

Unlocking the quantum design of photosynthesis for bio-inspired solar technologies



Tjaart Krüger
Associate Professor
Department of Physics
University of Pretoria



105 billion tons per year

of biomass is produced by
photosynthesis

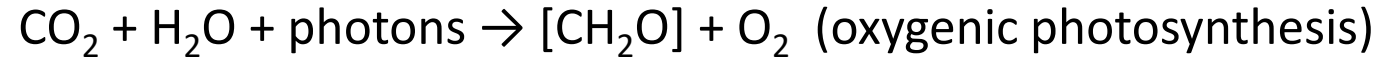
A wide-angle photograph of the Great Pyramids of Giza in Egypt. The pyramids are constructed from golden-brown stone blocks and are set against a blue sky with scattered white clouds. The foreground is a vast, flat, sandy desert. A small figure of a person on a camel is visible in the lower right corner, providing a sense of scale.

= two great pyramids of Giza
per hour... every hour

~50% of global photosynthesis occurs in water



Photosynthesis: inspiration for solar tech



cheap molecules + light $\rightarrow$ fuels

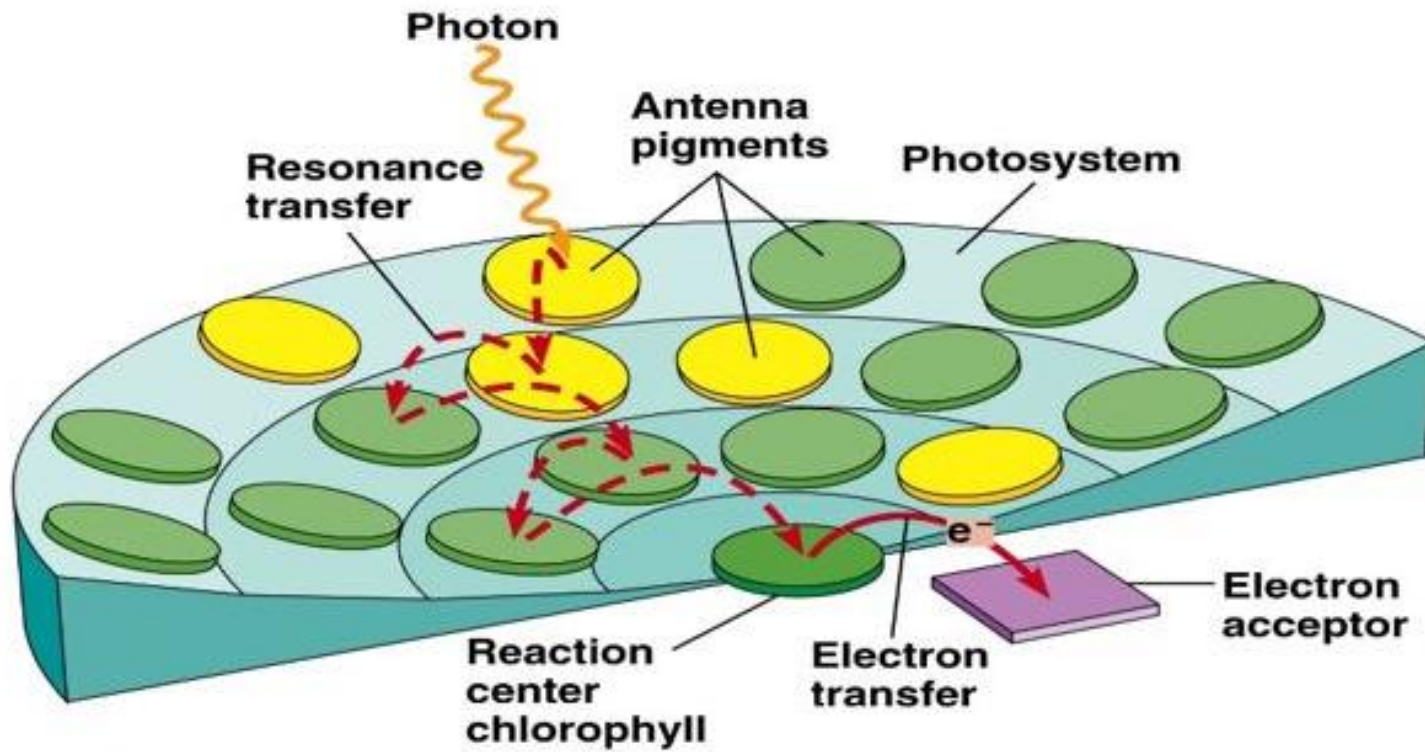
carbohydrates $\rightarrow$ liquid fuels

