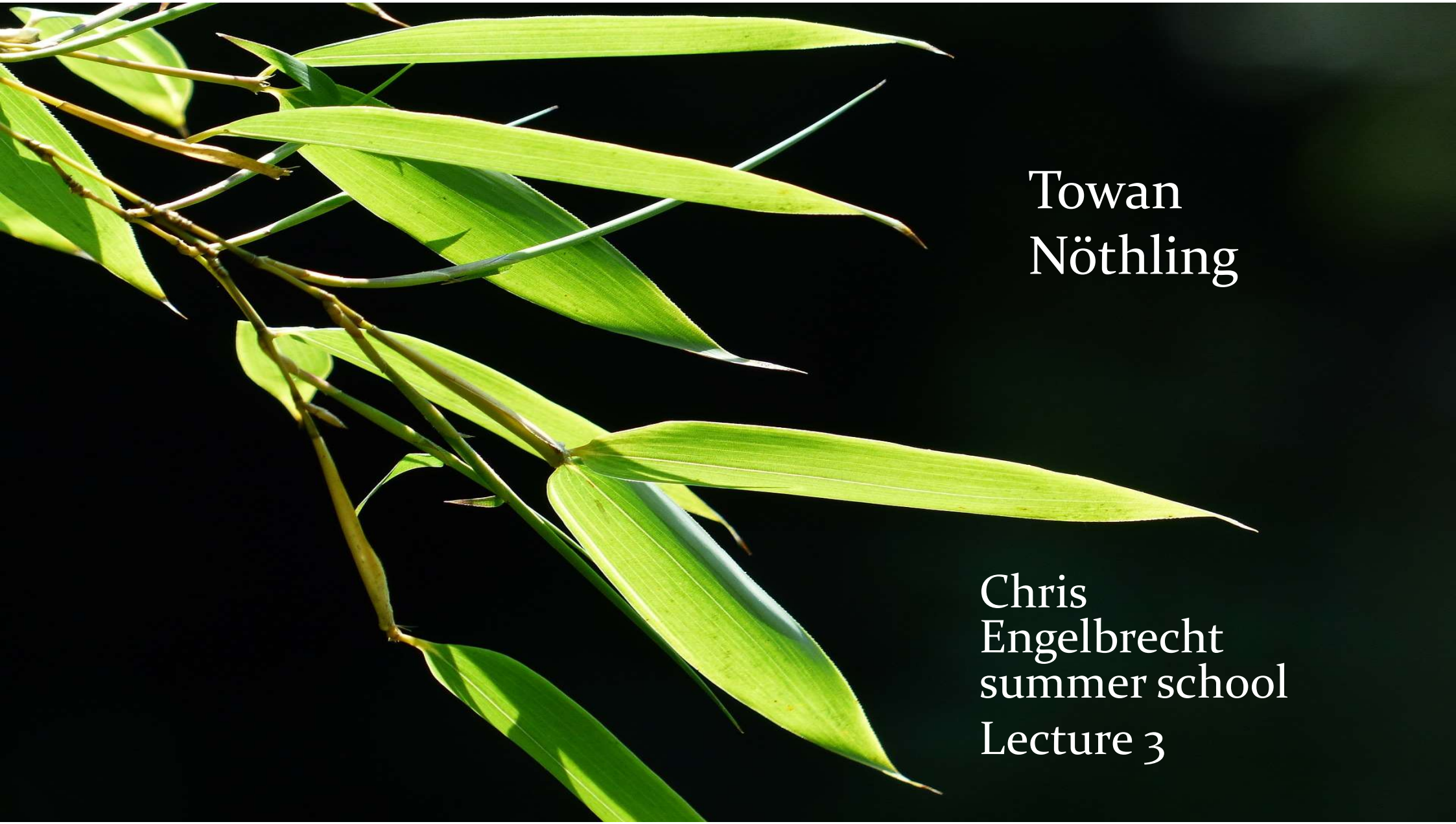
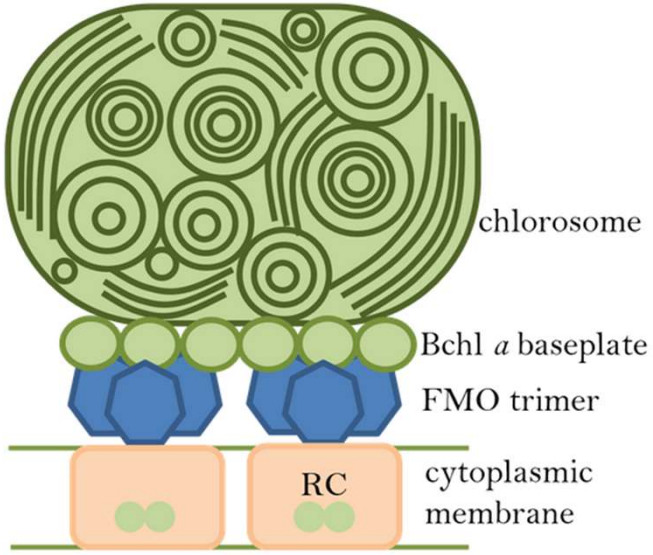
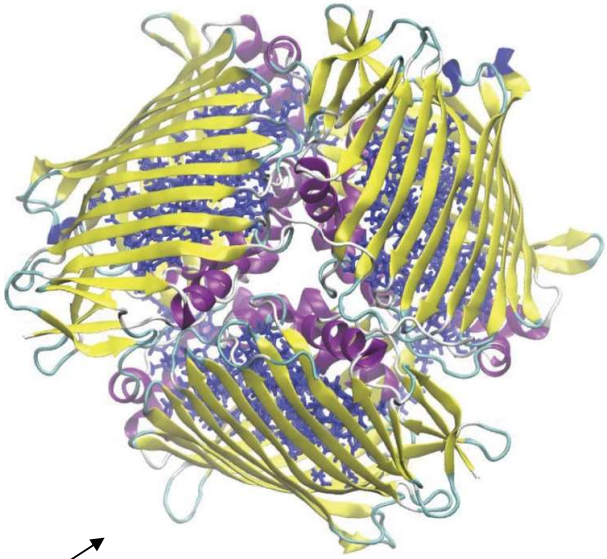

Towan
Nöthling
Chris
Engelbrecht
summer school
Lecture 3

Overview of quantum mechanics in biological systems





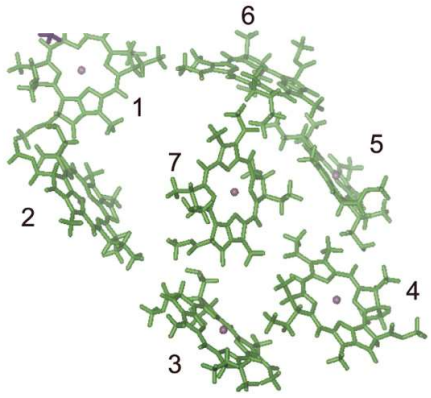
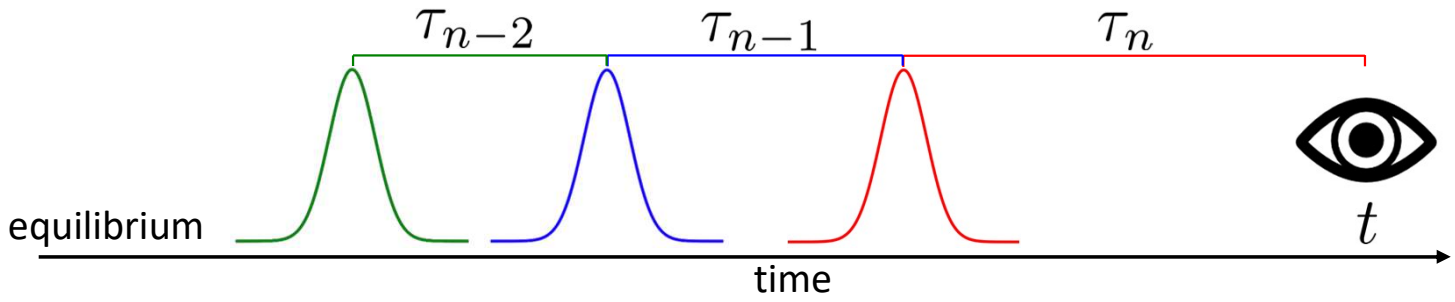


Figure credit: Jia, X., Mei, Y., Zhang, J. *et al*. *Sci Rep* **5**, 17096 (2015). CC BY 4.0

QM of linear response

$$P^{(n)}(t) = \int_0^\infty d\tau_n \int_0^\infty d\tau_{n-1} \ldots \int_0^\infty d\tau_1 \mathcal{R}^{(n)}(\tau_n, \tau_{n-1}, \ldots, \tau_1) E(t-\tau_n) E(t-\tau_n-\tau_{n-1}) \ldots E(t-\tau_n-\tau_{n-1}-\ldots-\tau_1)$$



$$\mathcal{R}^{(n)}(\tau_n, \tau_{n-1}, \ldots, \tau_1) = i^n \mathrm{Tr}[\hat{\mu}\mathcal{U}_{\mathrm{mol}}(\tau_n)\mathcal{V}\mathcal{U}_{\mathrm{mol}}(\tau_{n-1})\mathcal{V}\ldots\mathcal{U}_{\mathrm{mol}}(\tau_1)\mathcal{V}\rho^{\mathrm{eq}}]$$

$$\mathcal{R}^{(1)}(t) = i\mathrm{Tr}[\hat{\mu}\mathcal{U}_{\mathrm{mol}}(t)\mathcal{V}\rho^{\mathrm{eq}}]$$

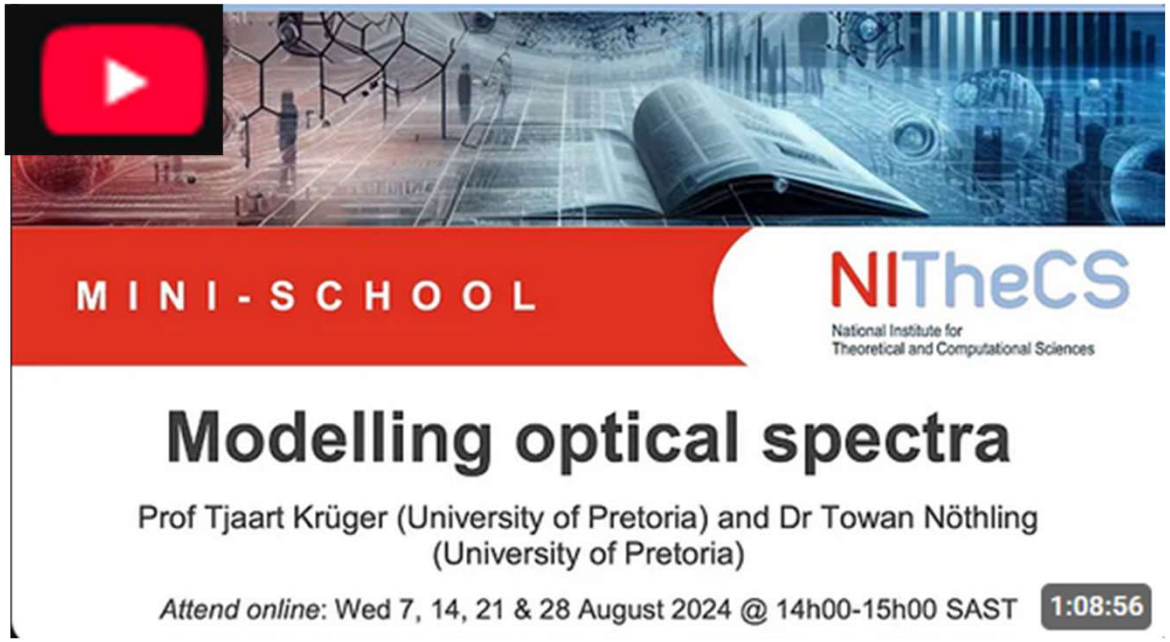
$$\mathcal{V}\bullet = [\hat{\mu}, \bullet]$$

