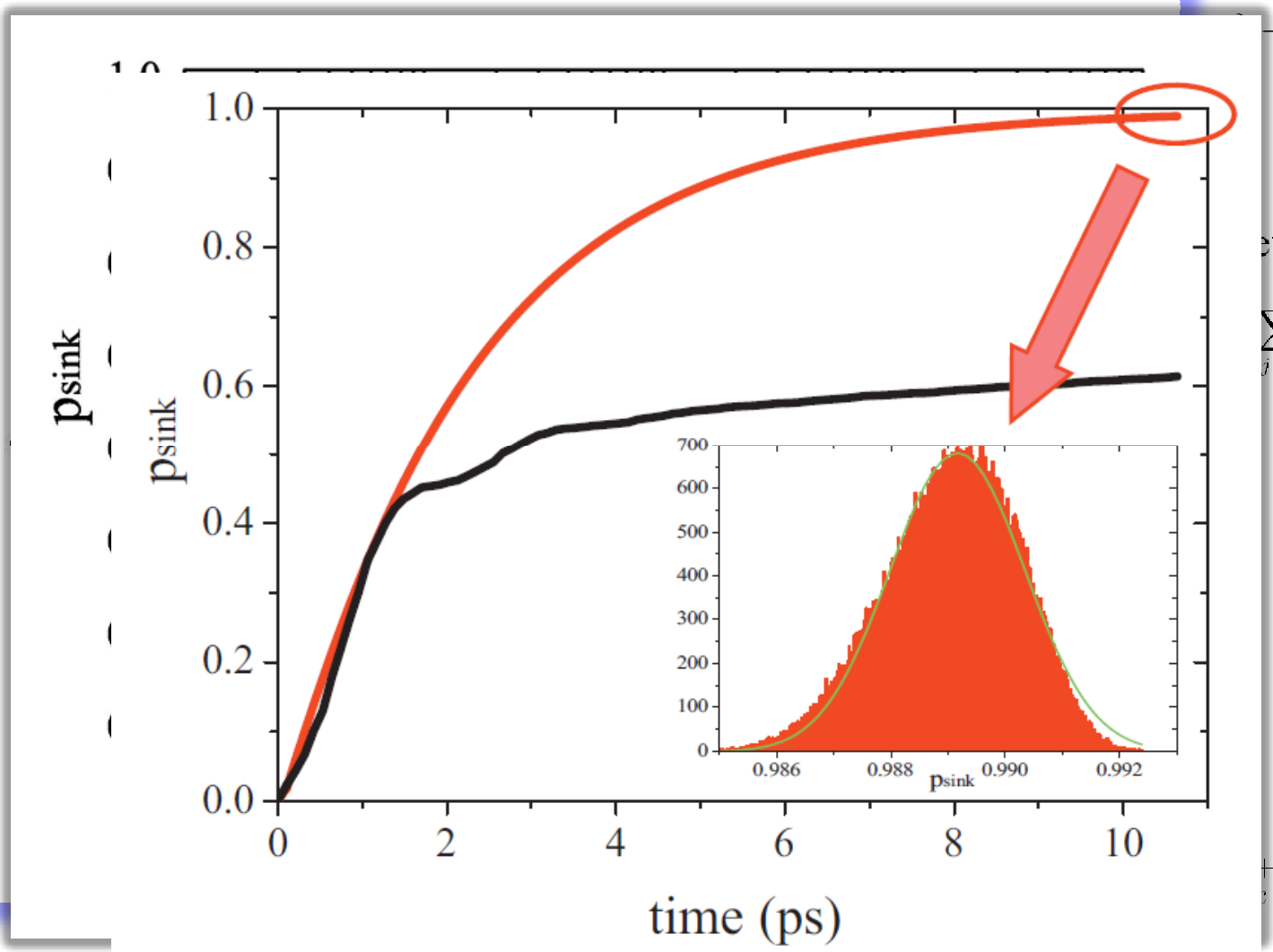
Coherence and noise for optimal & robust transport



$+ 2\sigma_j^+\sigma_j^-\rho\sigma_j^+\sigma_j^-]$

xcitation

$\sum_{j\neq l}\hbar v_{j,l}(\sigma_j^-\sigma_l^+ + \sigma_j^+\sigma_l^-)$

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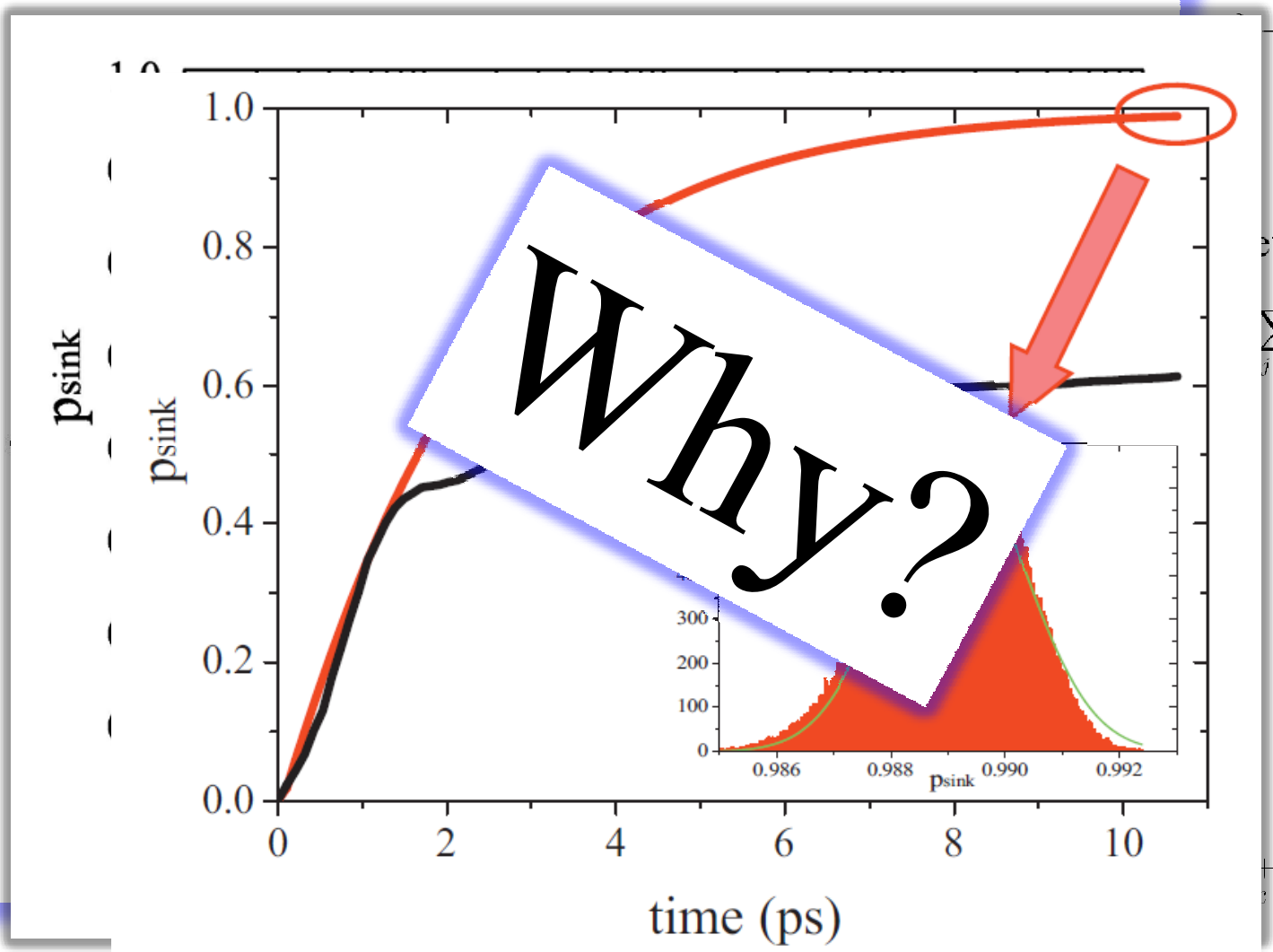

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Deconstructing the dynamics

Opinion: This is obvious

$$H = \begin{pmatrix} 215 & -104.1 & 5.1 & -4.3 & 4.7 & -15.1 & -7.8 \\ -104.1 & 220.0 & 32.6 & 7.1 & 5.4 & 8.3 & 0.8 \\ 5.1 & 32.6 & 0.0 & -46.8 & 1.0 & -8.1 & 5.1 \\ -4.3 & 7.1 & -46.8 & 125.0 & -70.7 & -14.7 & -61.5 \\ 4.7 & 5.4 & 1.0 & -70.7 & 450.0 & 89.7 & -2.5 \\ -15.1 & 8.3 & -8.1 & -14.7 & 89.7 & 330.0 & 32.7 \\ -7.8 & 0.8 & 5.1 & -61.5 & -2.5 & 32.7 & 280.0 \end{pmatrix}$$

Site basis

Deconstructing the dynamics

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Site basis

$$H = \begin{pmatrix} 513 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 332 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 307 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 268 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 121 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 102 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -23 \end{pmatrix}$$

Exciton basis

⇓

No coherent dynamics left

⇓

Noise supports transport

Deconstructing the dynamics

Opinion: This is obvious

$$H = \begin{pmatrix} 215 & -104.1 & 5.1 & -4.3 & 4.7 & -15.1 & -7.8 \\ -104.1 & 220.0 & 32.6 & 7.1 & 5.4 & 8.3 & 0.8 \\ 5.1 & 32.6 & 0.0 & -46.8 & 1.0 & -8.1 & 5.1 \\ -4.3 & 7.1 & -46.8 & 125.0 & -70.7 & -14.7 & -61.5 \\ 4.7 & 5.4 & 1.0 & -70.7 & 450.0 & 89.7 & -2.5 \\ -15.1 & 8.3 & -8.1 & -14.7 & 89.7 & 330.0 & 32.7 \\ -7.8 & 0.8 & 5.1 & -61.5 & -2.5 & 32.7 & 280.0 \end{pmatrix}$$

Site basis

$$H = \begin{pmatrix} 513 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 332 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 307 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 268 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 121 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 102 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -23 \end{pmatrix}$$