electrons $\rightarrow$ electricity

protons $\rightarrow$ H₂

NITheCS minischool on Energy Materials: <https://www.youtube.com/watch?v=J7pb-yRV4zs>

“Natural” solar cells



100% quantum efficiency



The diagram illustrates the chemical structure of chlorophyll *a*. It features a central magnesium atom (Mg) coordinated by four nitrogen atoms within a porphyrin-like ring system, with a fifth coordination site occupied by a phytyl ester group. The structure is divided into five pyrrole rings labeled A through E. Key substituents include a methyl group at C2, an ethyl group at C7, a phytol chain at C15, and a methyl ester at C16. Various other groups like R¹, R², Y, and X are indicated at specific positions.

1 nm

The image displays the chemical structures of Lutein and Zeaxanthin. Lutein is shown at the top, featuring a long polyene chain with two substituted cyclohexene rings at each end; the left ring has a hydroxyl group and two methyl groups, while the right ring has a hydroxyl group and three methyl groups. Zeaxanthin is shown below it, with a similar structure but the right ring has two methyl groups instead of three. Both structures are labeled with their respective names, 'Lutein' and 'Zeaxanthin', centered below each molecule.

>3 nm

A micrograph of skeletal muscle tissue, showing characteristic striations (alternating light and dark bands) and a large, pale, circular structure, likely a nucleus or a blood vessel.

3 Proteins + 54 pigments

Photosystem II

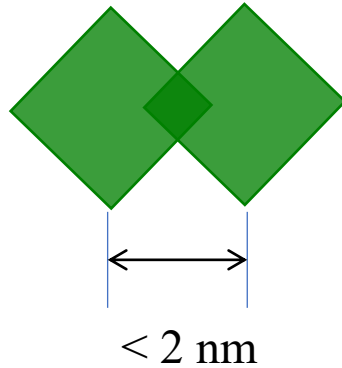
- Diameter ~ 7 nm
- Thickness ~ 4 nm

LHCII

Molecular excitons: quantum coherence

$$\Psi_{1,2} = \frac{1}{\sqrt{2}} (\varphi_1^1 \varphi_2^0 \pm \varphi_1^0 \varphi_2^1)$$