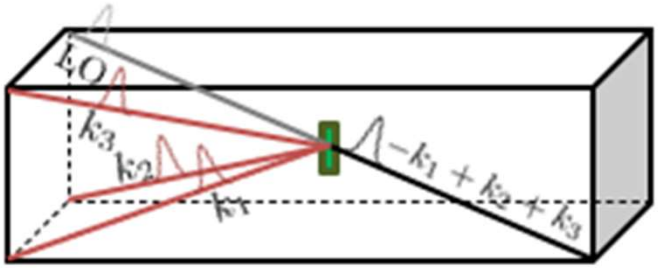
QM of linear response

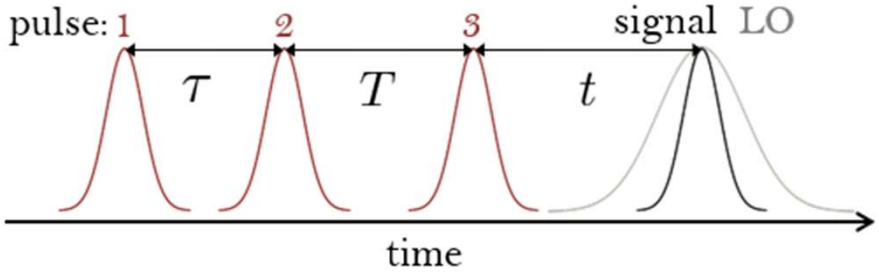
$$\mathrm{S}^{\mathrm{A}}(\omega) \propto 2\mathrm{Re} \int_0^\infty dt\, e^{i\omega t} R^{(1)}(t)$$

QM of linear response

$$\mathrm{S}^{\mathrm{A}}(\omega) \propto 2\mathrm{Re} \int_0^\infty dt\, e^{i\omega t} R^{(1)}(t)$$

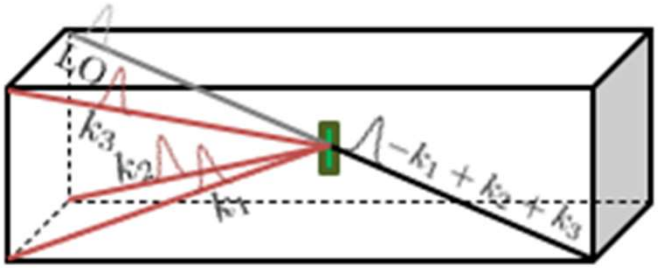


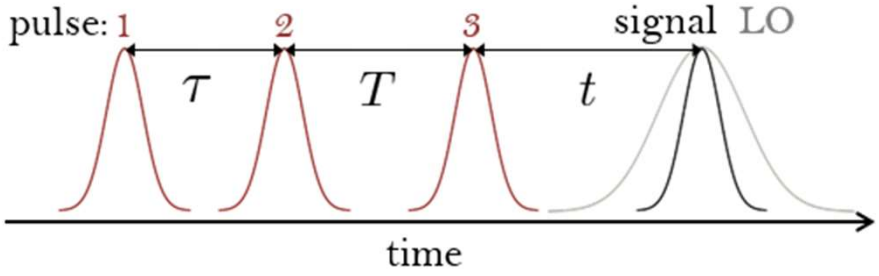


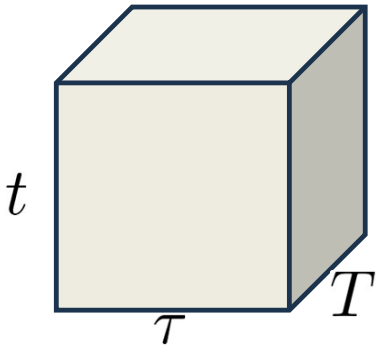


2D-electronic spectroscopy

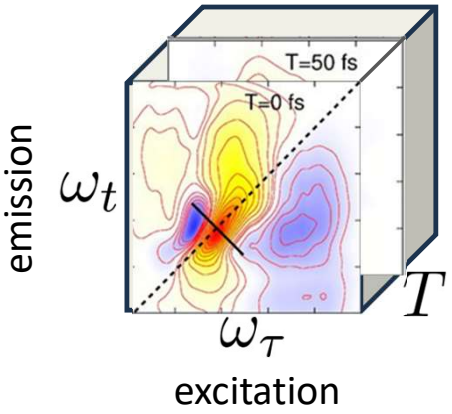
(third order linear spectroscopy)

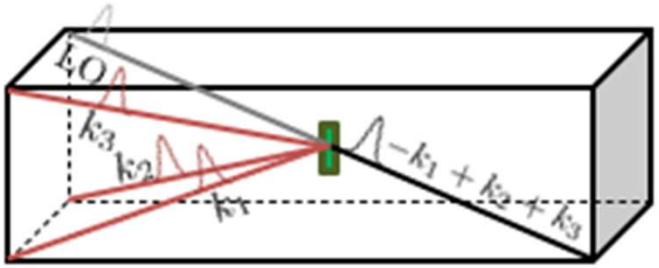


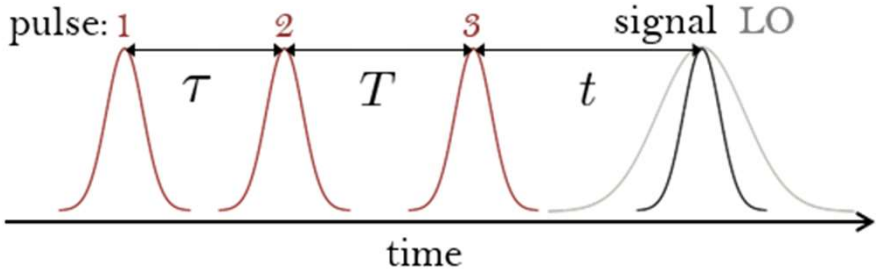


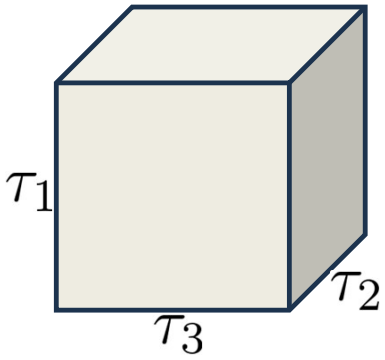


FT over τ and t

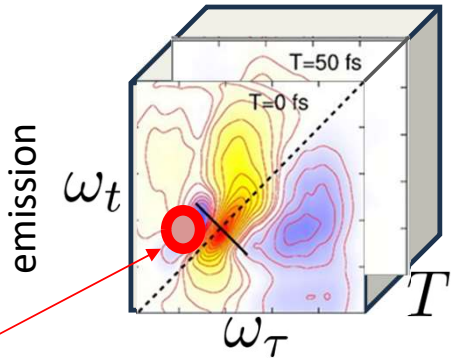




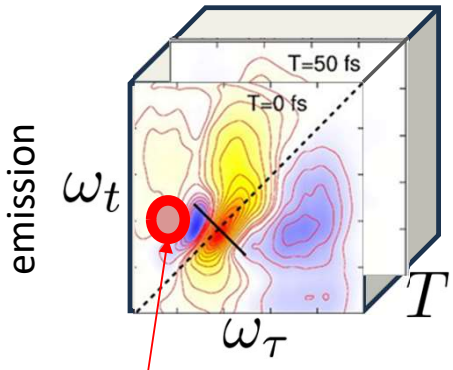


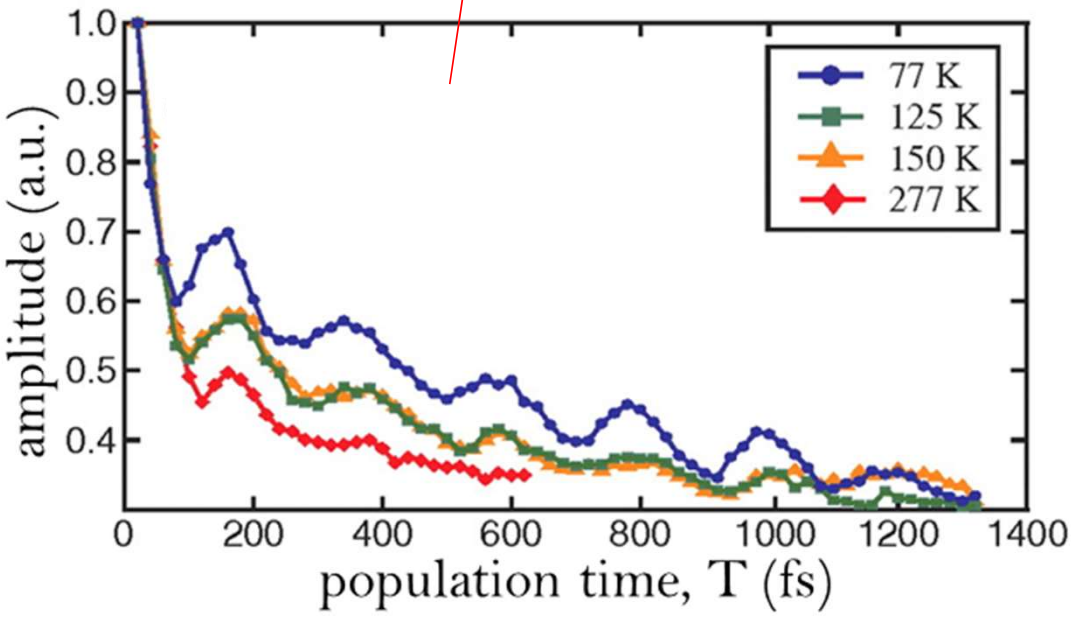


FT over τ and t



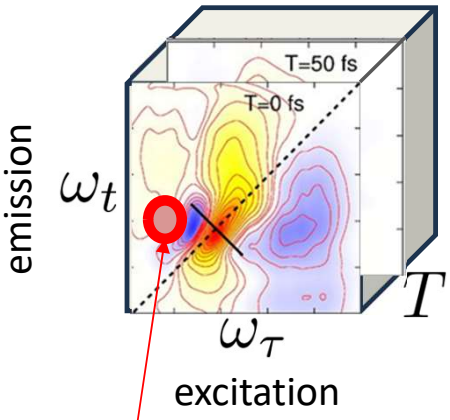
coherence between different exciton states

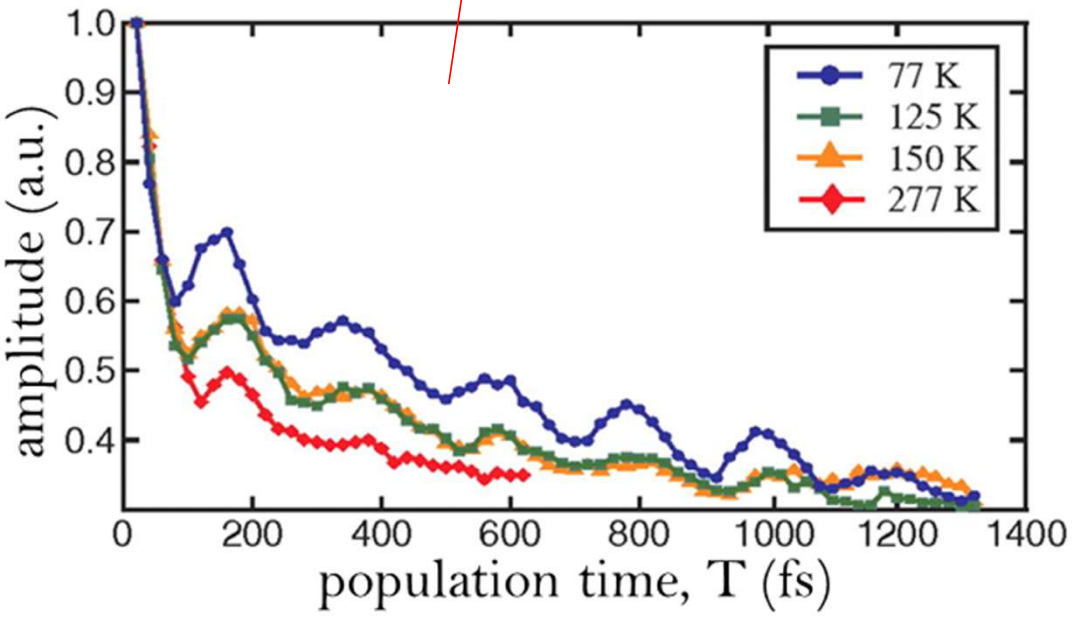




coherence last for longer than what is expected for electronic coherence between exciton states .