Exciton basis

⇓

No coherent dynamics left

⇓

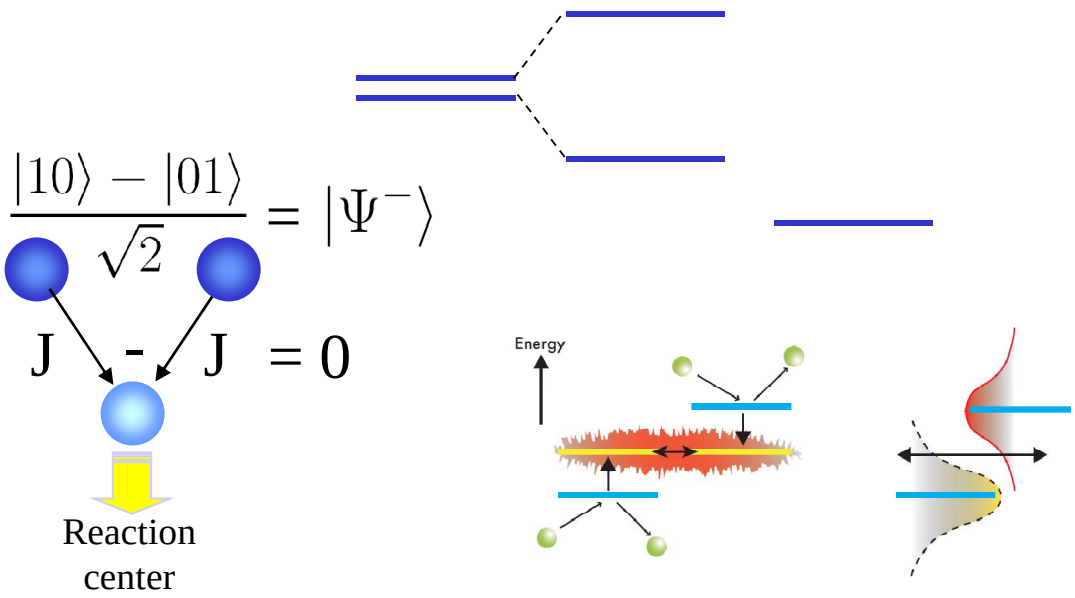
Noise supports transport

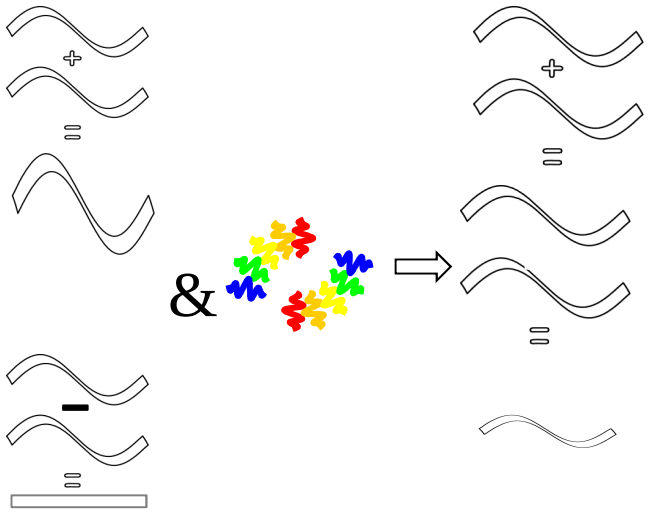
But: Answer depends on structure of network

Sometimes noise helps
sometimes it hinders transport

Deconstructing the dynamics

Deconstructing the dynamics





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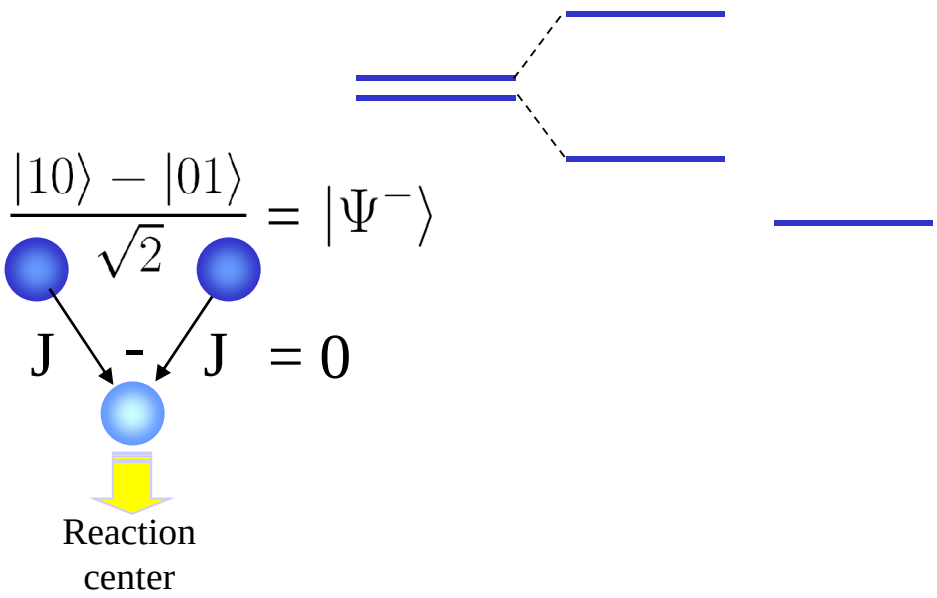
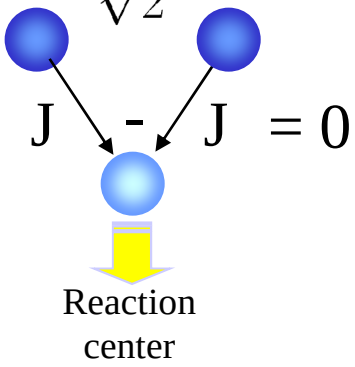
Chin, Huelga, Plenio, Phil. Trans. Roy. Soc. 2011

Deconstructing the dynamics



Plenio & Huelga, New J. Phys. 2008
Caruso, Chin, Datta, Huelga, Plenio, J. Chem. Phys. 2009
Chin, Caruso, Datta, Huelga, Plenio, New J. Phys. 2010
Chin, Huelga, Plenio, Phil. Trans. Roy. Soc. 2011

$$\frac{|10\rangle - |01\rangle}{\sqrt{2}} = |\Psi^-\rangle$$



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Chin, Caruso, Datta, Huelga, Plenio, New J. Phys. 2010
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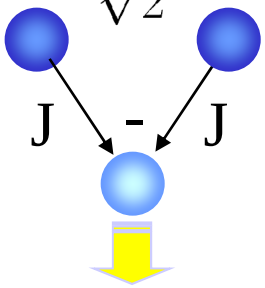
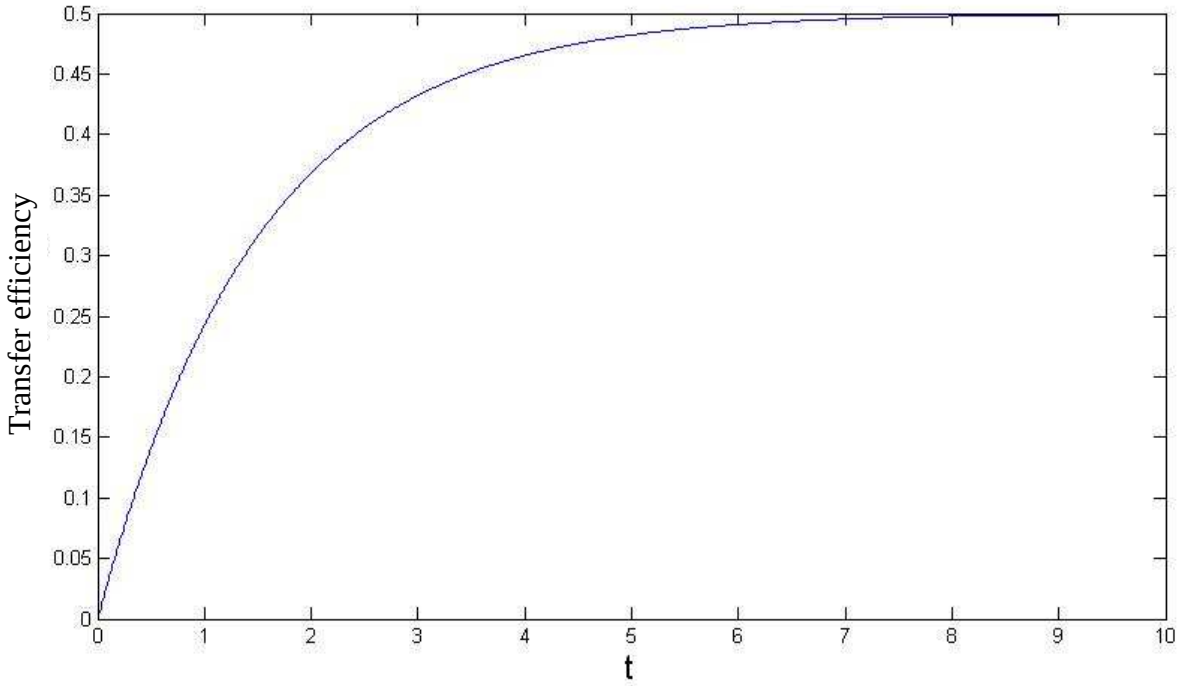
$$\frac{|10\rangle - |01\rangle}{\sqrt{2}} = |\Psi^-\rangle$$



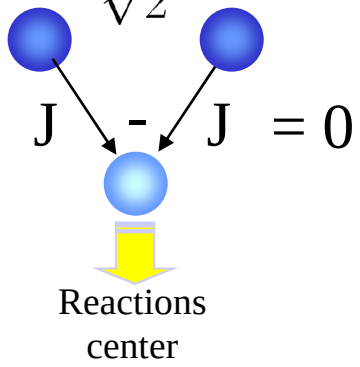
$$|01\rangle = \frac{1}{\sqrt{2}}\left[\frac{|01\rangle - |10\rangle}{\sqrt{2}} + \frac{|01\rangle + |10\rangle}{\sqrt{2}}\right]$$

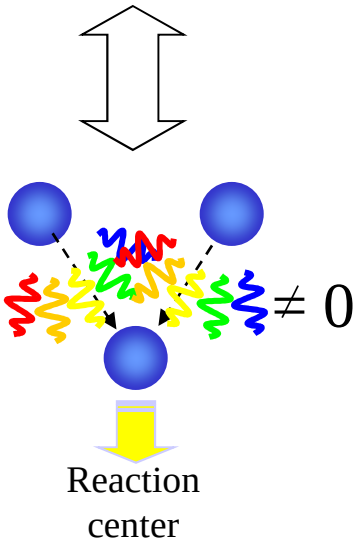
$$\Downarrow$$

$$\rho = \frac{1}{2}|\psi^-\rangle\langle\psi^-| + \frac{1}{2}|RC\rangle\langle RC|$$