The chlorophyll dimer

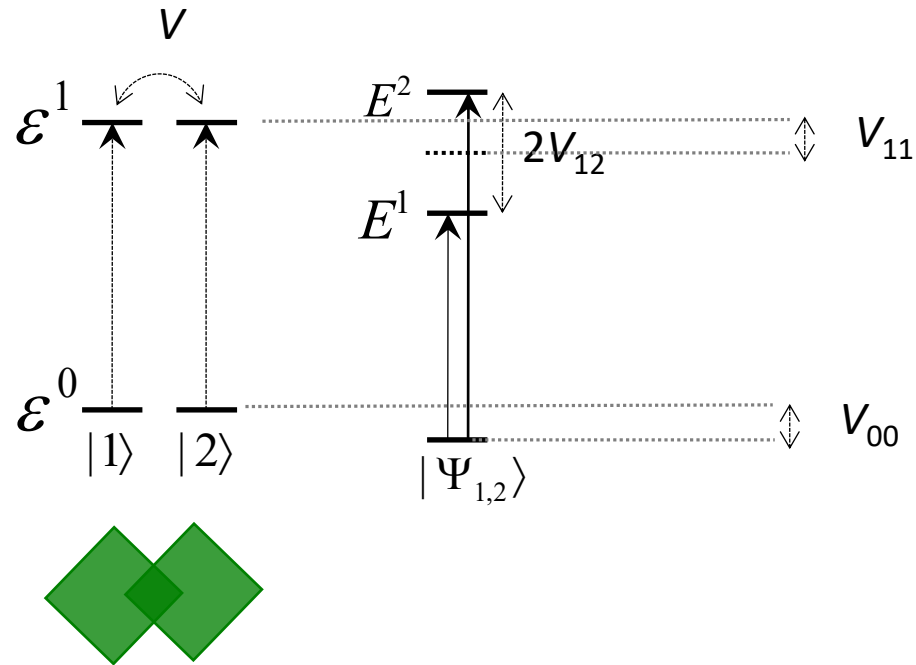


Physiological benefits:

1. Enhanced light absorption
2. Enhanced energy funnelling
3. Enhanced energy transfer: >10x
4. Less trapping and energy loss in antennas
5. Faster charge separation in reaction centres

Molecular excitons: quantum coherence

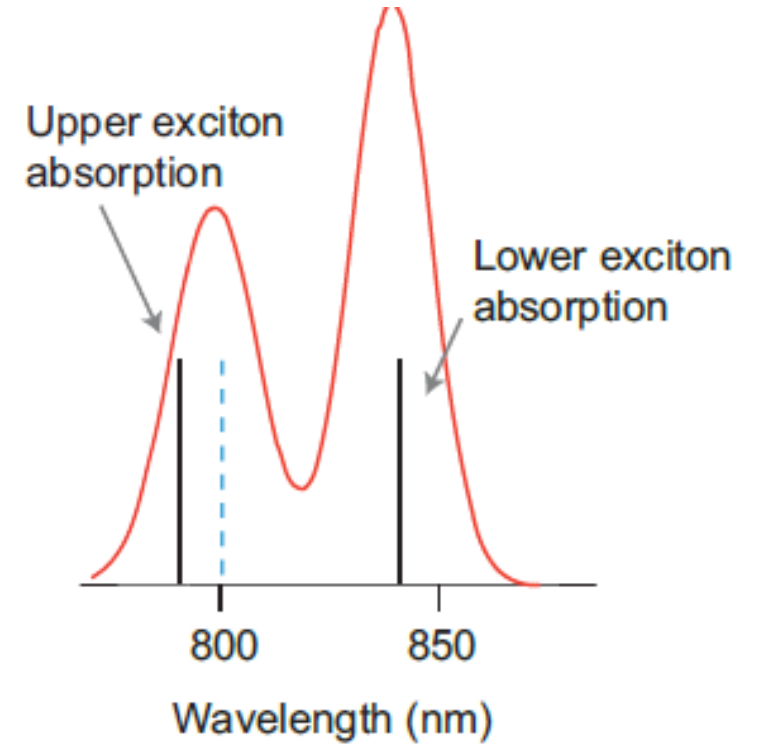
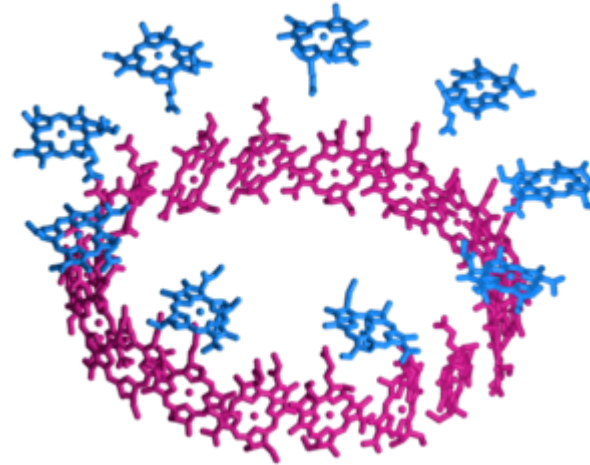
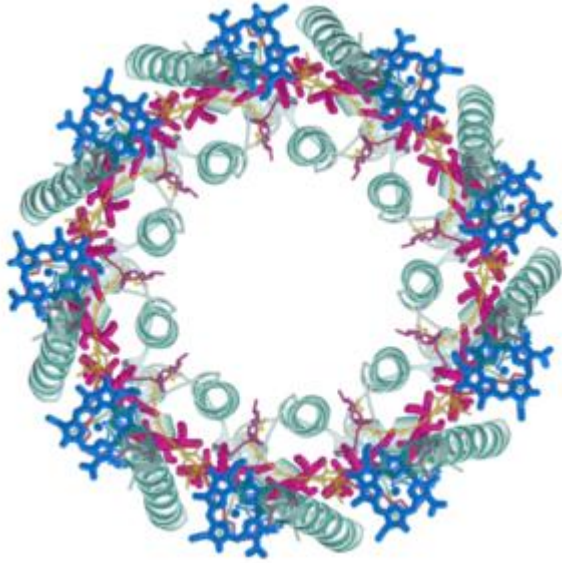
$$\Psi_{1,2} = \frac{1}{\sqrt{2}} (\phi_1^1 \phi_2^0 \pm \phi_1^0 \phi_2^1)$$