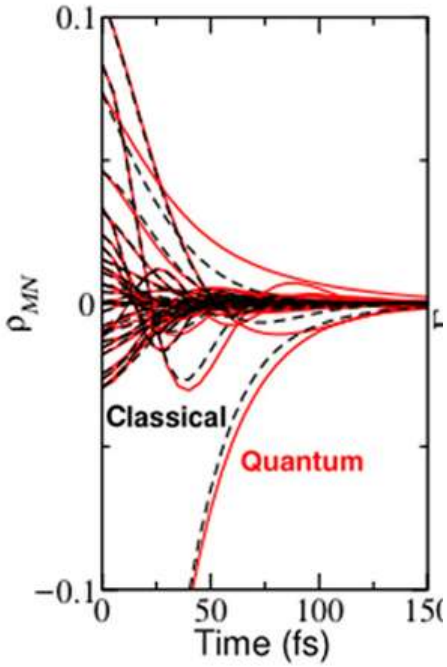
Panitchayangkoon *et al.* Proc. Natl. Acad. Sci. U.S.A., 107(29). PNAS licence



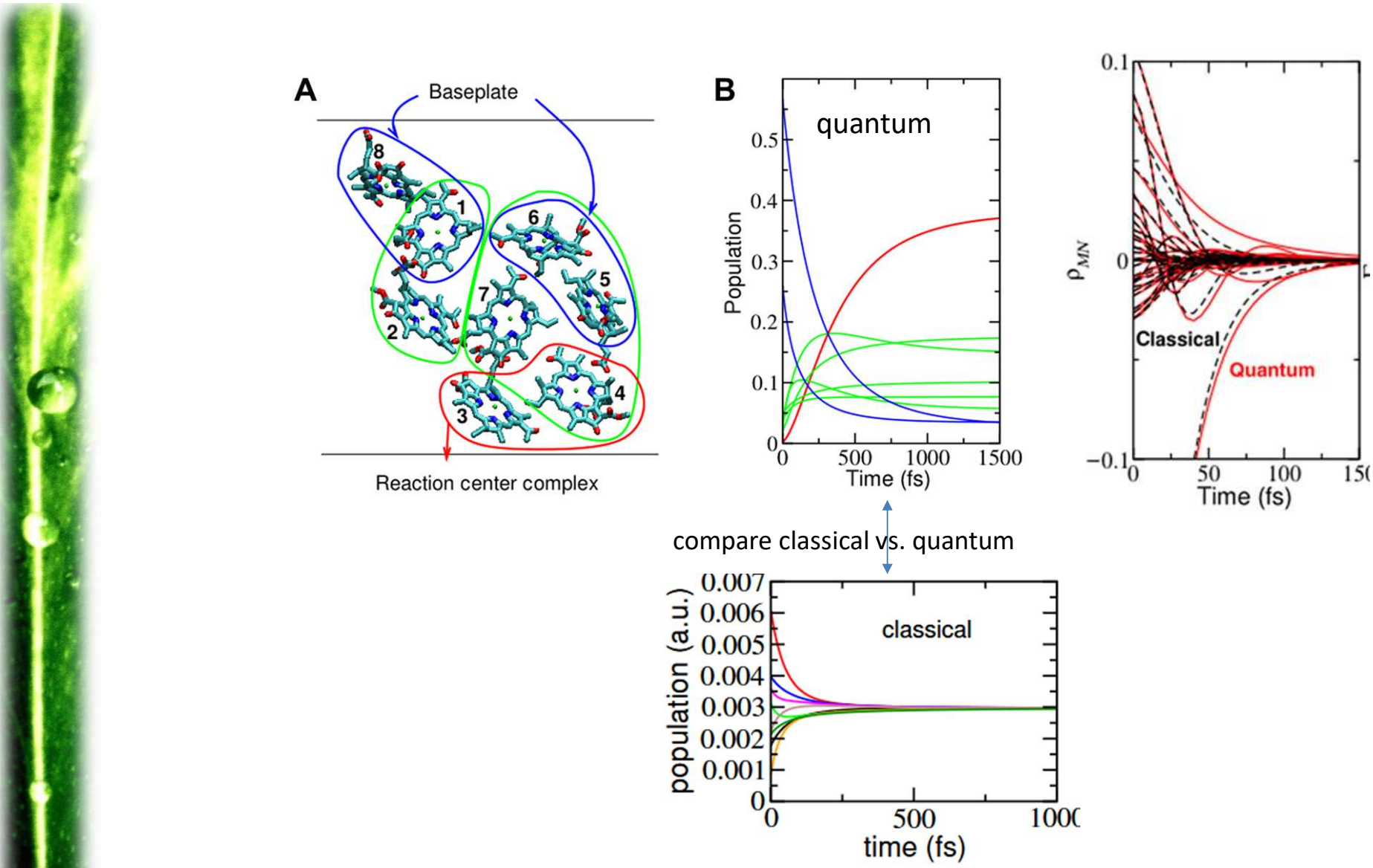


Panitchayangkoon *et al.* Proc. Natl. Acad. Sci. U.S.A., 107(29). PNAS licence

coherence last for longer than what is expected from simulations.

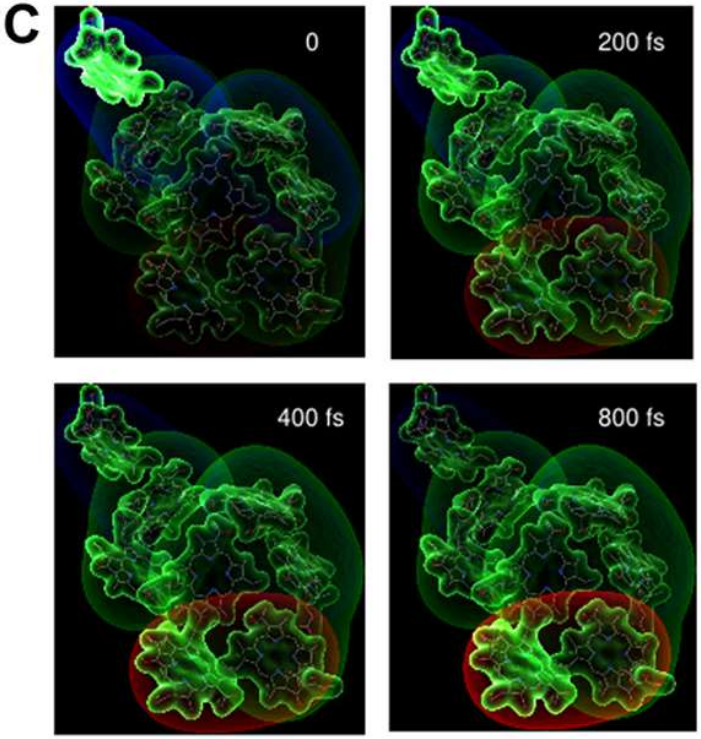


Cao *et al. 2020. Science Advances* 6(14) CC BY-NC 4.0.



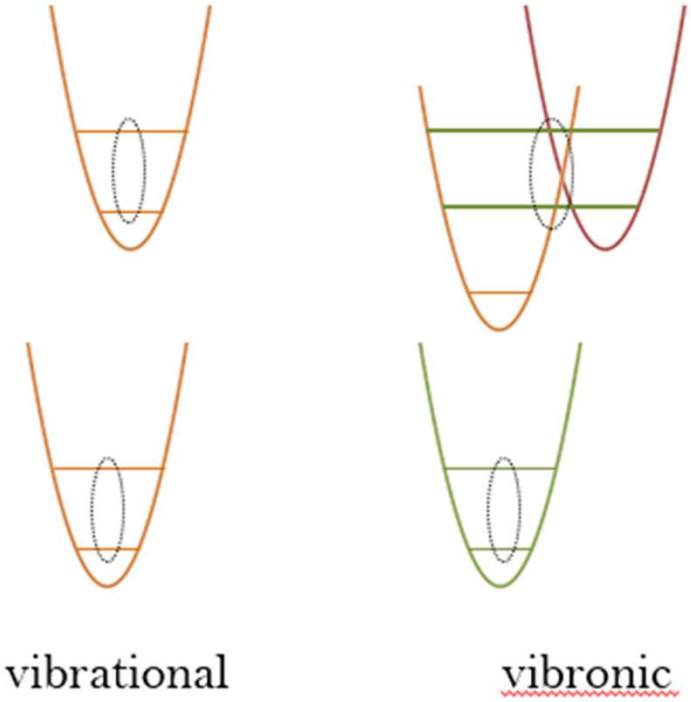
Figures from Cao *et al.* 2020. *Science Advances* 6(14). CC BY-NC 4.0.

Cao *et al.* 2020. *Science Advances* 6(14). CC BY-NC 4.0.



In photosynthesis, the interaction between pigments and the coupling to the bath is fine-tuned.

Reviews: Cao *et al.* 2020. *Science Advances* 6(14)
Fleming *et al.* 2012. *Faraday Discuss* 155.

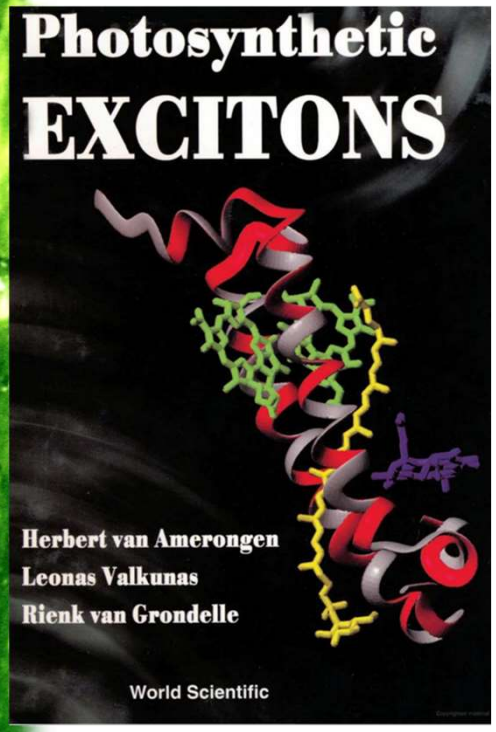


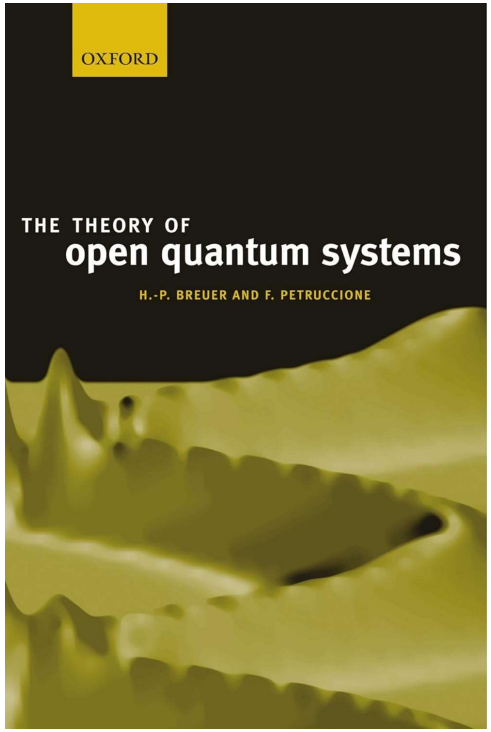
Dephasing of coherence in these models are slow, because the two vibrational levels are **on the same pigment** and therefore couple to the same bath.