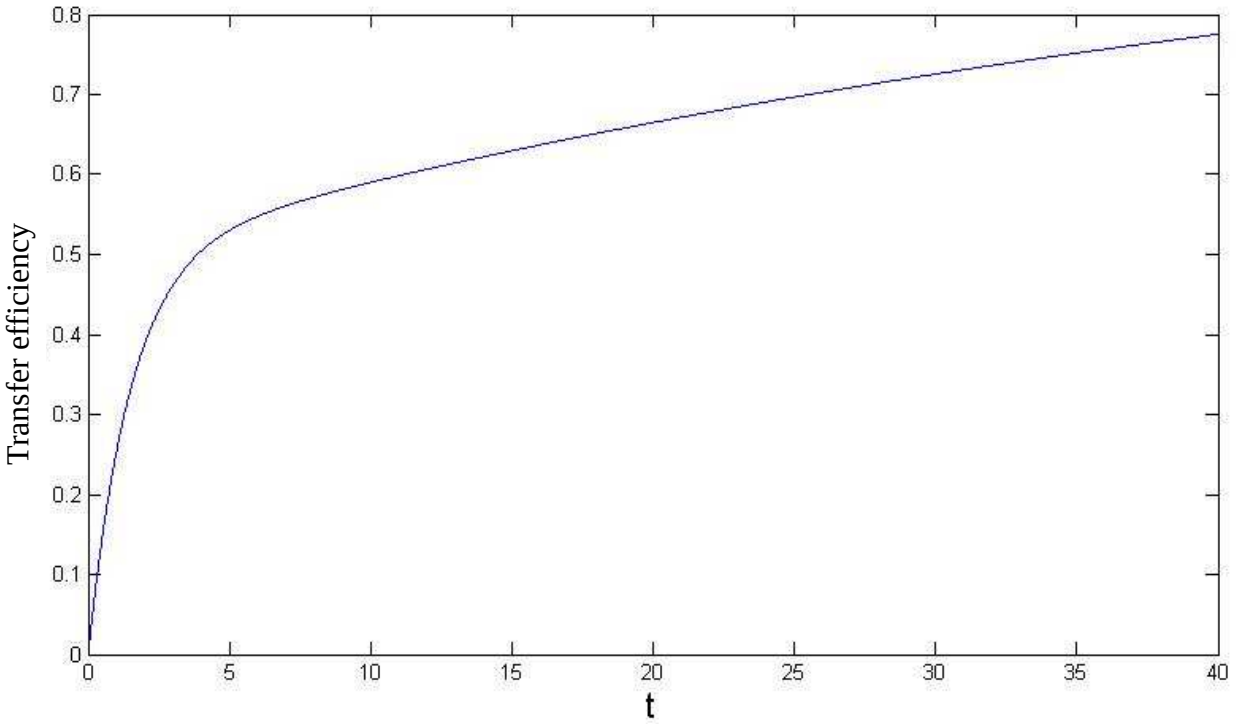
$$\frac{|10\rangle - |01\rangle}{\sqrt{2}} = |\Psi^-\rangle$$

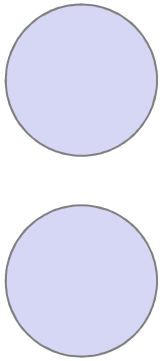


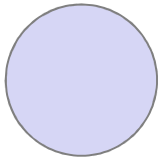


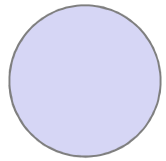
Reduction of destructive interference

Add noise to sacrifice some good coherence (slight slowdown) to fight the bad coherence (higher speed up).

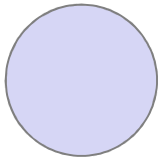


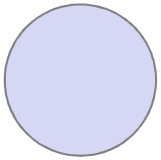


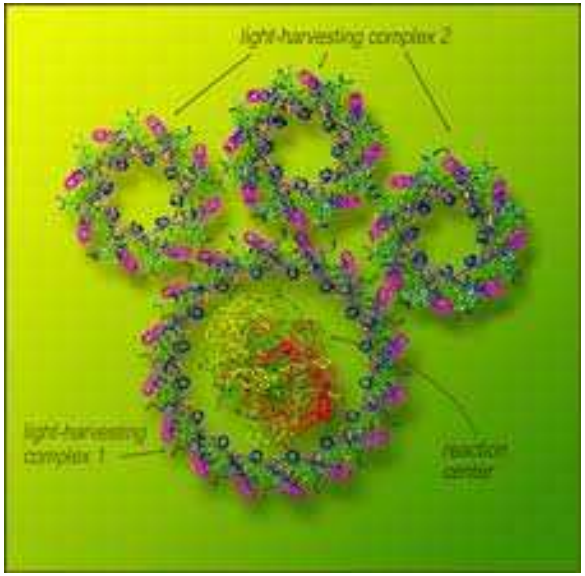


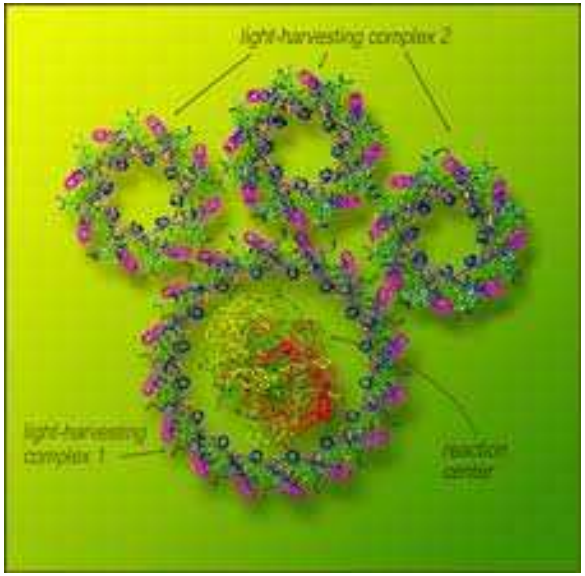


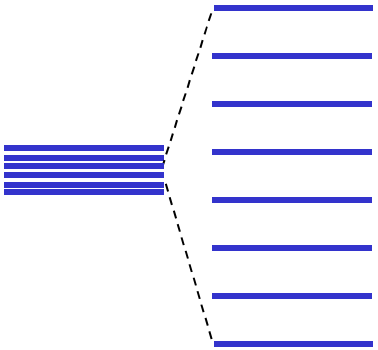
With noise



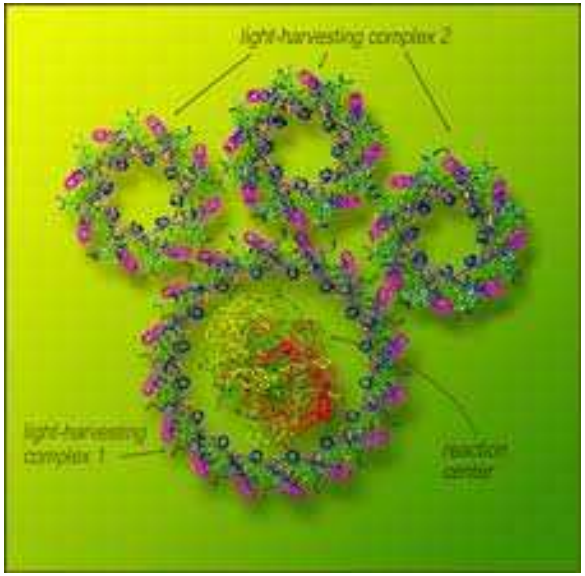


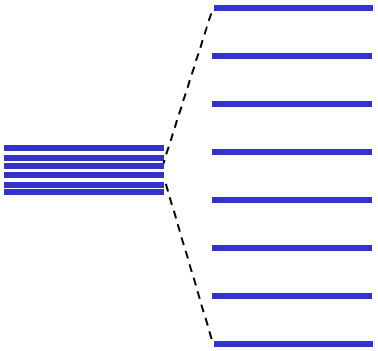

light-harvesting complex 2
light-harvesting complex 1
reaction center



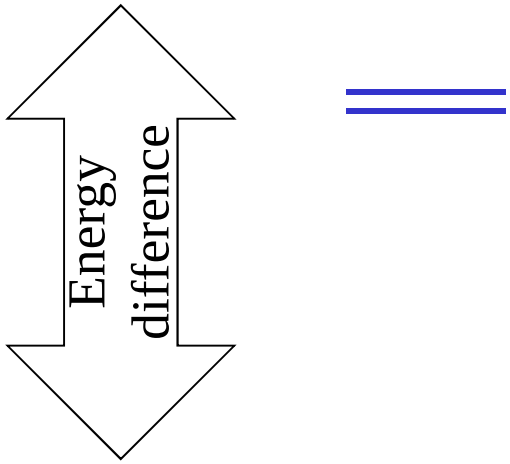


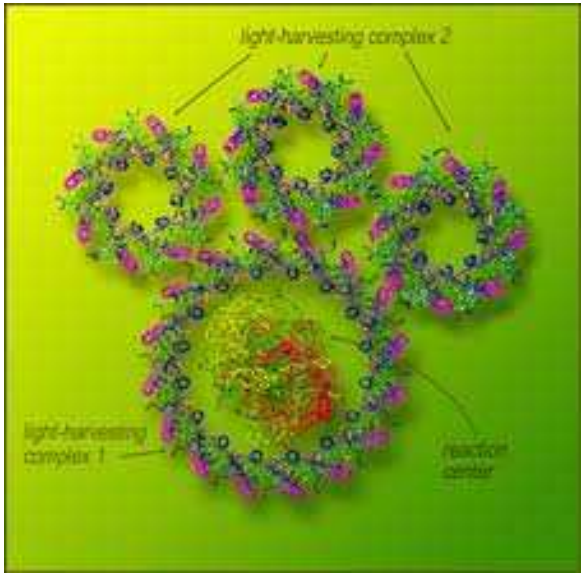
Antennae absorbs over broader range of frequencies