Physiological benefits:

1. Enhanced light absorption
2. Enhanced energy funnelling
3. Enhanced energy transfer: >10x
4. Less trapping and energy loss in antennas
5. Faster charge separation in reaction centres

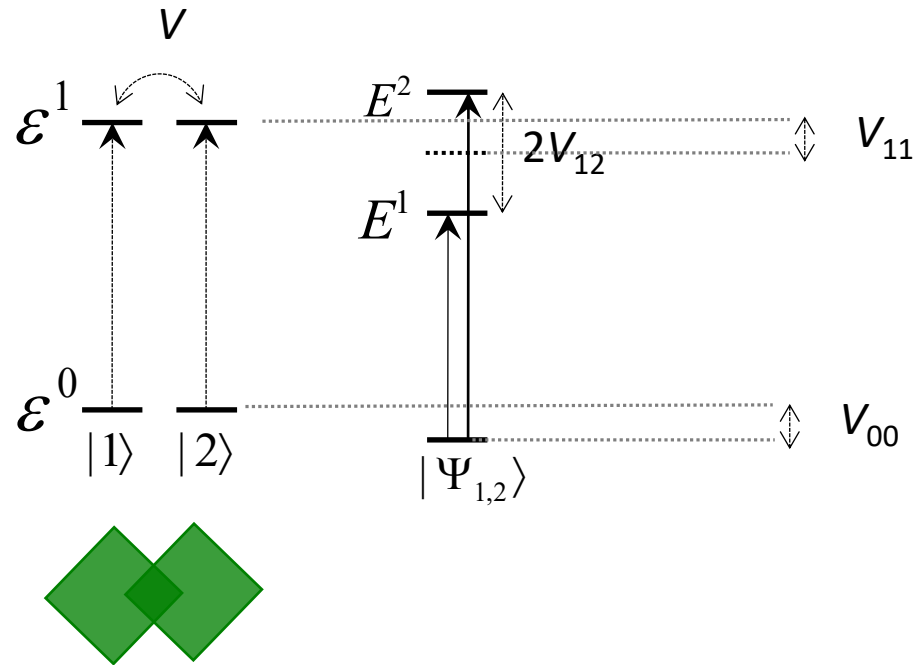
1. Electronic coherence “creates” pigments