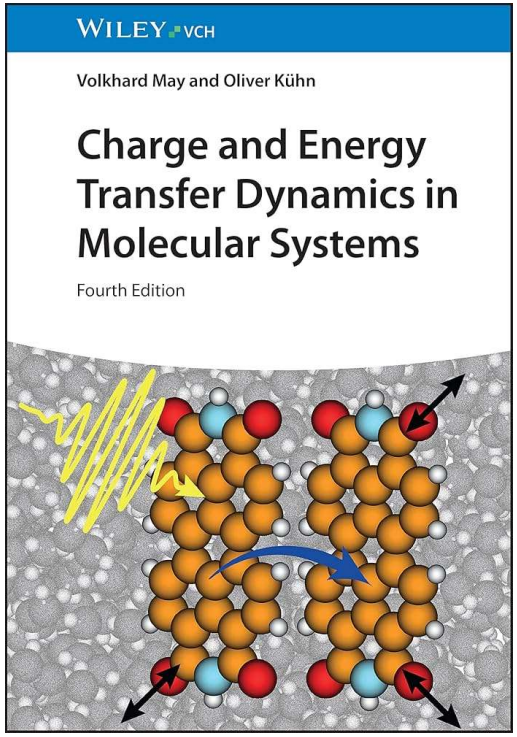
ground-state vibrations — Maiuri *et al.* 2018. *Nat. Chem*. 10(2)

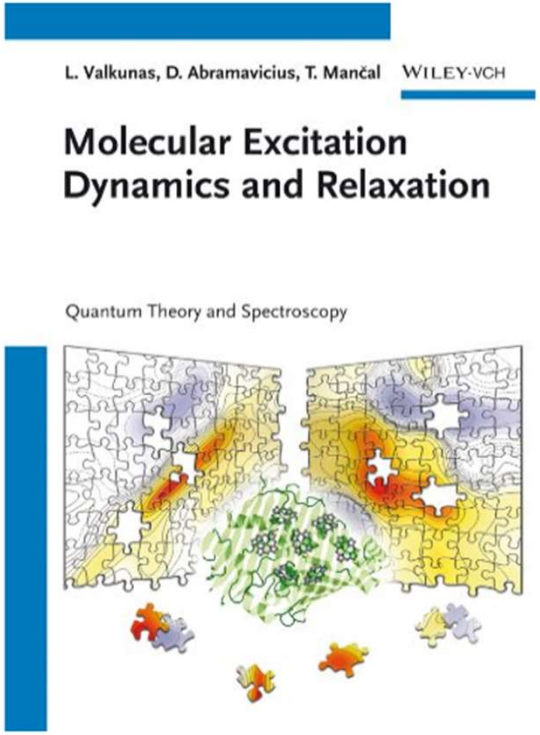
Vibronic states and role of resonant vibrations in LHCs — Malý *et al.* 2016. *ChemPhysChem*, 17(9); Dean *et al.* 2016, *Chem*, 1(6)

Resources


Photosynthetic
EXCITONS
Herbert van Amerongen
Leonas Valkunas
Rienk van Grondelle
World Scientific


OXFORD
THE THEORY OF
open quantum systems
H.-P. BREUER AND F. PETRUCCIONE


WILEY VCH
Volkhard May and Oliver Kühn
Charge and Energy
Transfer Dynamics in
Molecular Systems
Fourth Edition

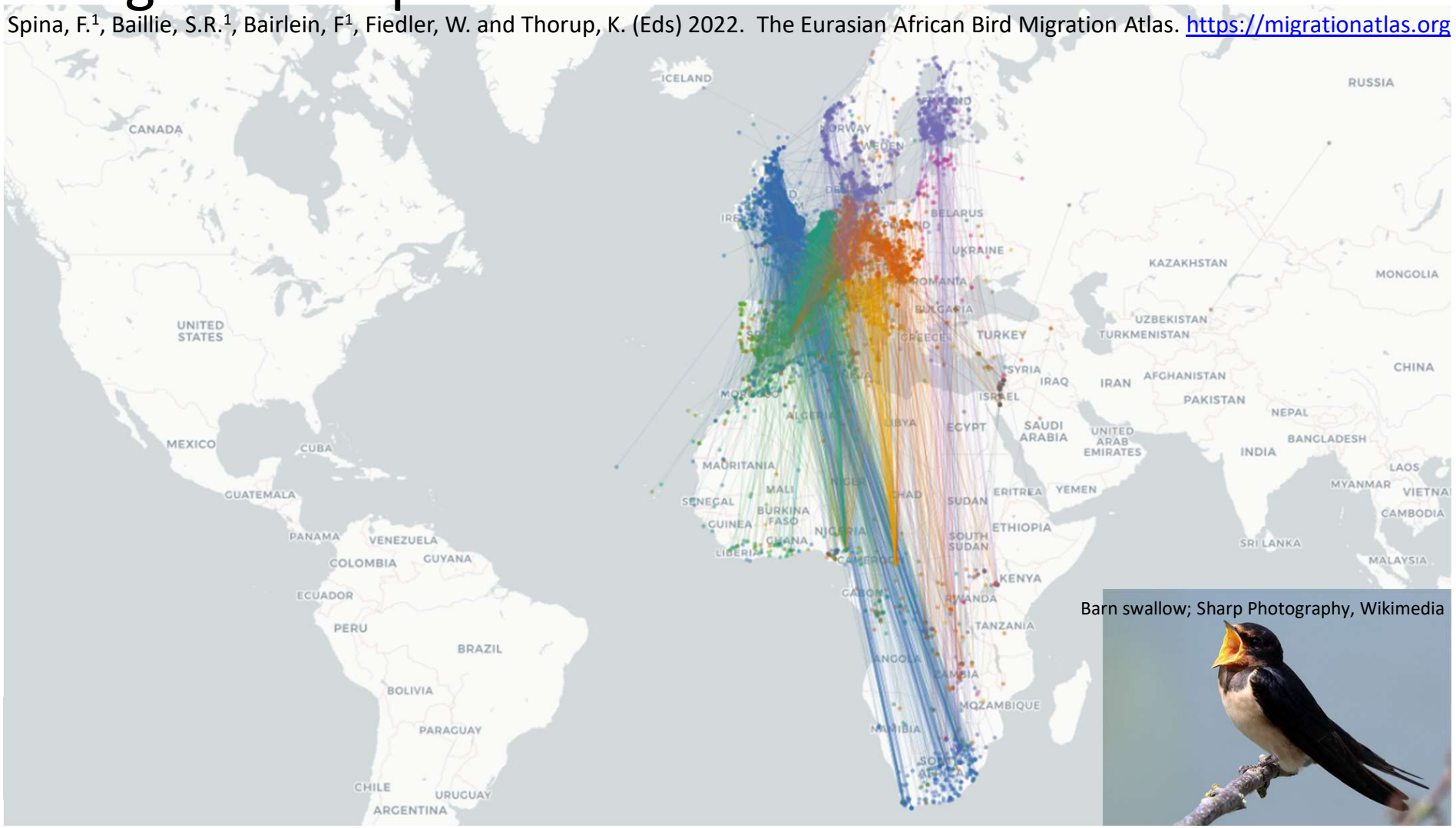

L. Valkunas, D. Abramavicius, T. Mančal
WILEY-VCH
Molecular Excitation
Dynamics and Relaxation
Quantum Theory and Spectroscopy

- How birds (may) know where to go
- How we (may) smell
- How our enzymes (may) keep us alive
- How we (may) think

or maybe not…

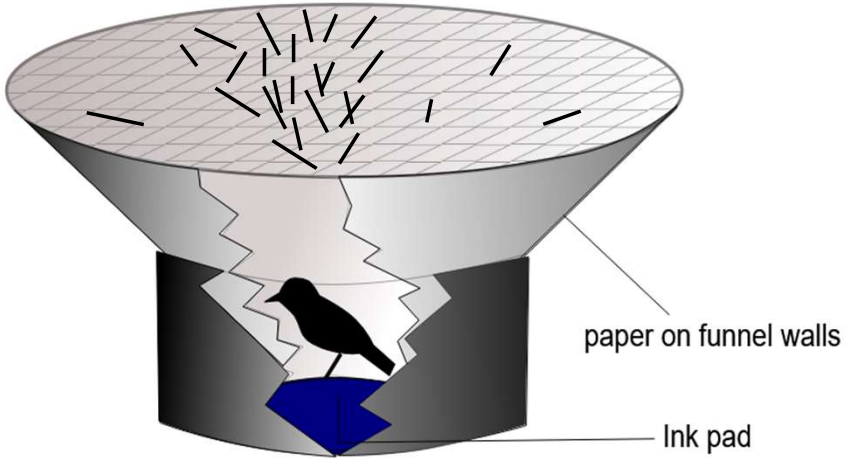
Magnetoreception in Birds

Spina, F.[1], Baillie, S.R.[1], Bairlein, F[1], Fiedler, W. and Thorup, K. (Eds) 2022. The Eurasian African Bird Migration Atlas. https://migrationatlas.org



Barn swallow; Sharp Photography, Wikimedia

Magnetoreception in Birds



Emlen Funnel


Poor sense of direction


Good sense of direction

Engels, S. *et al.* Nature 509. 2014

Magnetoreception in Birds

Zeitschrift für Physikalische Chemie Neue Folge, Bd. 111, S. 1–5 (1978)
© by Akademische Verlagsgesellschaft, Wiesbaden 1978

A Biomagnetic Sensory Mechanism Based on Magnetic Field Modulated Coherent Electron Spin Motion

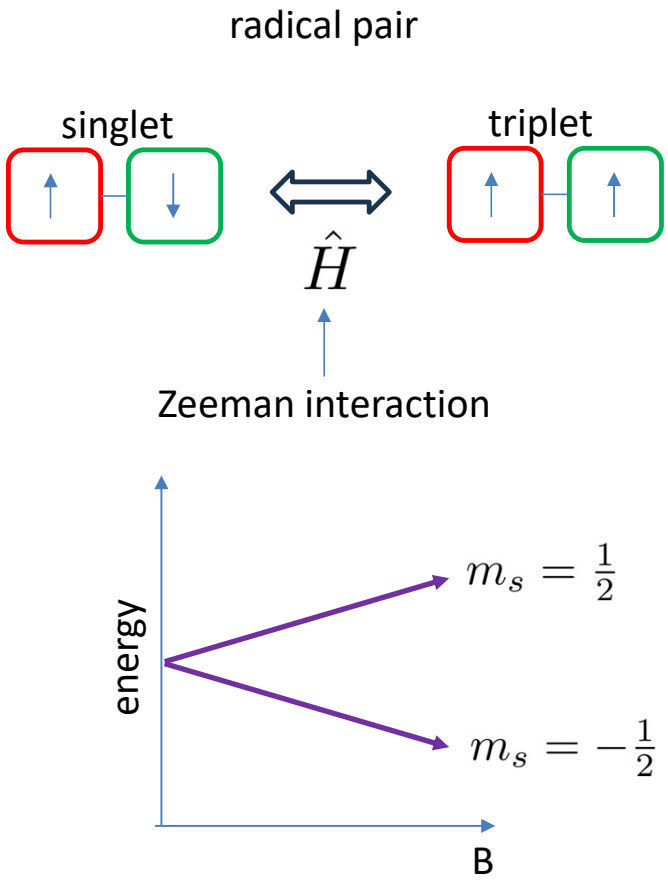
By

Klaus Schulten, Charles E. Swenberg* and Albert Weller

Max-Planck-Institut für biophysikalische Chemie, Abteilung Spektroskopie, D-3400 Göttingen, Federal Republic of Germany

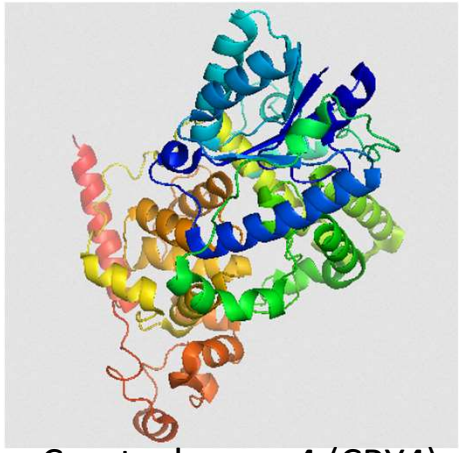
(Received July 20, 1978)

Biomagnetism / Electron spin states / Hyperfine interaction

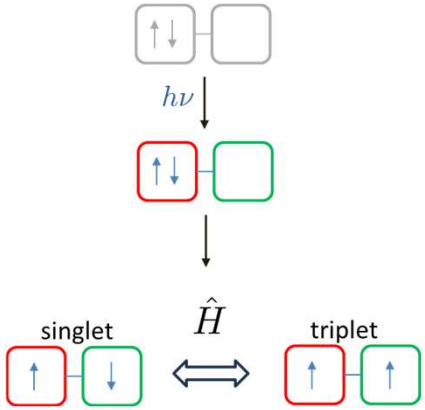


Review: Wiltschko *et al. J. R. Soc. Interface 16.* 2019

Magnetoreception in Birds



Cryptochrome 4 (CRY4)



Article

Magnetic sensitivity of cryptochrome 4 from a migratory songbird

https://doi.org/10.1038/s41586-021-03618-9
Received: 17 July 2019
Accepted: 6 May 2021
Published online: 23 June 2021
Check for updates

Jingjing Xu[1], Lauren E. Jarocha[2], Tilo Zollitsch[2], Marcin Konowalczyk[3], Kevin B. Henbest[2,3], Sabine Richert[4], Matthew J. Golesworthy[3], Jessica Schmidt[1], Victoire Déjean[3], Daniel J. C. Sowood[2], Marco Bassetto[1,2], Jiate Luo[2], Jessica R. Walton[2], Jessica Fleming[2], Yujing Wei[2], Tommy L. Pitcher[3], Gabriel Moise[3], Maike Herrmann[1], Hang Yin[5], Haijia Wu[6], Rabea Bartölke[1], Stefanie J. Käsehagen[1], Simon Horst[1], Glen Dautaj[1], Patrick D. F. Murton[2], Angela S. Gehrckens[2], Yogarany Chelliah[7,8], Joseph S. Takahashi[7,8], Karl-Wilhelm Koch[6,9], Stefan Weber[4], Ilia A. Solov'yov[9,10]✉, Can Xie[11,12]✉, Stuart R. Mackenzie[2]✉, Christiane R. Timmel[3,13]✉, Henrik Mouritsen[1,9]✉ & P. J. Hore[2]✉