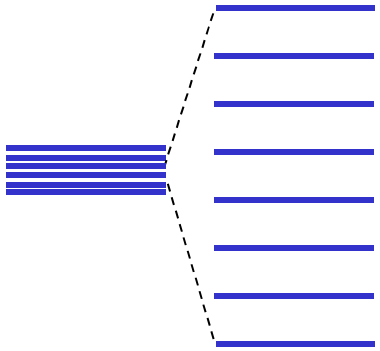




Antennae absorbs over broader range of frequencies

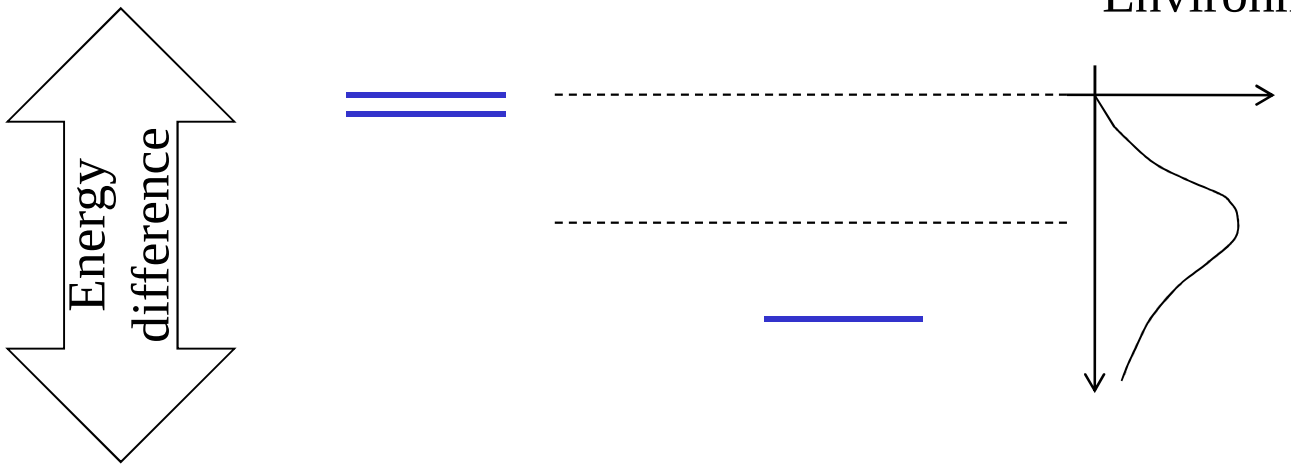


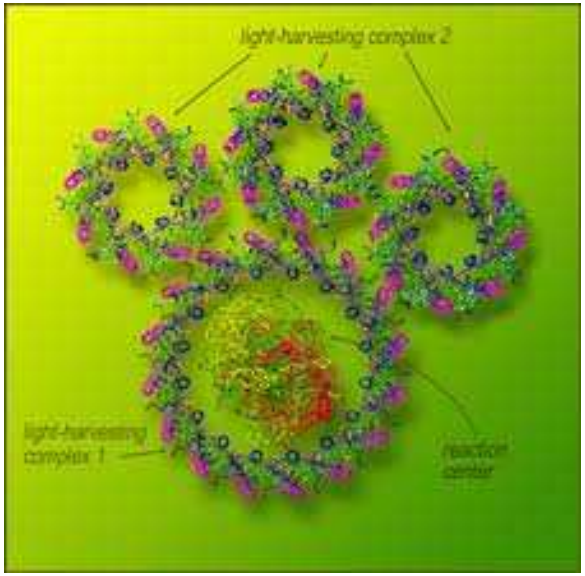


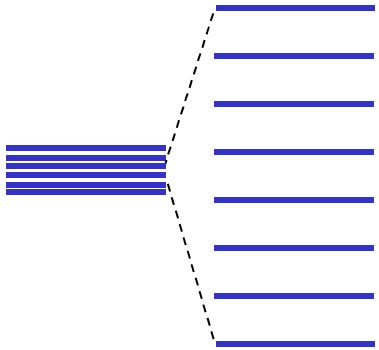


Antennae absorbs over broader range of frequencies

Environment spectral density

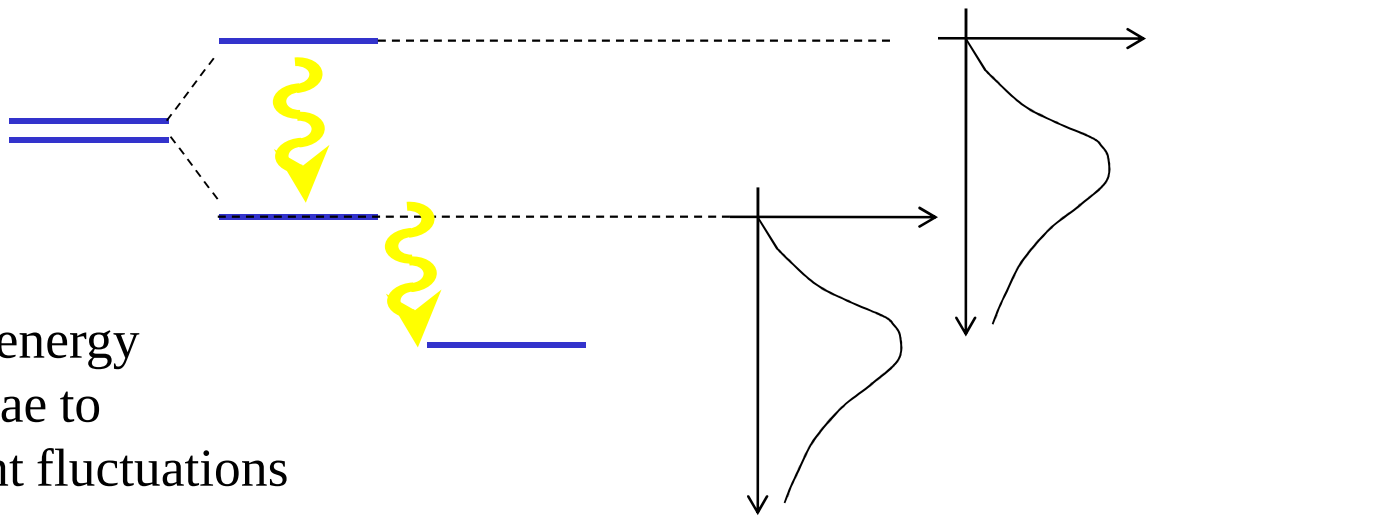




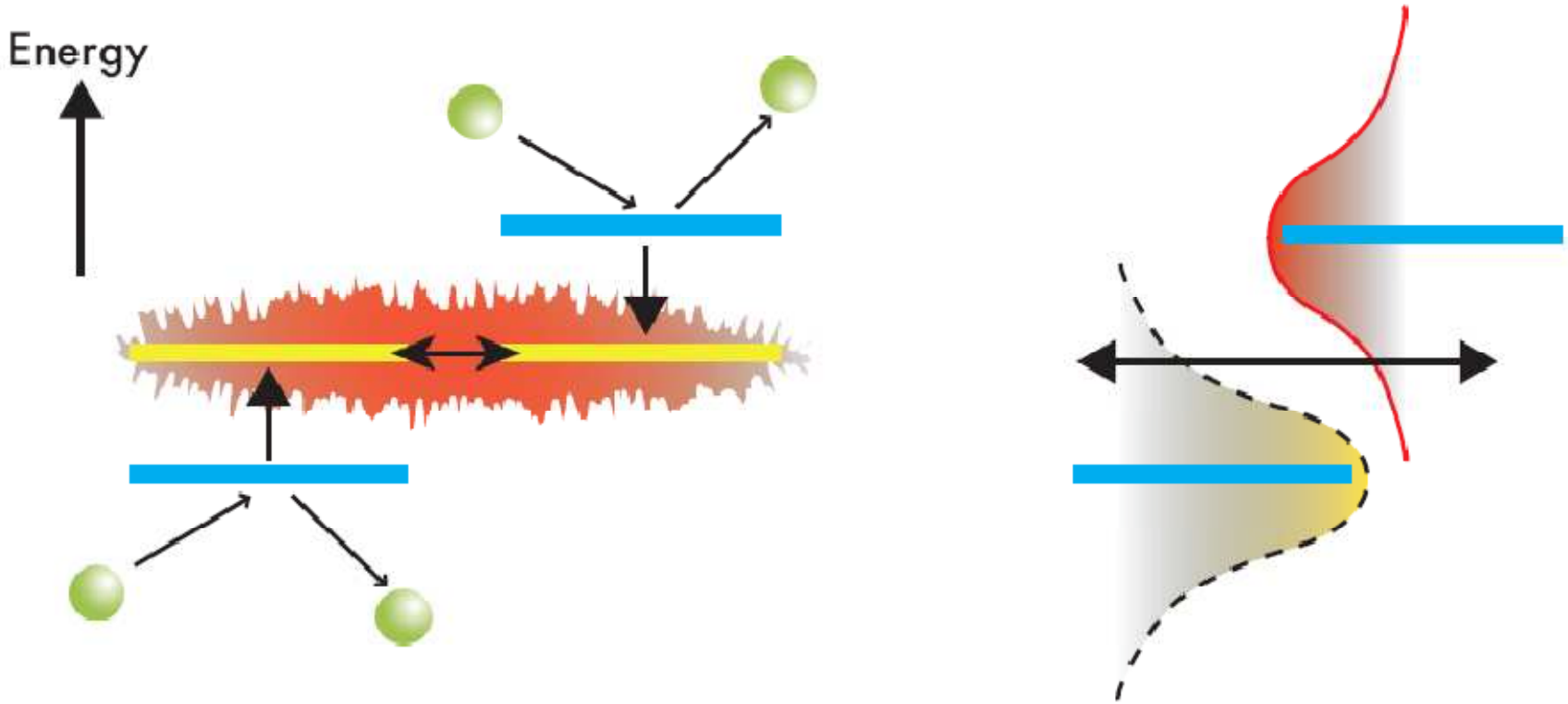


Antennae absorbs over broader range of frequencies

Environment spectral density



Coherently shifted energy levels act as antennae to harvest environment fluctuations