Purple bacteria

Molecular excitons: quantum coherence

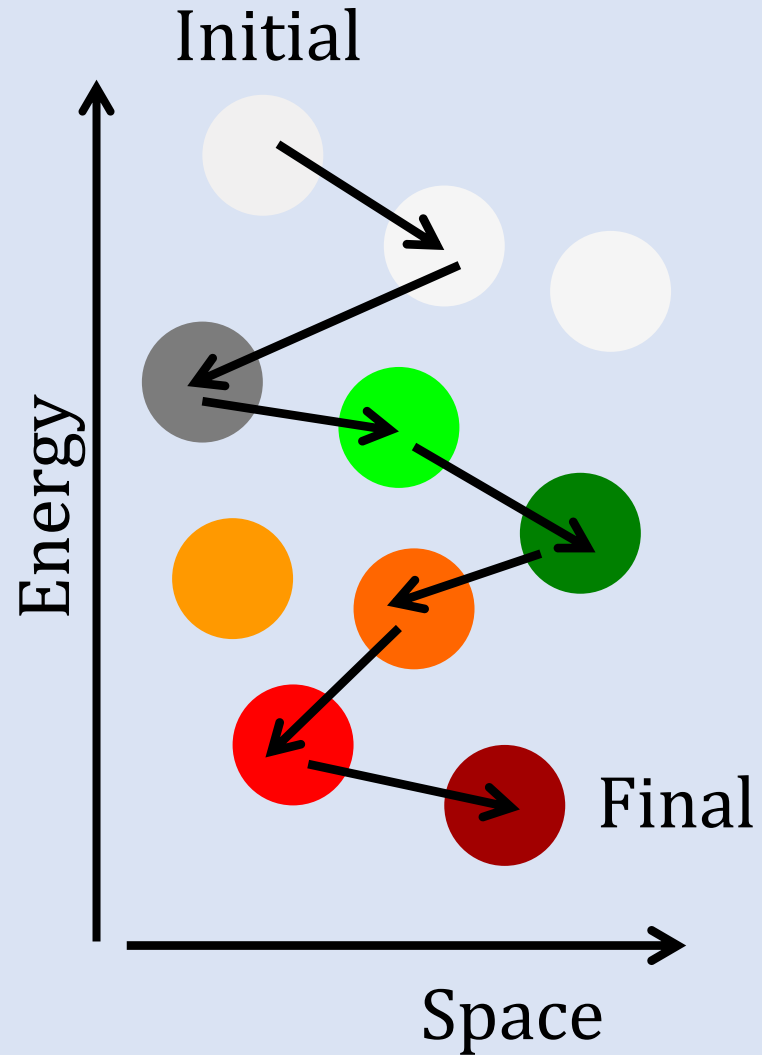
$$\Psi_{1,2} = \frac{1}{\sqrt{2}} (\phi_1^1 \phi_2^0 \pm \phi_1^0 \phi_2^1)$$