Sharp Photography, CC BY SA 4.0, wikimedia

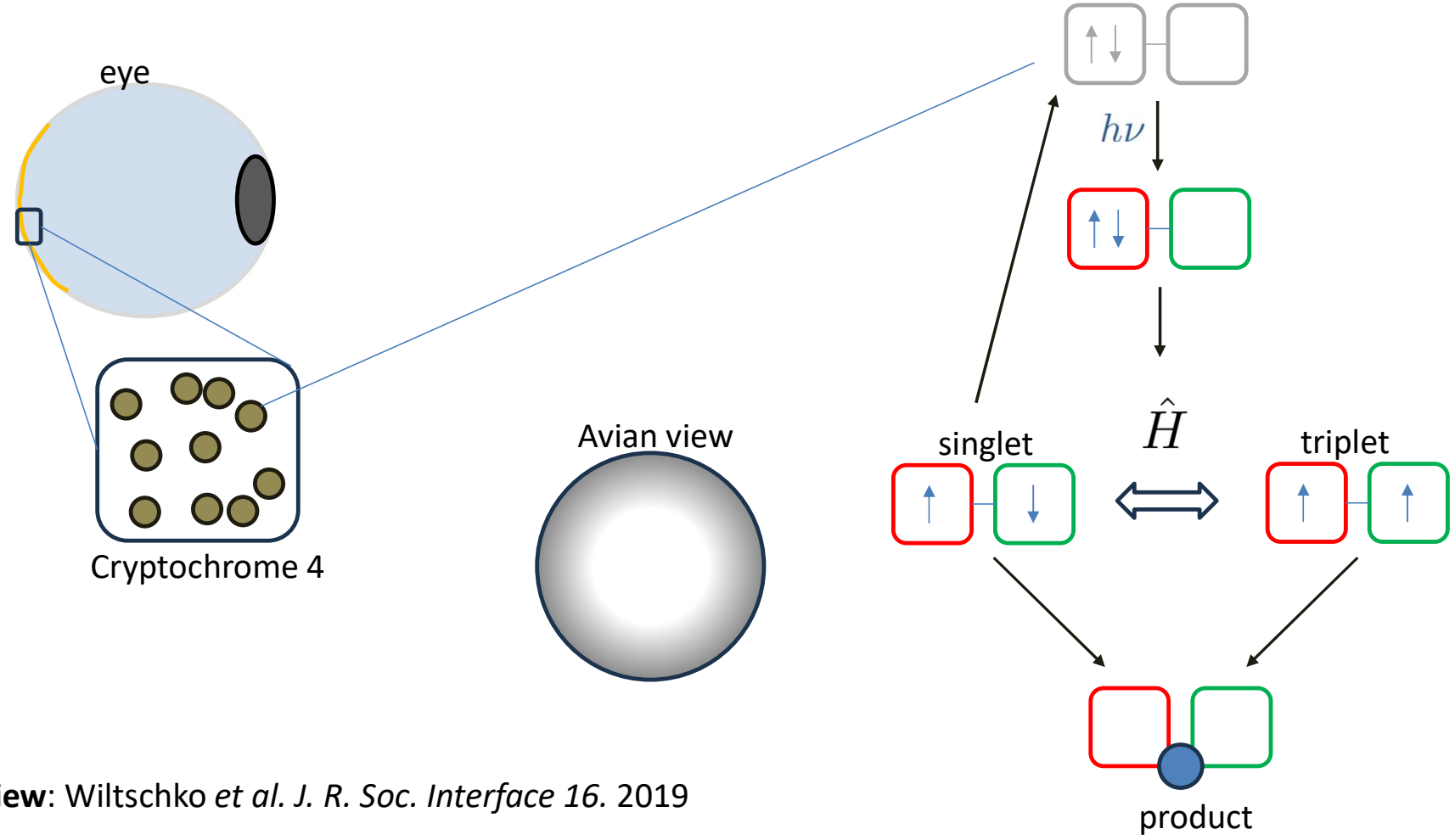
(CRY4) sensitive

Andrei Niemimäki, , CC BY SA 2.0, wikimedia

(CRY4) less sensitive

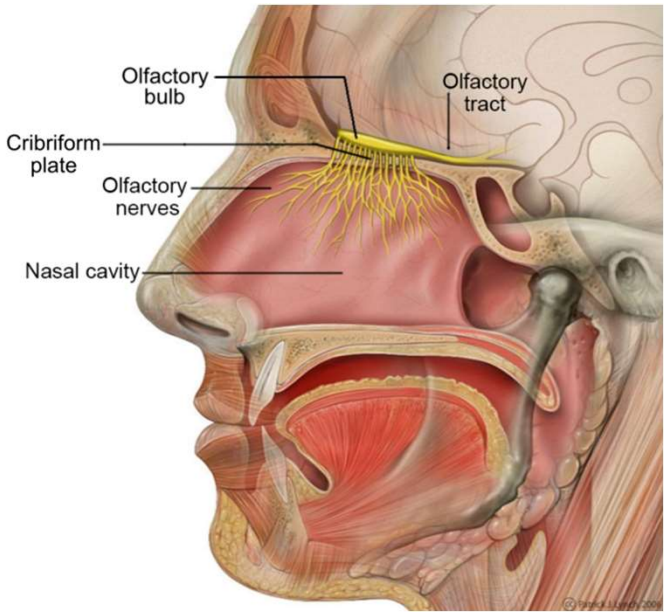
Review: Wiltschko *et al. J. R. Soc. Interface 16.* 2019

Magnetoreception in Birds

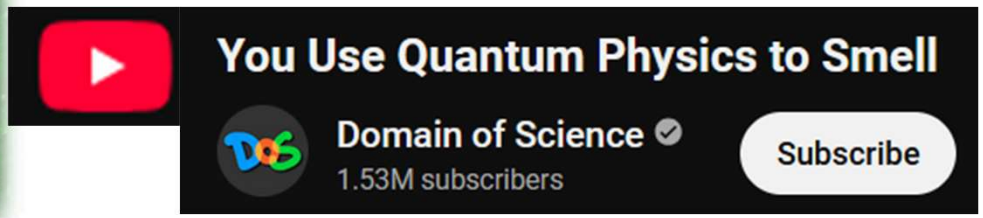


Review: Wiltschko *et al. J. R. Soc. Interface 16.* 2019

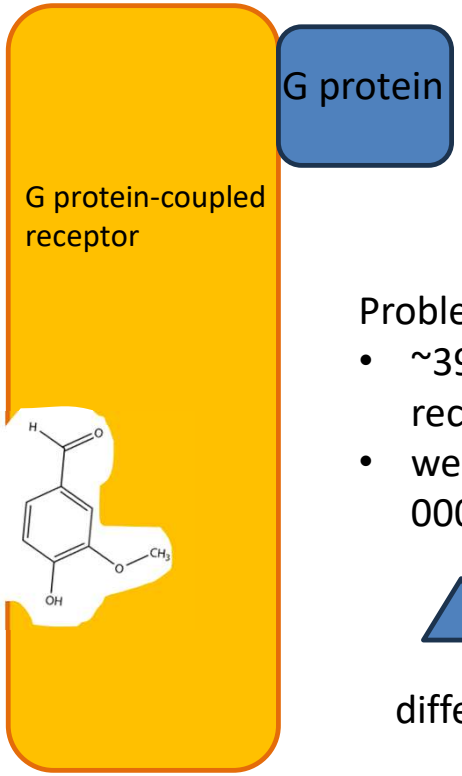
Olfaction



Patrick J. Lynch CC BY SA 4.0, wikimedia

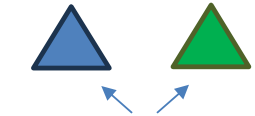


lock and key model of olfaction

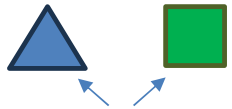


Problem:

- ~390 types of receptors
- we can smell ~10 000 smells!

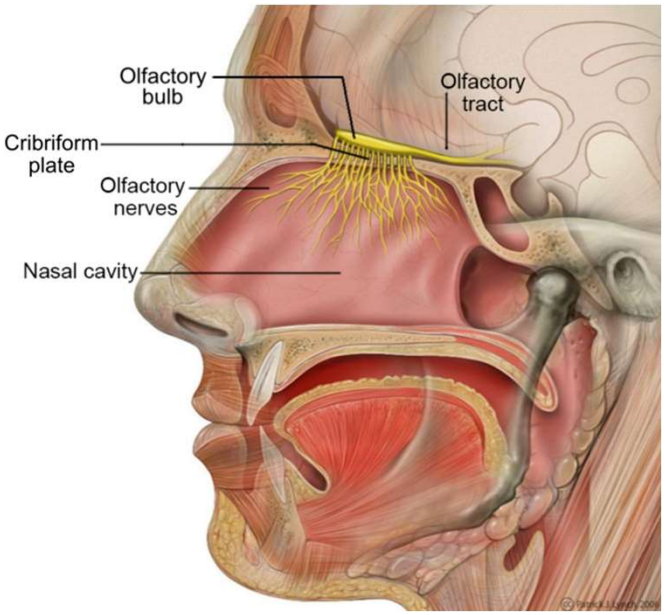


different smell



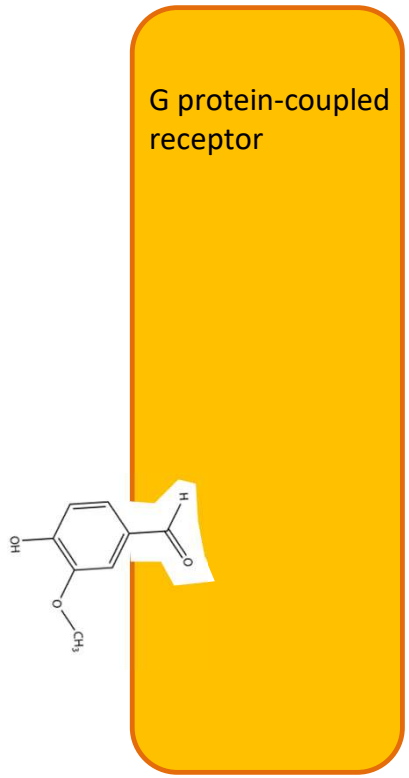
same smell

Olfaction



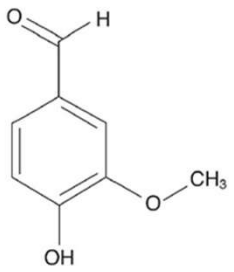
Patrick J. Lynch CC

partial lock and key model

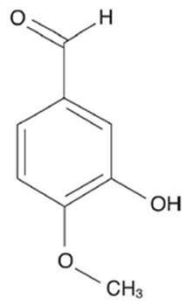


Problem:

- Different arrangements of functional groups smell differently

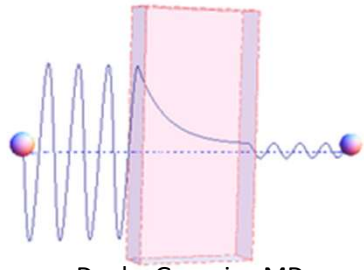


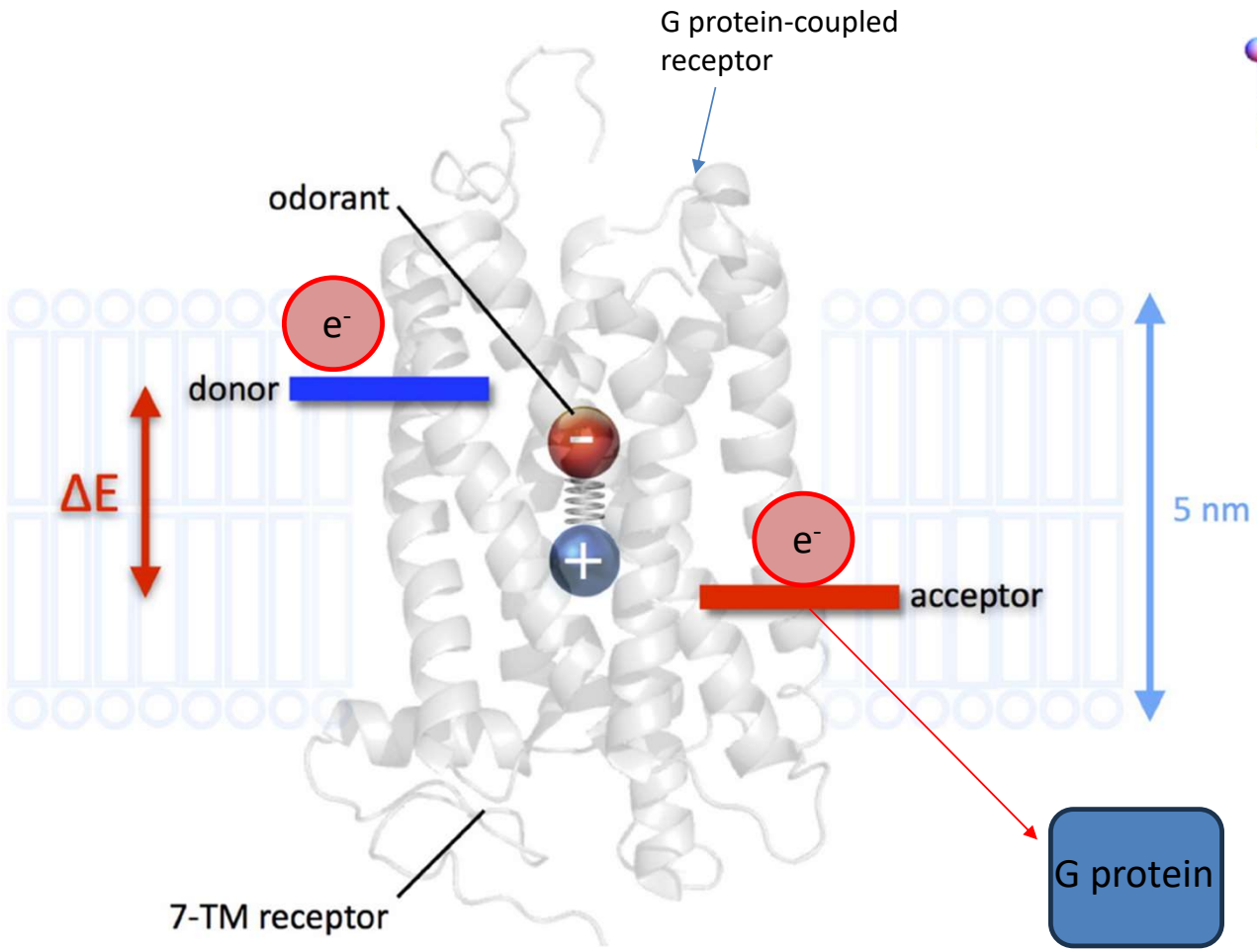
Vanillin



Isovanillin

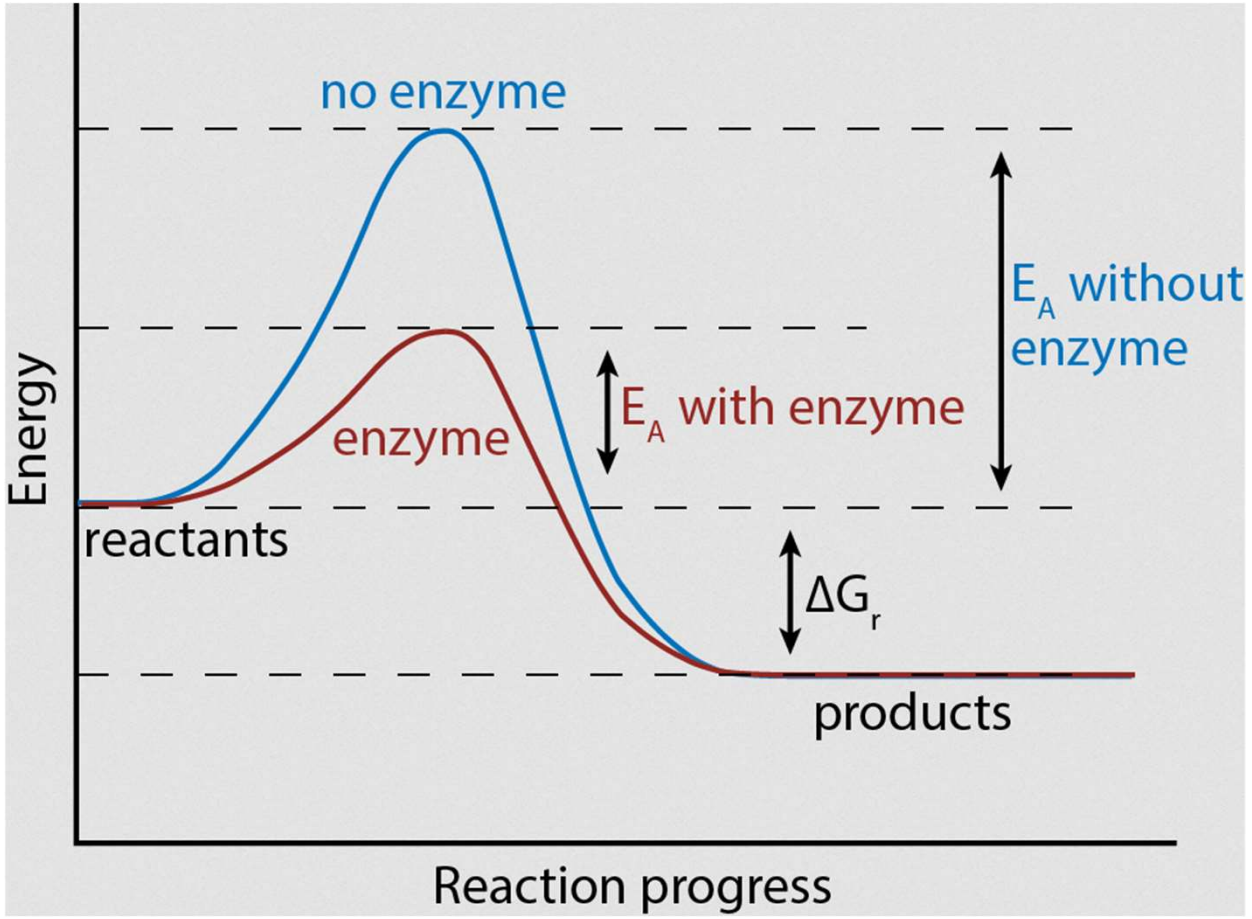
Olfaction





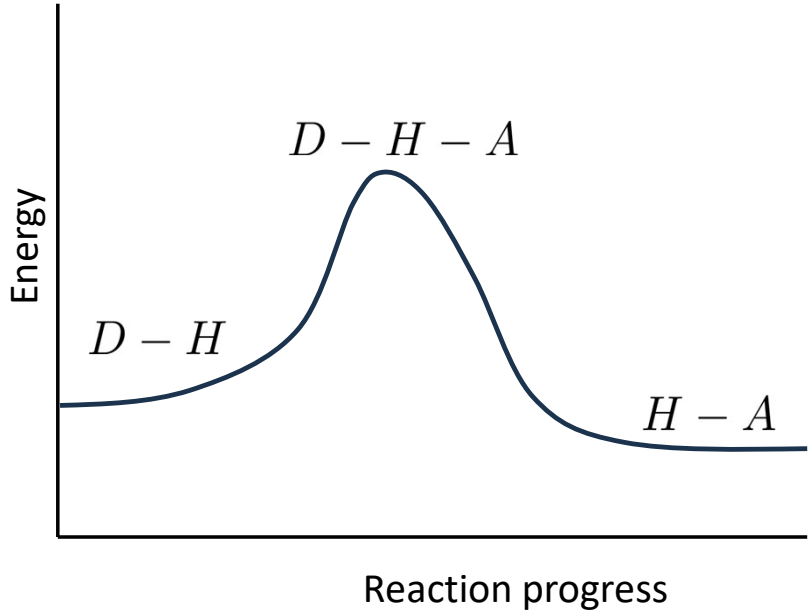
Adapted from Horsfield *et al. Advances in Physics: X*. 2017.

Enzyme function



Microbialmatt, CC BY SA 4.0, wikimedia

Enzyme function

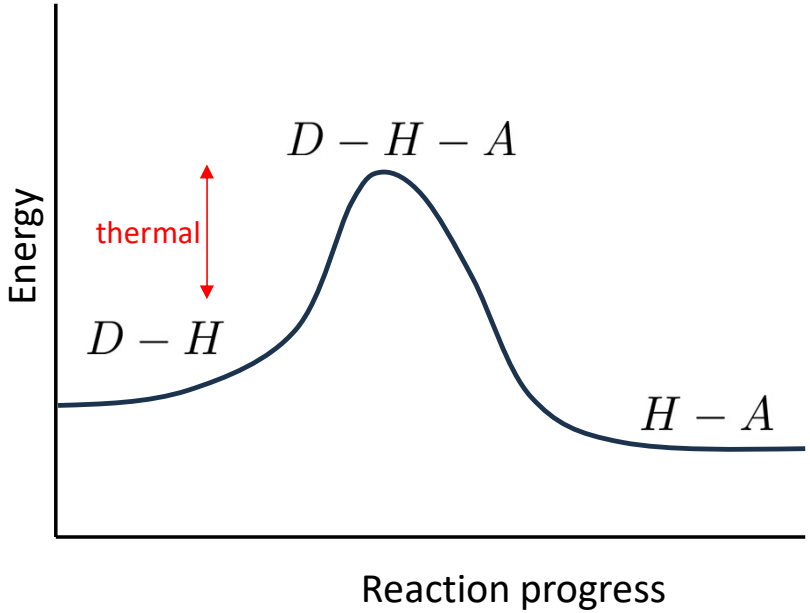


Hydrogen-transfer enzymes

- Replacing hydrogen with deuterium slows the reaction down much more than would be expected classically.

Review of H-tunnelling in enzymes: Klinman and Kohen. Annu. Rev. Biochem. 2013.

Enzyme function



Hydrogen-transfer enzymes

- Replacing hydrogen with deuterium slows the reaction down much more than would be expected classically.
- At very low temperatures, the reaction still takes place. Thermal energy can therefore not be the only way to cross the energy barrier.

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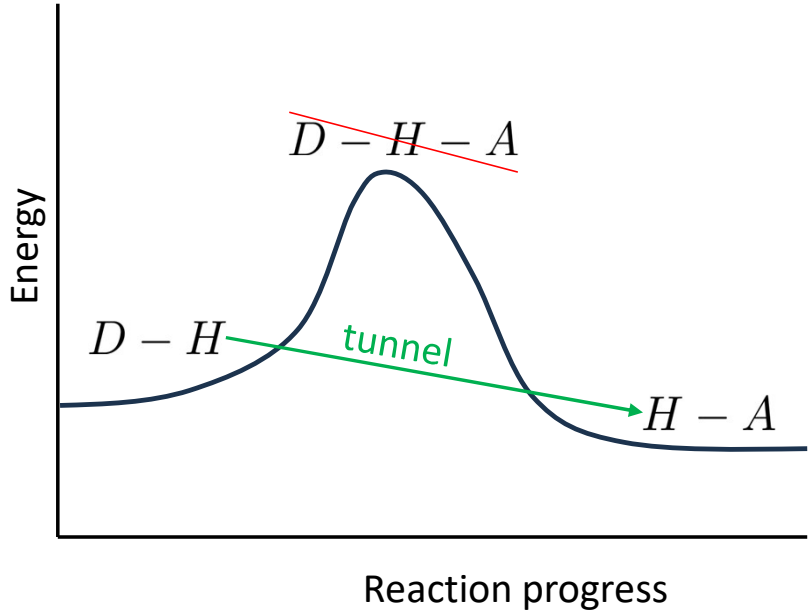

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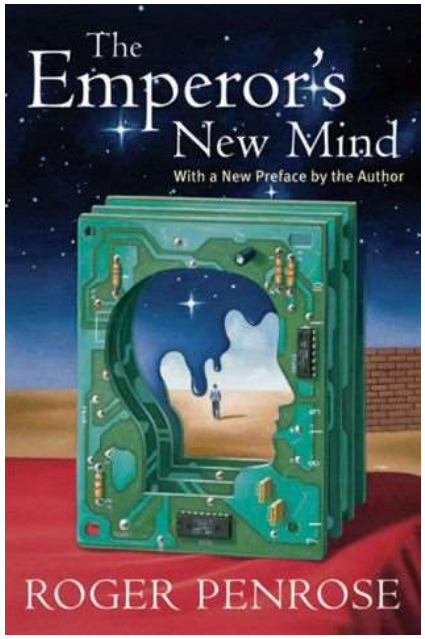
QM in brain

Orchestrated Objective Reduction (Orch-OR) theory

Developed by Roger Penrose and Stuart Hameroff



1989

Review: Hameroff and Penrose. *Physics of Life Reviews* 11(1). 2014.