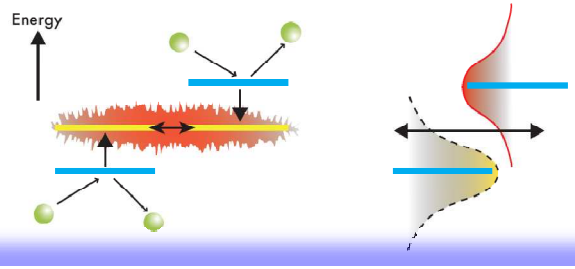

Energy

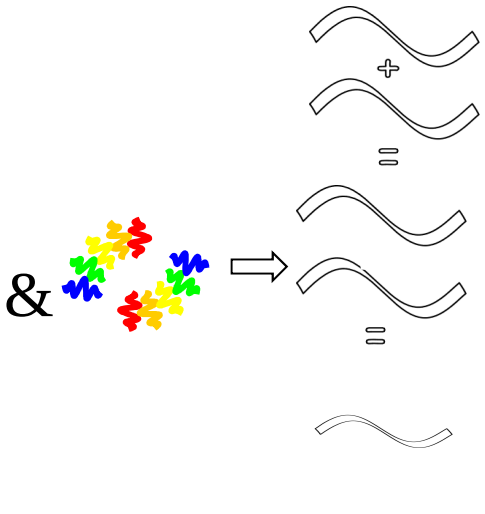
Deconstructing the dynamics

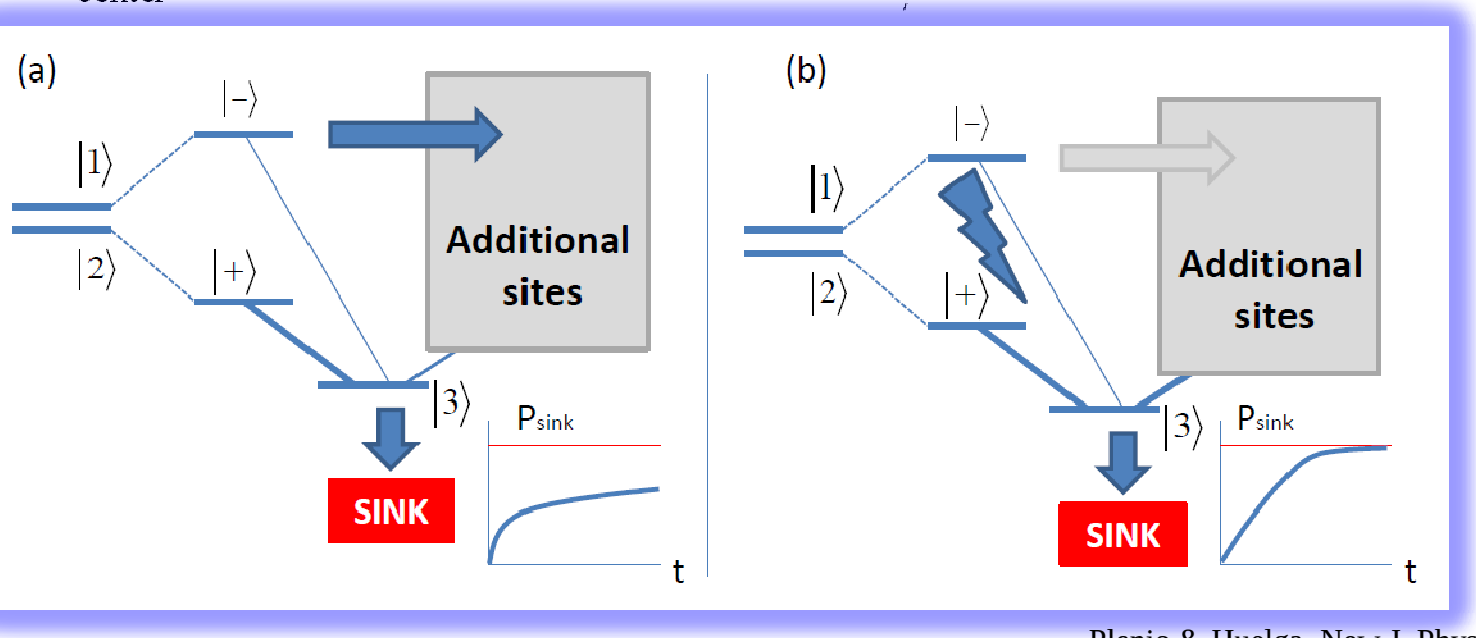
$$\frac{|10\rangle - |01\rangle}{\sqrt{2}} = |\Psi^-\rangle$$

J - J = 0

Reaction center







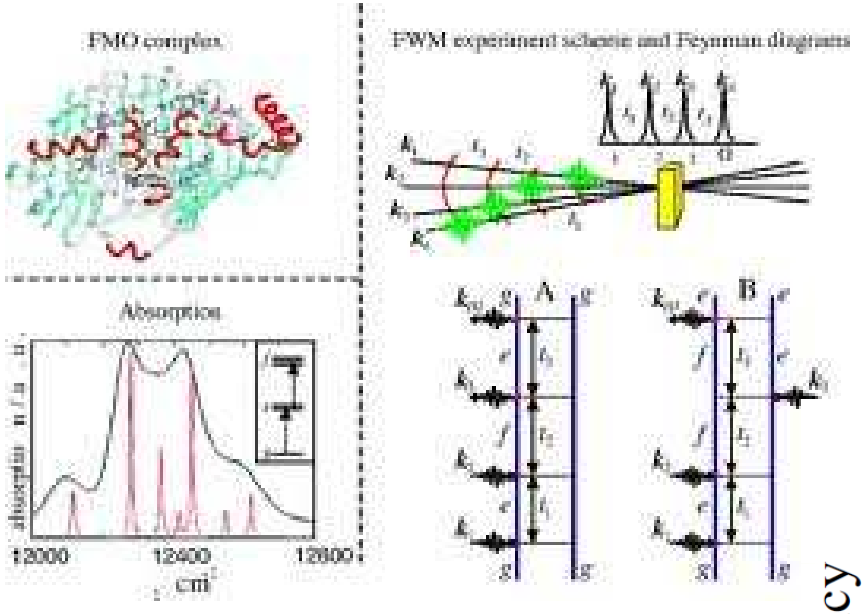
Plenio & Huelga, New J. Phys. 2008
Caruso, Chin, Datta, Huelga, Plenio, J. Chem. Phys. 2009
Chin, Caruso, Datta, Huelga, Plenio, New J. Phys. 2010
Chin, Huelga, Plenio, Phil. Trans. Roy. Soc. 2011

$$H = \begin{pmatrix} 215 & -104.1 & 5.1 & -4.3 & 4.7 & -15.1 & -7.8 \\ -104.1 & 220.0 & 32.6 & 7.1 & 5.4 & 8.3 & 0.8 \\ 5.1 & 32.6 & 0.0 & -46.8 & 1.0 & -8.1 & 5.1 \\ -4.3 & 7.1 & -46.8 & 125.0 & -70.7 & -14.7 & -61.5 \\ 4.7 & 5.4 & 1.0 & -70.7 & 450.0 & 89.7 & -2.5 \\ -15.1 & 8.3 & -8.1 & -14.7 & 89.7 & 330.0 & 32.7 \\ -7.8 & 0.8 & 5.1 & -61.5 & -2.5 & 32.7 & 280.0 \end{pmatrix}$$

where we have shifted the zero of energy by 12 230 (all numbers are given in the units of $1.988\,865 \times 10^{-23}$ nm $= 1.2414 \times 10^{-4}$ eV) for all sites corresponding to a wavelength of $\cong$800 nm.

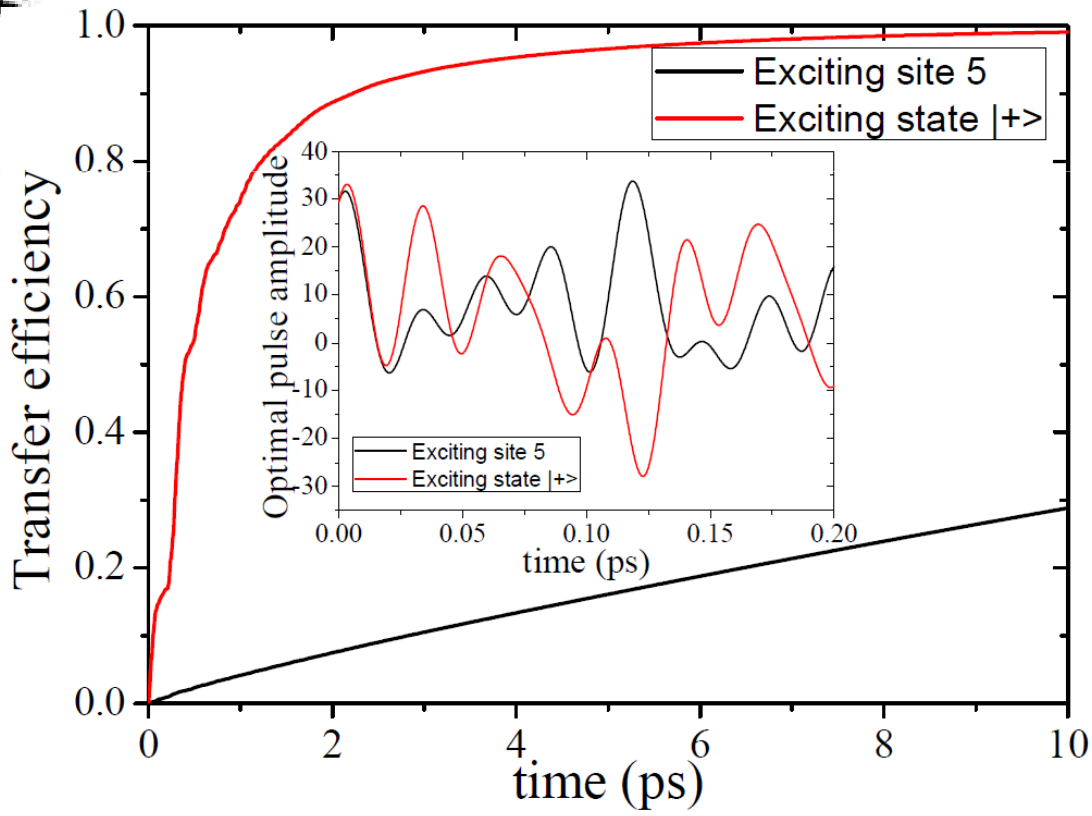
Can test the relevance of structural elements for dynamics by selectively adding noise in computer simulation, but ...

... test in real system would be more convincing



Prepare initial states and control dynamics for strongest separation in signal for different hypotheses

Sites are not spectrally resolved hence laser pulses need to be shaped optimally.



Caruso, Montangero, Calarco, Huelga, Plenio, arxiv:1103.0929

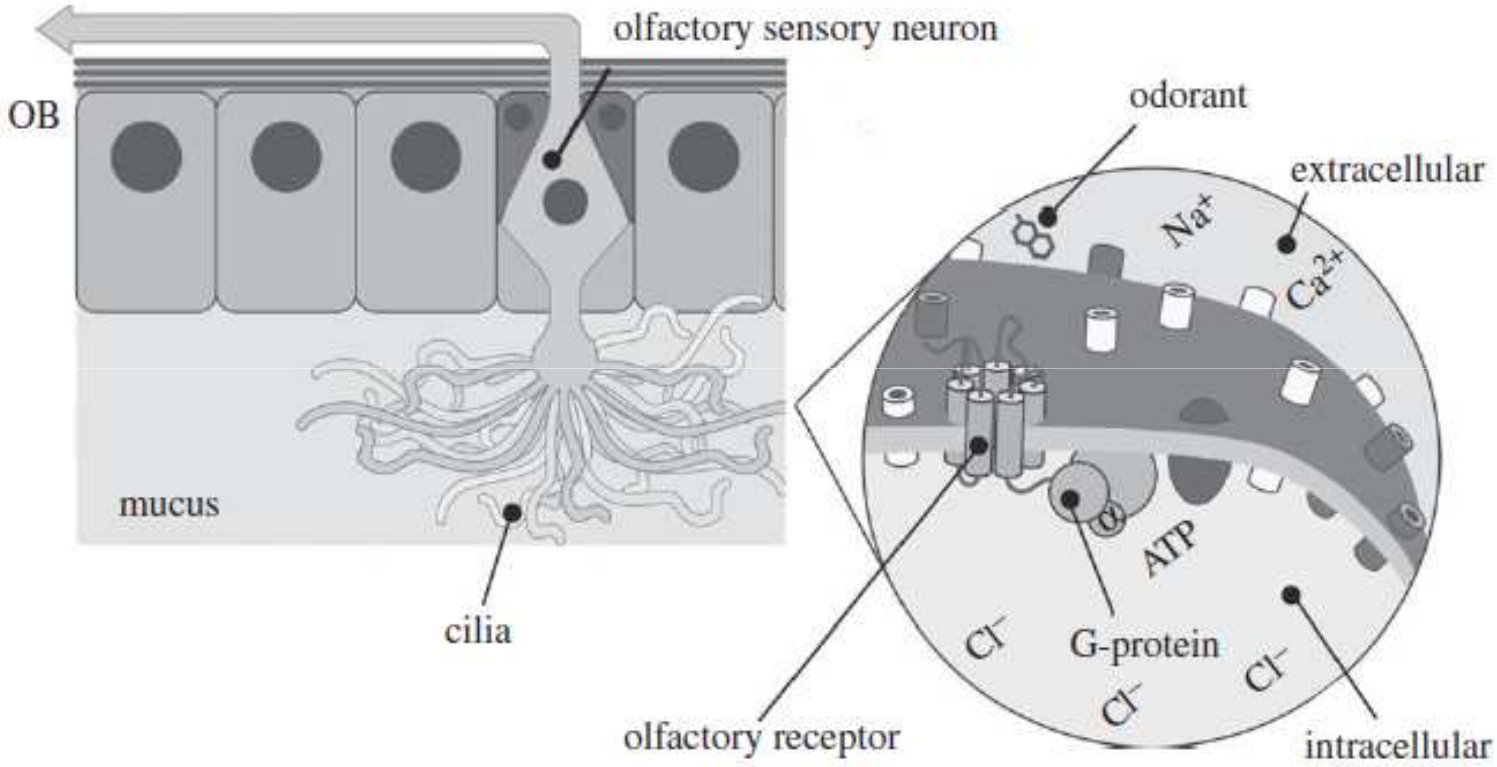
Observe Nature to discover the design principles of network dynamics in strong contact with environment

Engineer system to generate constructive interplay between quantum dynamics and noise for optimal performance in man-made nanostructures.

Build an artificial leaf

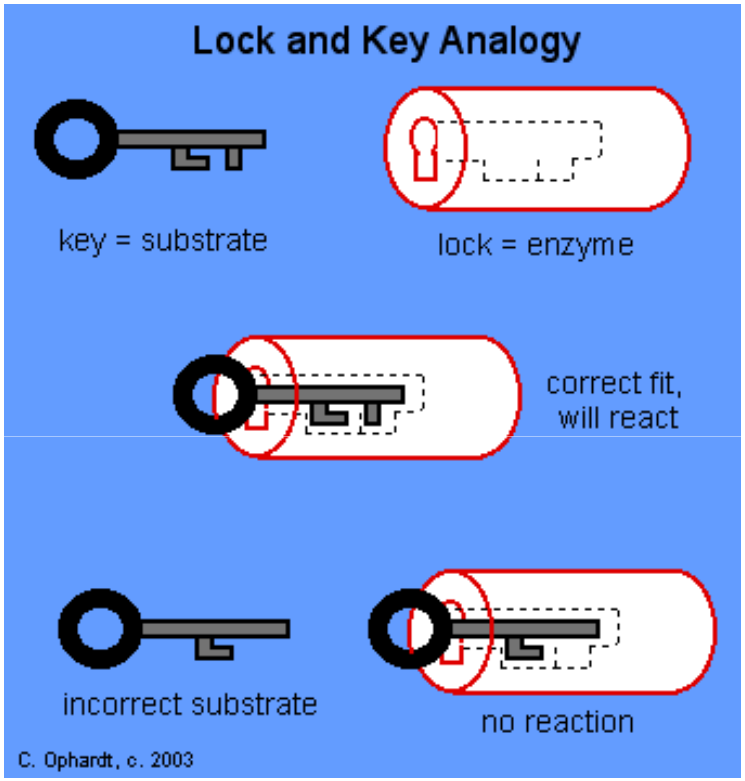
Electron Tunneling and Olfaction

How does smell work?

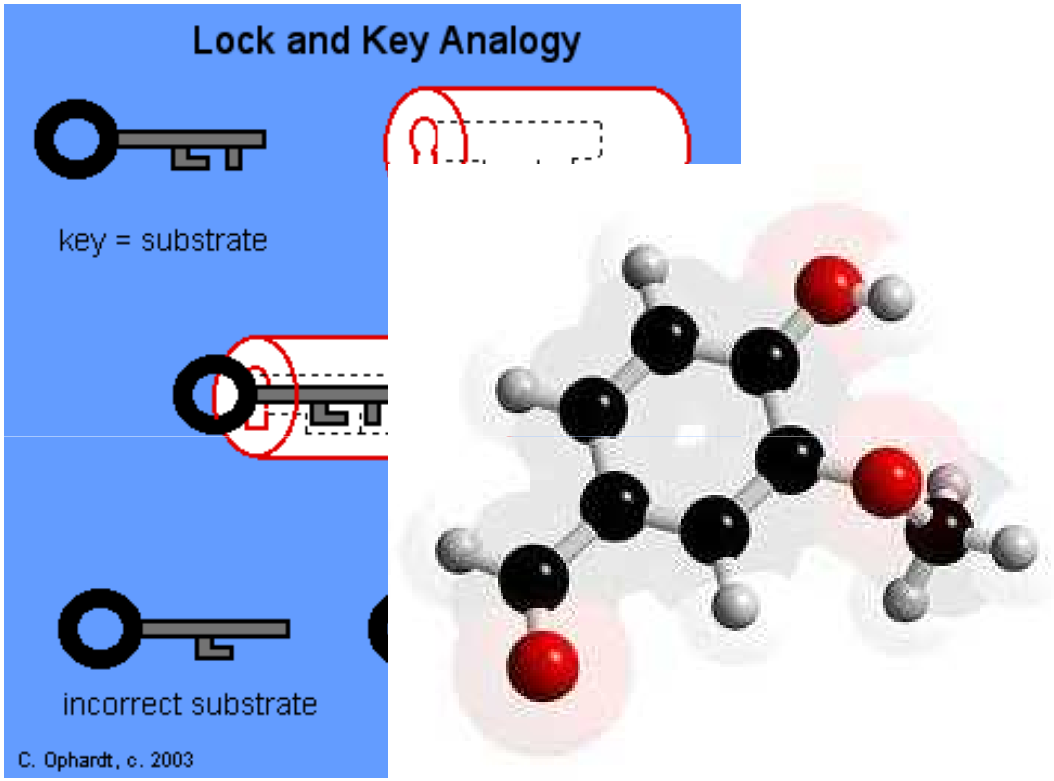


Different receptors are sensitive to different scents, but how ?

Lock and key: Receptors chose shape of molecule

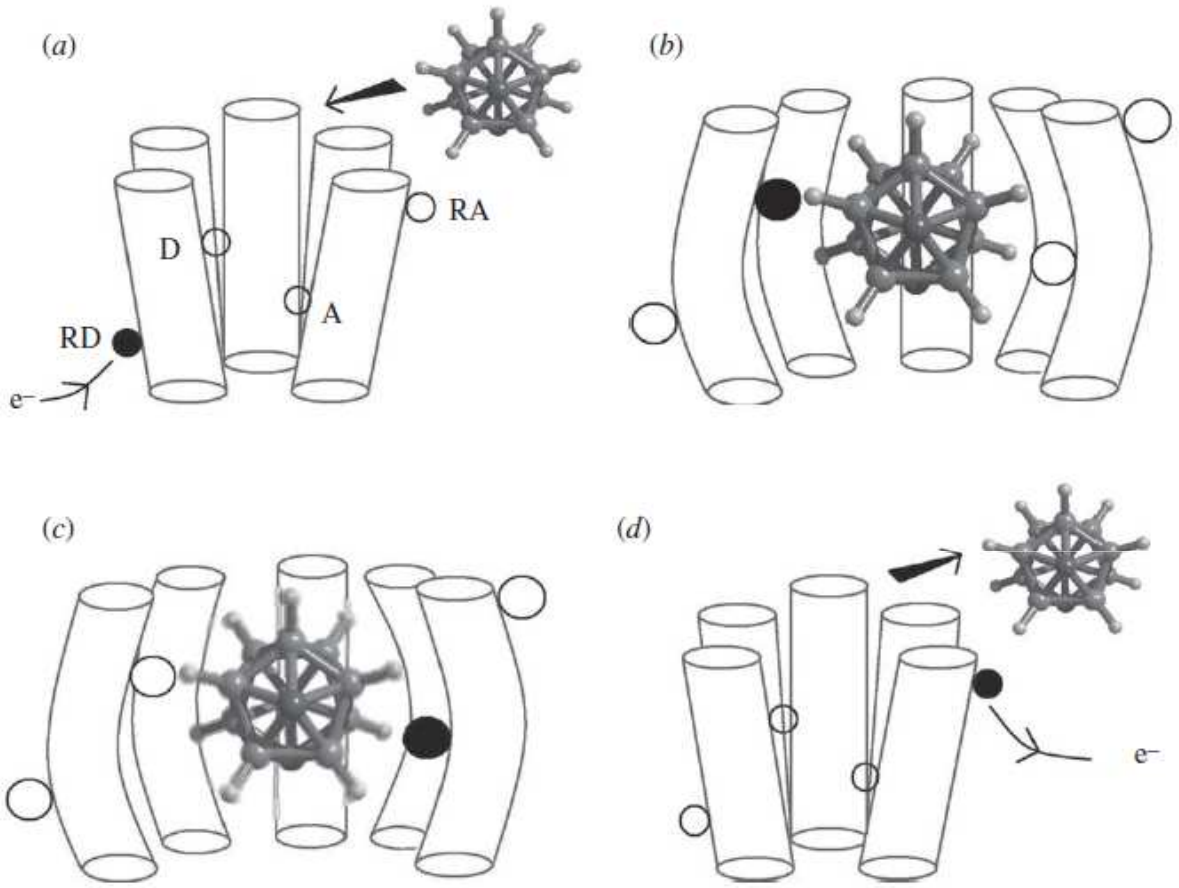


Lock and key: Receptors chose shape of molecule



Weakness: Odorants are small molecules, often very similar in shape

Replace hydrogen by deuterium, should smell the same
but does not appear so.