QM in brain

Orchestrated Objective Reduction (Orch-OR) theory

Developed by Roger Penrose and Stuart Hameroff

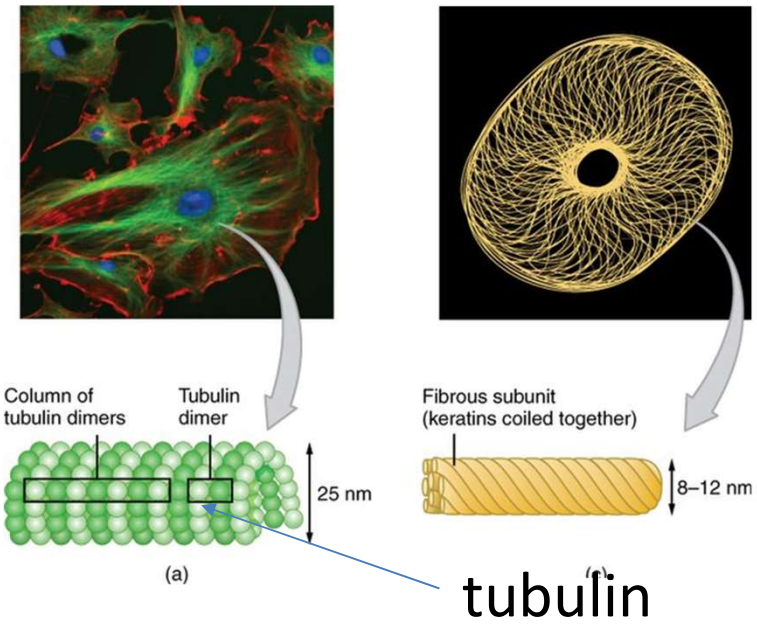
- Based on the believe that Gödel's incompleteness theorems imply that the human brain is not just a sophisticated computer, i.e., consciousness is not purely computational.
- They suggest that quantum collapse (which cannot be predicted with certainty) are integral to consciousness.
- Quantum processes in the brain are orchestrated by structures in the neurons

Review: Hameroff and Penrose. *Physics of Life Reviews* 11(1). 2014.

QM in brain

Orchestrated Objective Reduction (Orch-OR) theory

OpenStax, CC BY SA 4.0, wikimedia



- Tubulin proteins can be in different configurations (like qubits).
- Quantum coherence exist between different tubulin proteins and lasts long enough for quantum computation.
- Quantum collapse is objective and the brain can control how and when it occurs (e.g., when enough mass or energy is involved).

Review: Hameroff and Penrose. *Physics of Life Reviews* 11(1). 2014.

QM in brain

Article

Testing the Conjecture That Quantum Processes Create Conscious Experience

Hartmut Neven [1,*], Adam Zalcman [1], Peter Read [2], Kenneth S. Kosik [3], Tjitse van der Molen [3], Dirk Bouwmeester [4,5], Eve Bodnia [4], Luca Turin [6] and Christof Koch [7]

1 Google Quantum AI, Los Angeles, CA 90291, USA; viathor@google.com
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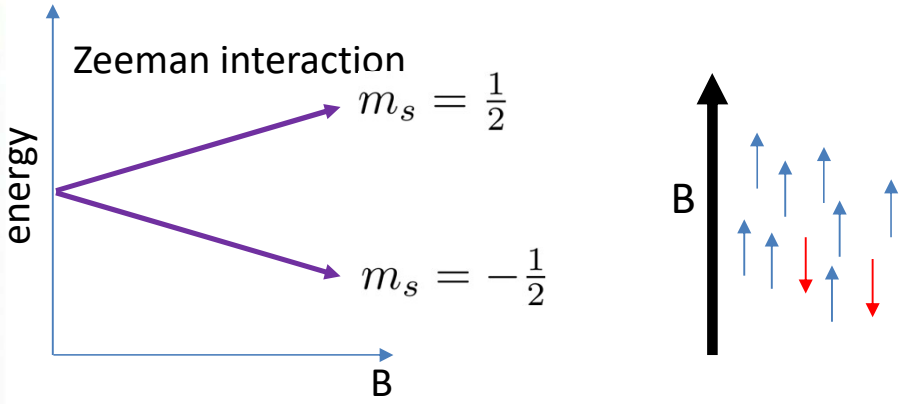
4 Department of Physics, UC Santa Barbara, Santa Barbara, CA 93106, USA; bouwmeester@ucsb.edu (D.B.); ebodnia@ucsb.edu (E.B.)
5 Huygens-Kamerlingh Onnes Laboratory, Leiden University, 2311 EZ Leiden, The Netherlands
6 Faculty of Medicine and Health Sciences | Biomedical Research, University of Buckingham, Buckingham MK18 1EG, UK; luca.turin@buckingham.ac.uk
7 Allen Institute, Seattle, WA 98109, USA; christofk@alleninstitute.org
* Correspondence: neven@google.com

Using quantum mechanics to probe biological systems

Medical imaging

MRI

Discovered by Felix Bloch and Edward Mills Purcell (Nobel prize 1952)



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Review: Grover *et al. J.* 2015. *Clin. Exp. Hepatol* 5(3)

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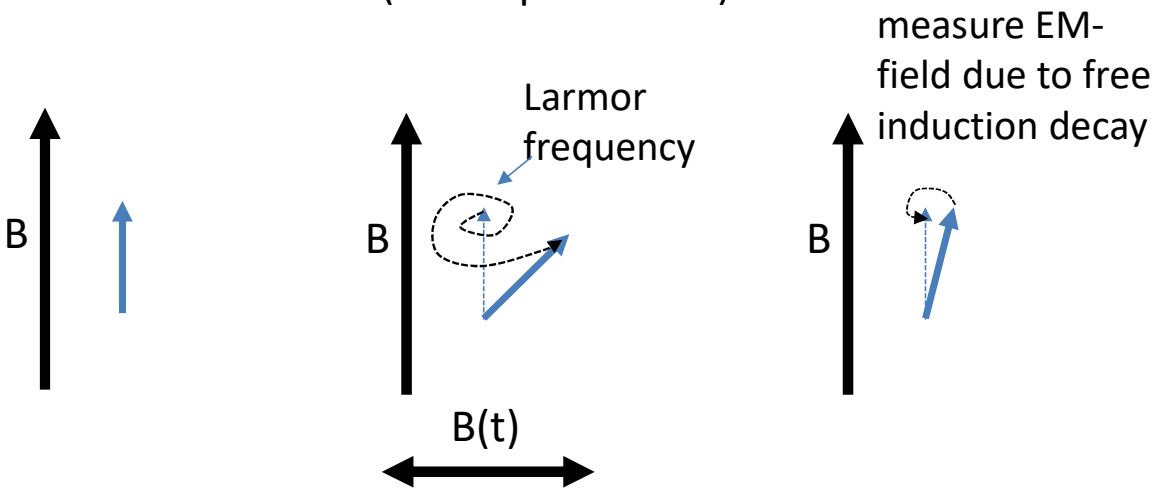

spin-lattice relaxation (T_1)
spin-spin relaxation (T_2)

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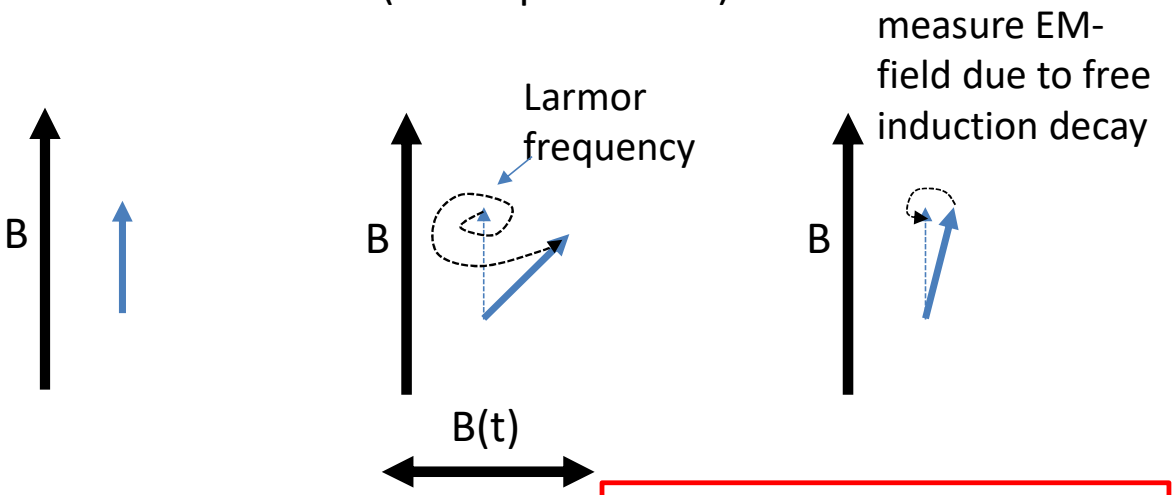

spin-lattice relaxation (T_1)
spin-spin relaxation (T_2)

dynamics calculated with…
Bloch equation

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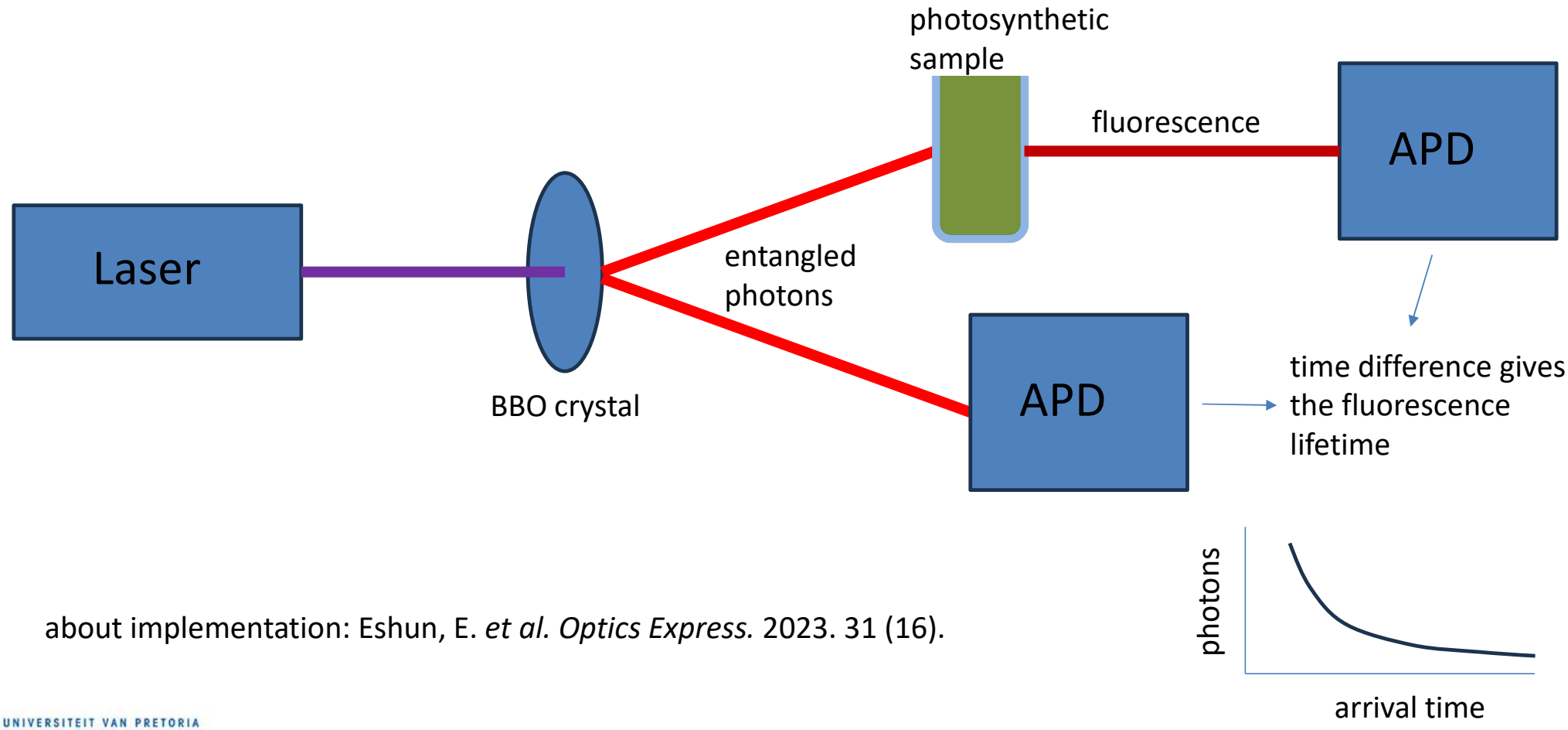
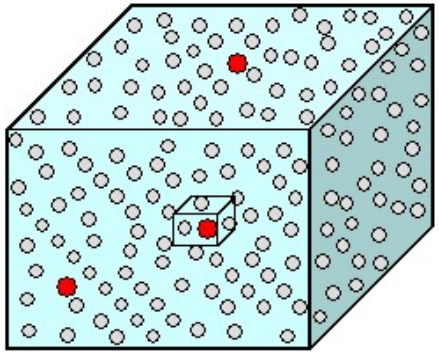
Review: Grover *et al. J.* 2015. *Clin. Exp. Hepatol* 5(3)