Odorant docks at receptor (maybe shape sensitive),

then

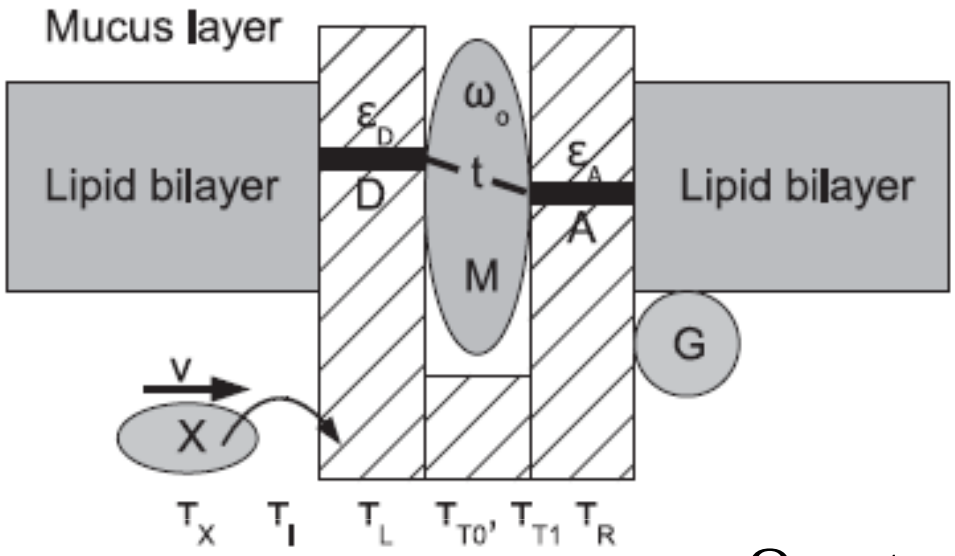
Phonon assisted electron transfer

Is

Sensitive to phonon spectrum of molecule

Test: Can you smell deuterium ? It seems drosophila can !

Turin, Chem. Senses 21, 773 (1996)

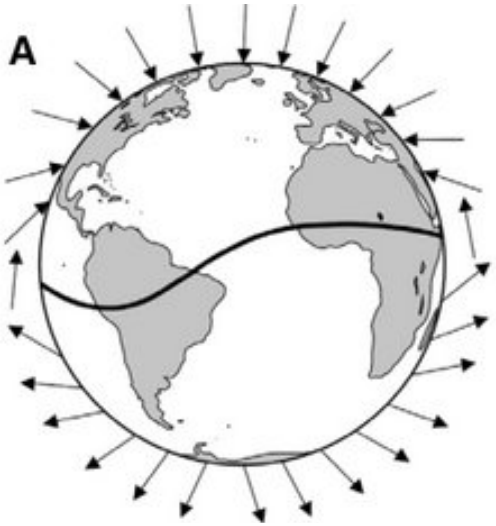


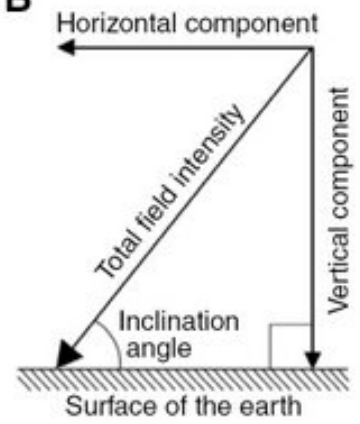
Quantum Theory of phonon-assisted electron tunneling confirms that the theory is at least theoretically plausible.

Summary: Some points in favour of Turins theory but no conclusive decision yet. Correct theory might well be a happy marriage between different approaches.

Brookes, Hartoutsiou, Horsfield and Stoneham, Phys. Rev. Lett. 98, 038101 (2007)

Spin Chemistry for Bird Navigation





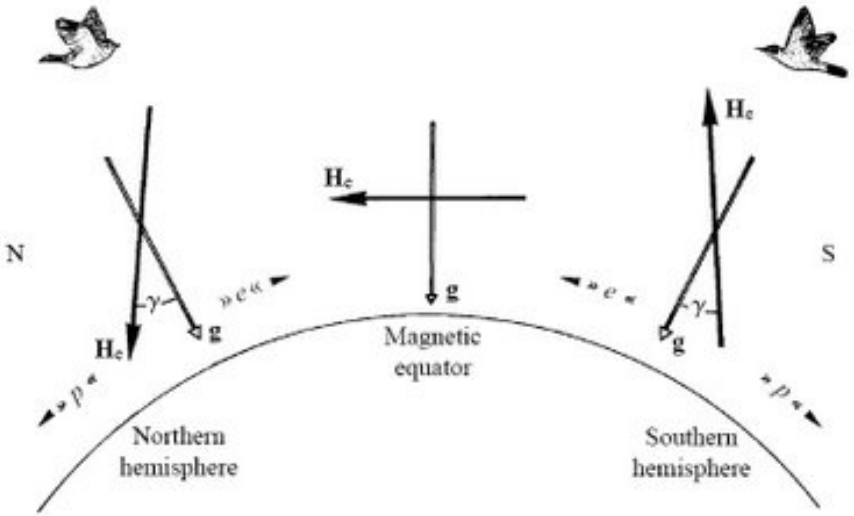
Northern autumn
September, October,
November

Southern autumn
March, April, May

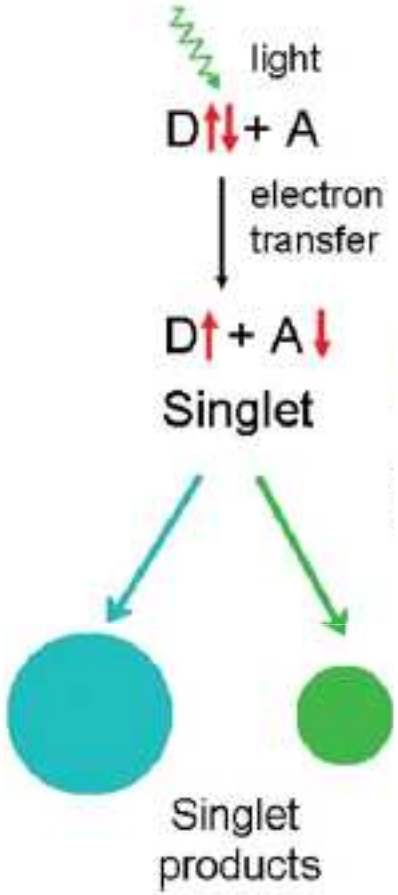
Birds and other animals sense the magnetic field.

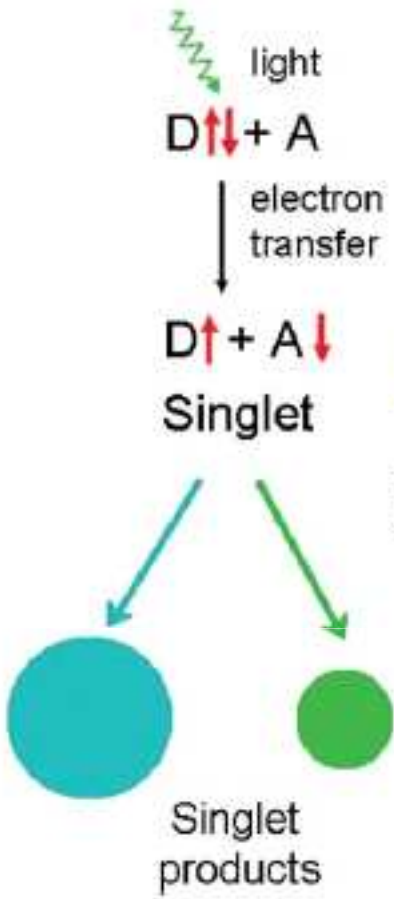
How do they do this ?

- Magnetic particles
- Chemical compass



Wiltschko & Wiltschko since the 1960‘s


light
D↑↓ + A
electron
transfer
D↑ + A↓
Singlet
Singlet
products

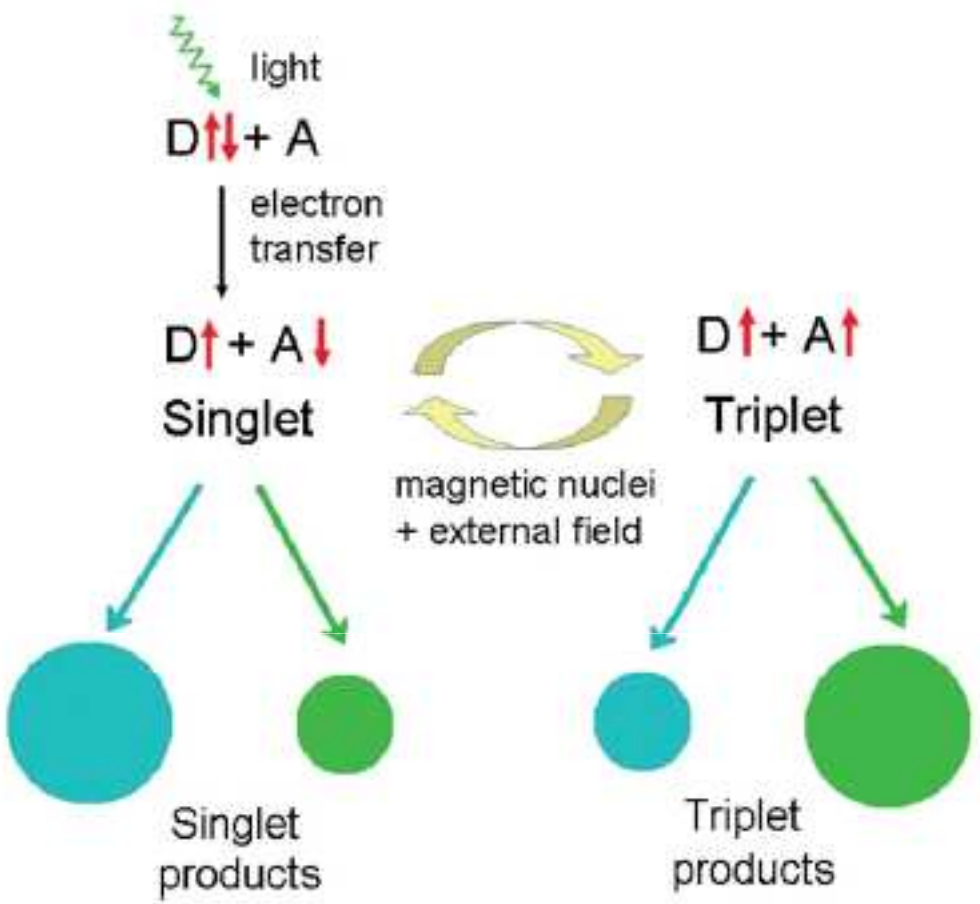


$$H = \sum_{k=A,D} H_k = -\gamma_e \sum_k \vec{B}_k \cdot \vec{S}_k + \sum_{k,j} \vec{S}_k \cdot \hat{\lambda}_{k_j} \cdot \vec{I}_{k_j}$$