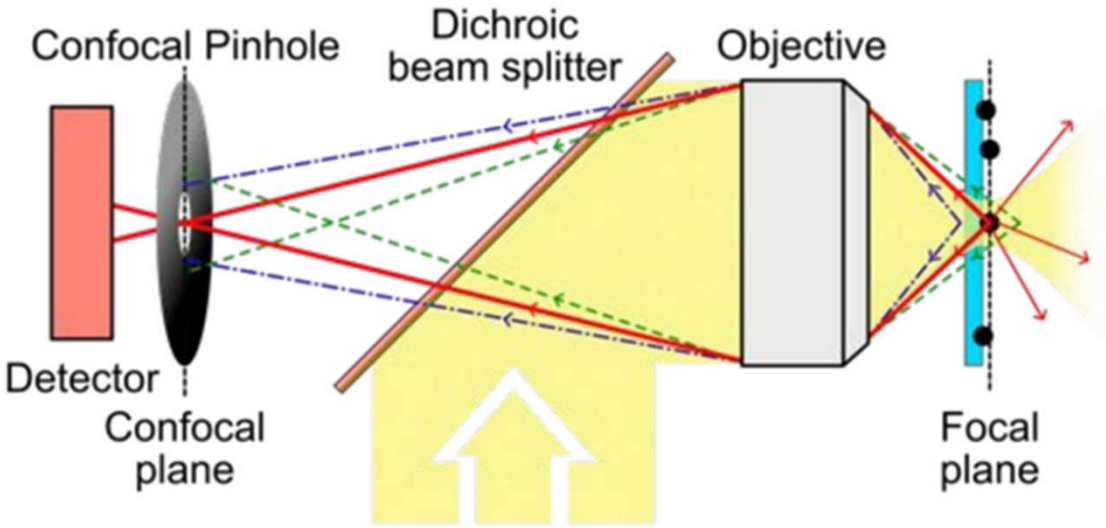
using entangled photons to measure fluorescence lifetimes



about implementation: Eshun, E. *et al. Optics Express.* 2023. 31 (16).

Single-molecule spectroscopy



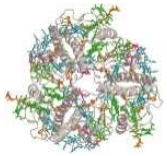


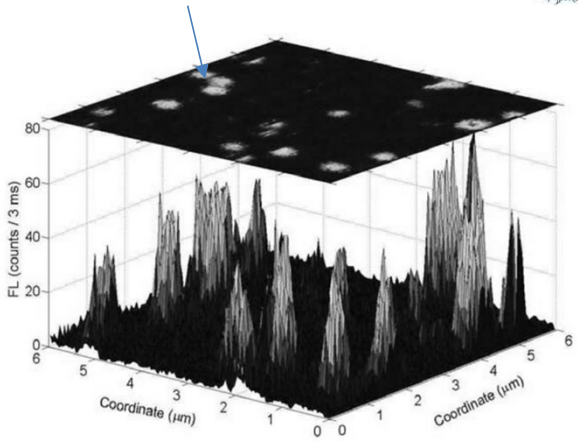
Joshua Botha, MSc. thesis

Reviews: Faraday Discuss., 2015, 184, 9
Malý *et al. ScI. Rep. 6(1).* 2016
T.P.J. Krüger, R. van Grondelle*, Physica B*. 2015

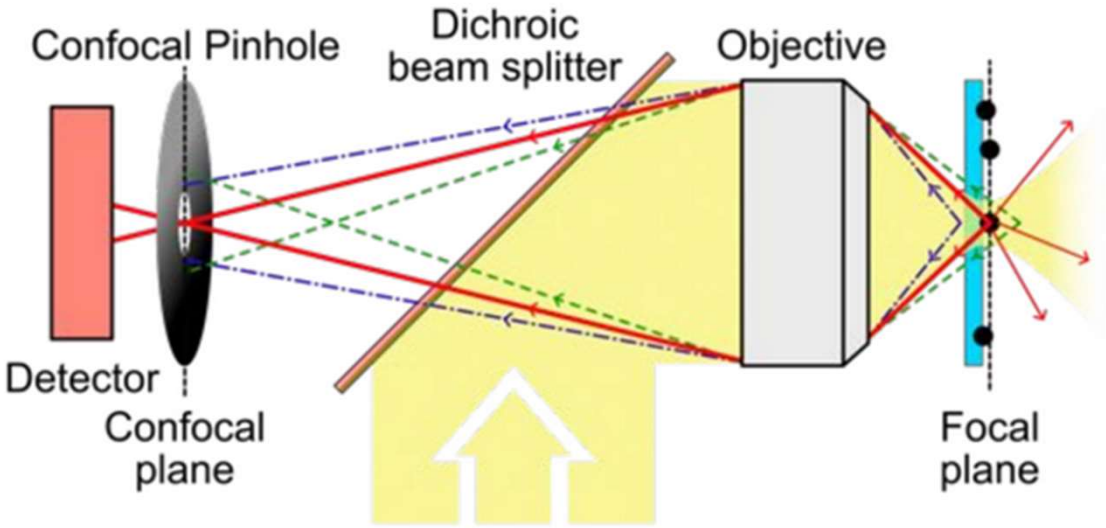
Single-molecule spectroscopy

single macromolecule (LHCII)





Tjaart Krüger, PhD. thesis



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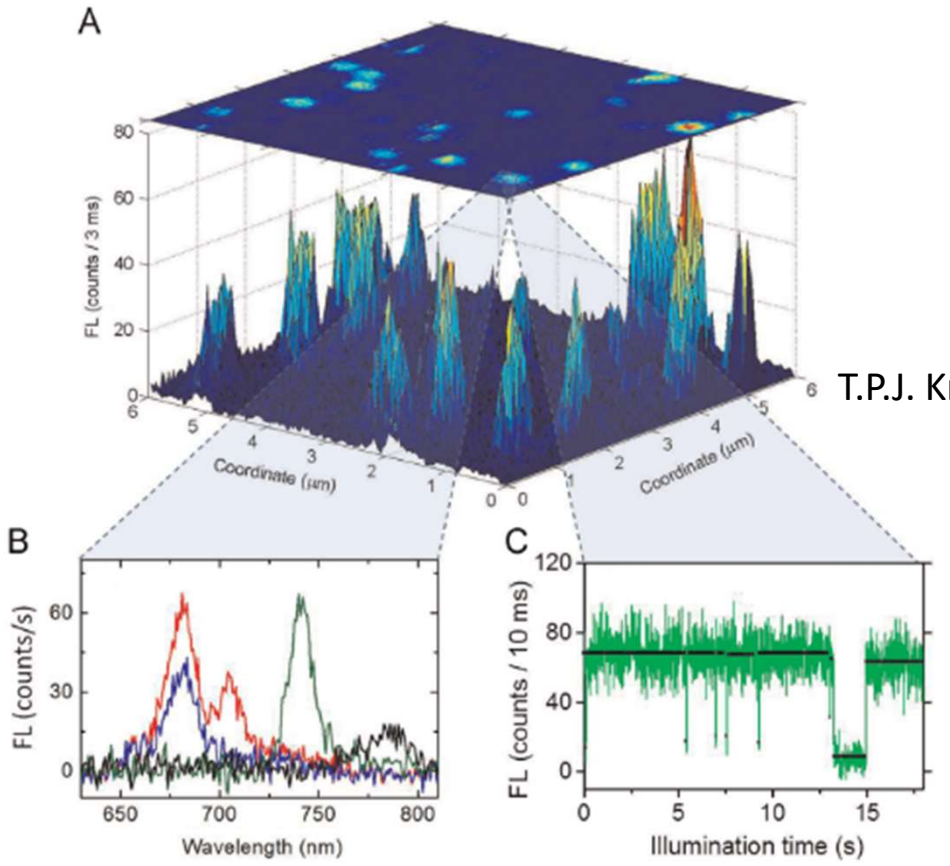

T.P.J. Krüger, R. van Grondelle, Physica B (2015),

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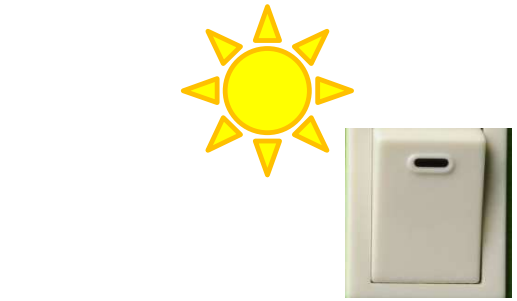
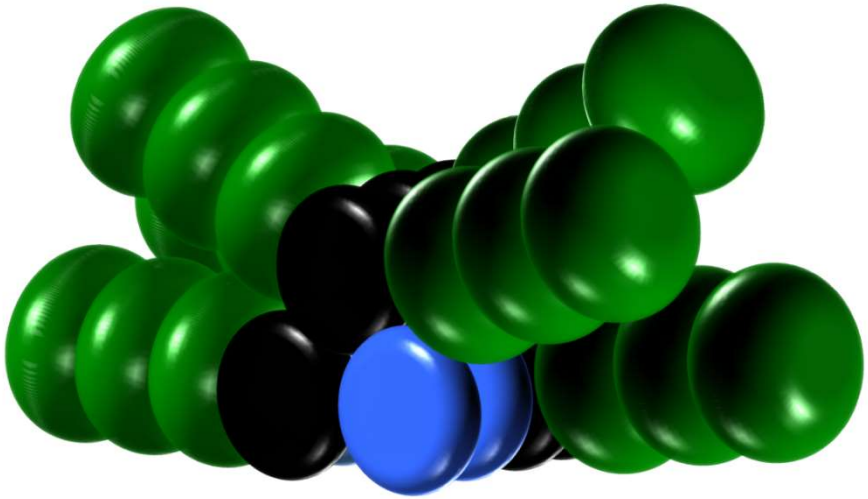
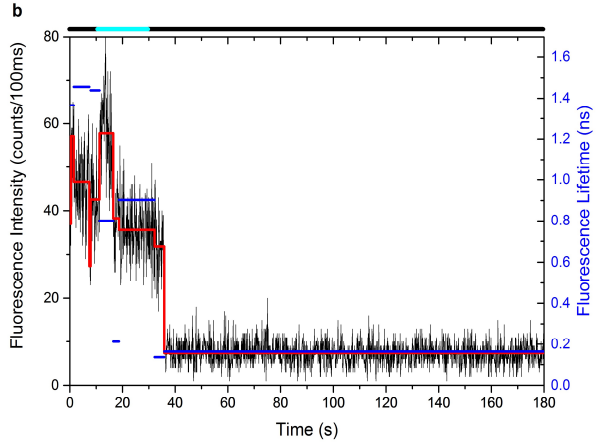
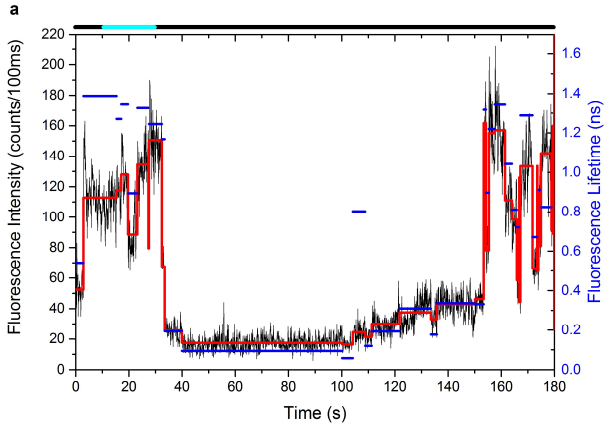


Phycobilisome







Gwizdala, Botha, Wilson, Kirilovsky, van Grondelle & TPJK, “Switching an individual phycobilisome off and on” *J Phys Chem Lett* 9:2426-2432 (2018)