Electron spins

Nuclear spins

Ritz, T., S. Adem, and K. Schulten., Biophys. J. 78:707–718 (2000)



Photon absorption leads to creation of radical pair

Initially in singlet state, internal and external magnetic fields lead to singlet-triplet interconversion

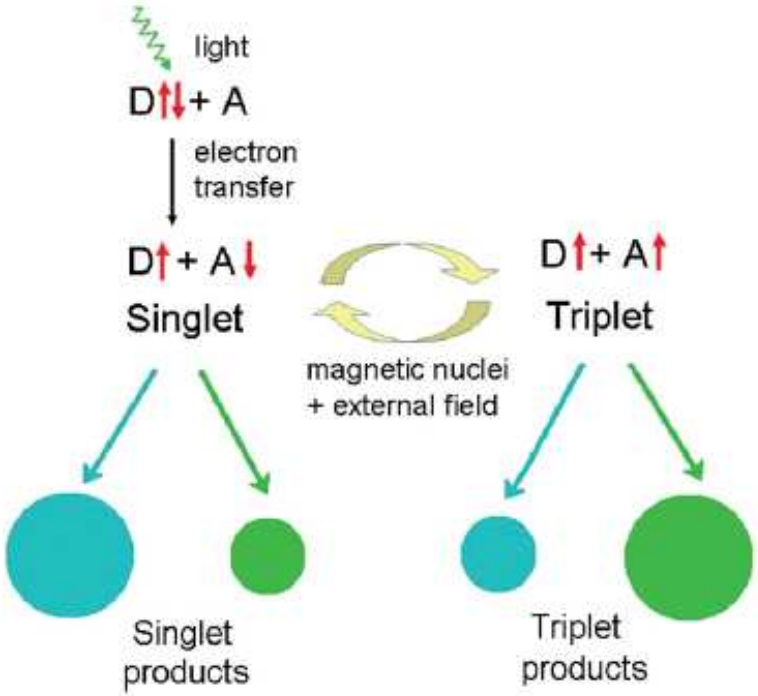
Reaction products are spin-dependent

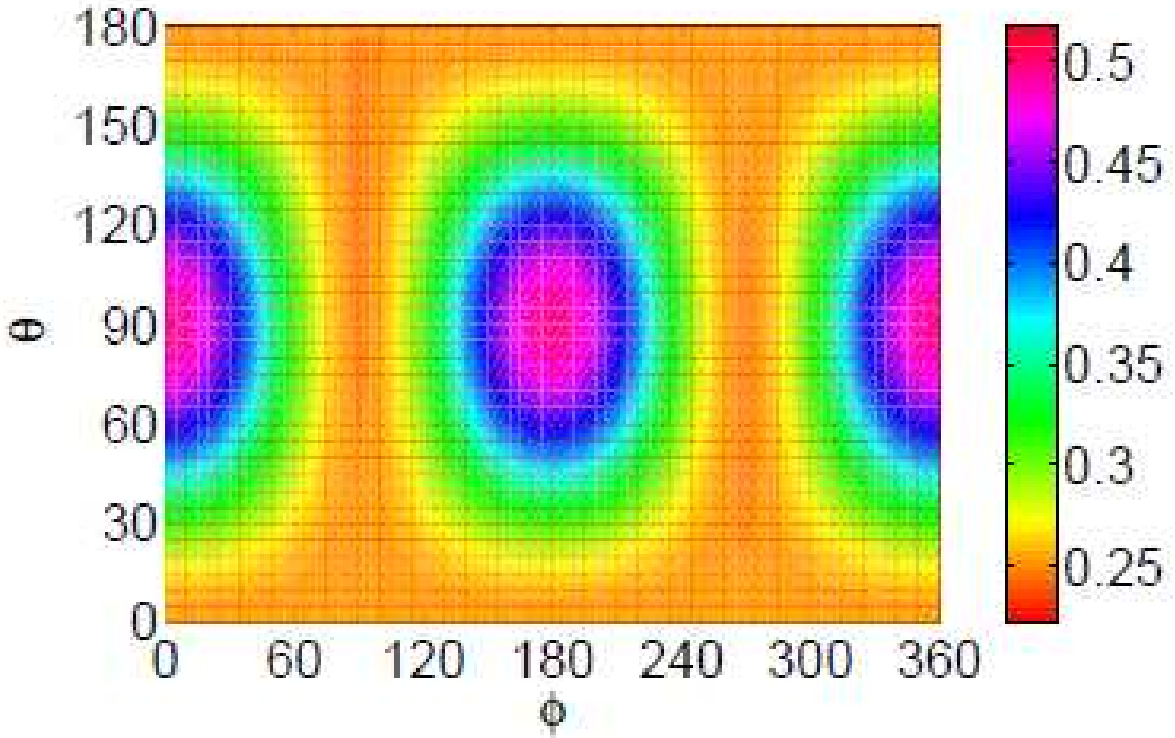
$$H = \sum_{k=A,D} H_k = -\gamma_e \sum_k \vec{B}_k \cdot \vec{S}_k + \sum_{k,j} \vec{S}_k \cdot \hat{\lambda}_{k_j} \cdot \vec{I}_{k_j}$$

Electron spins

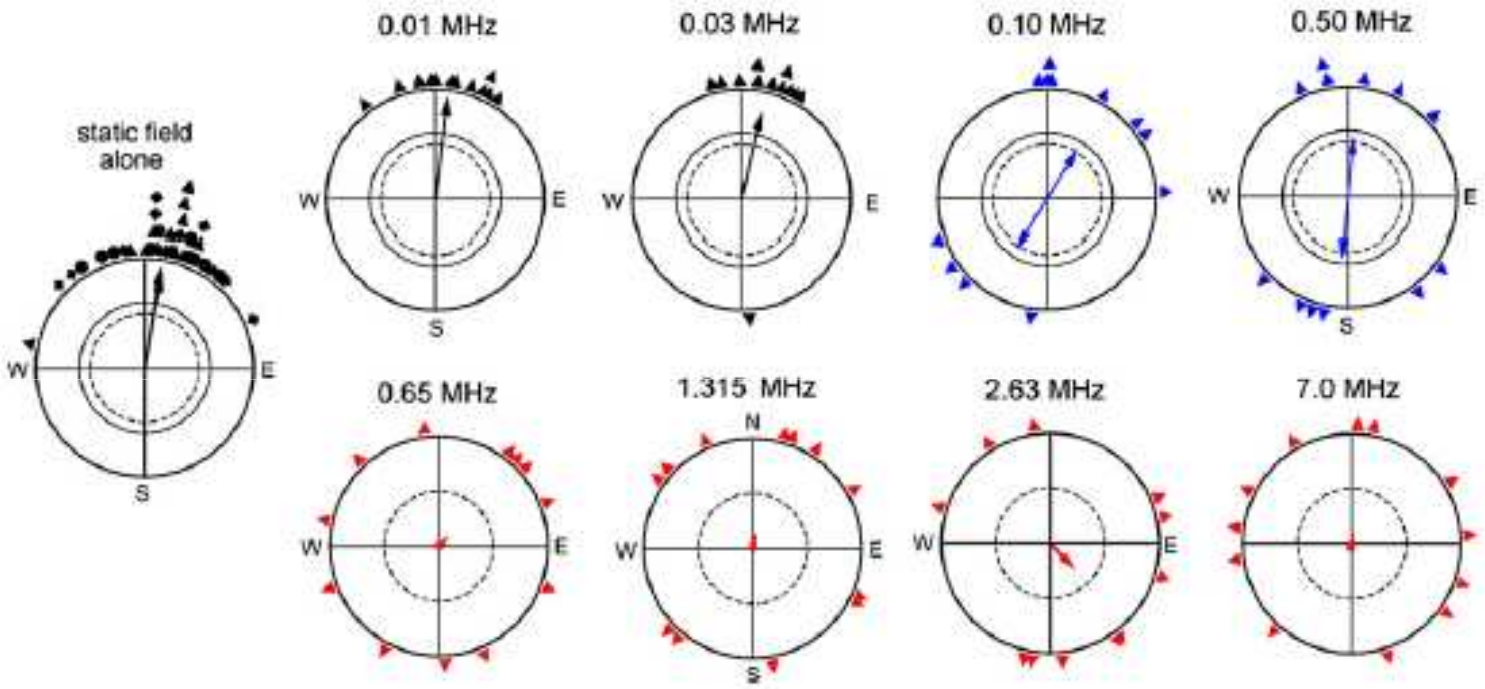
Nuclear spins

Ritz, T., S. Adem, and K. Schulten., Biophys. J. 78:707–718 (2000)


light
D↑↓ + A
electron transfer
D↑ + A↓
Singlet
D↑ + A↑
Triplet
magnetic nuclei + external field
Singlet products
Triplet products


180
150
120
90
60
30
0
Φ
0
60
120
180
240
300
360
Φ
0.5
0.45
0.4
0.35
0.3
0.25

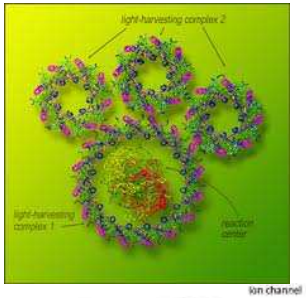
Triplet states split in magentic field, hence sensitive to radiation → Test



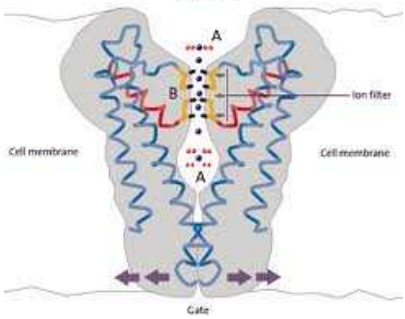
Birds are perturbed by specific frequencies of external radiation !
Without light no magnetic vision !

Ritz, Wiltschko, Hore, Rodgers, Stapput, Thalau, Timmel & Wiltschko, Biophys. J. 96, 3451 (2009)

- Photosynthesis

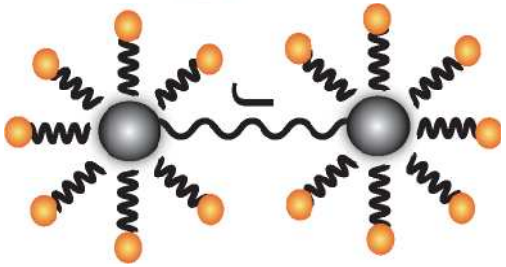


- Ion Channels



- Magnetic Vision

- Olfaction



- Theoretical Methods

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