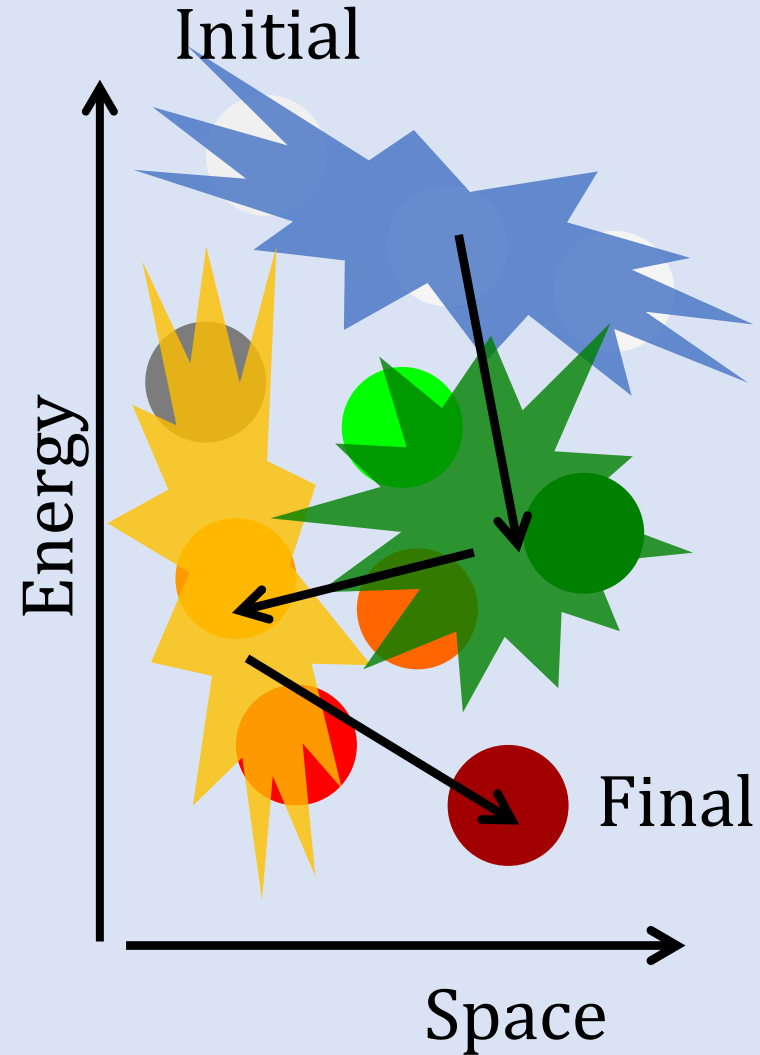
Physiological benefits:

1. Enhanced light absorption
2. Enhanced energy funnelling
3. Enhanced energy transfer: >10x
4. Less trapping and energy loss in antennas
5. Faster charge separation in reaction centres

2. Molecular excitons enhance energy funnelling



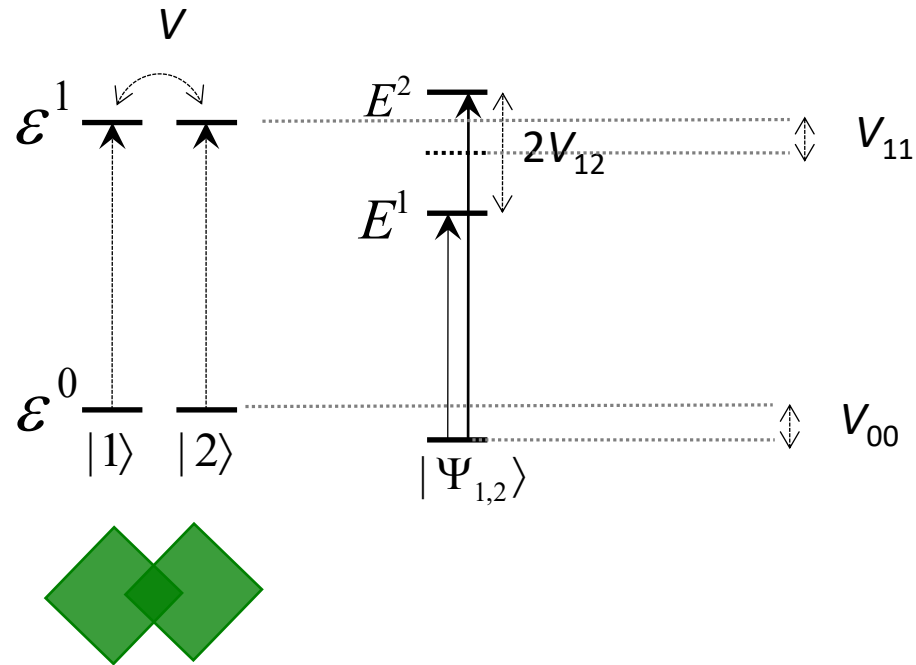
Individual pigments



Excitons

Molecular excitons: quantum coherence

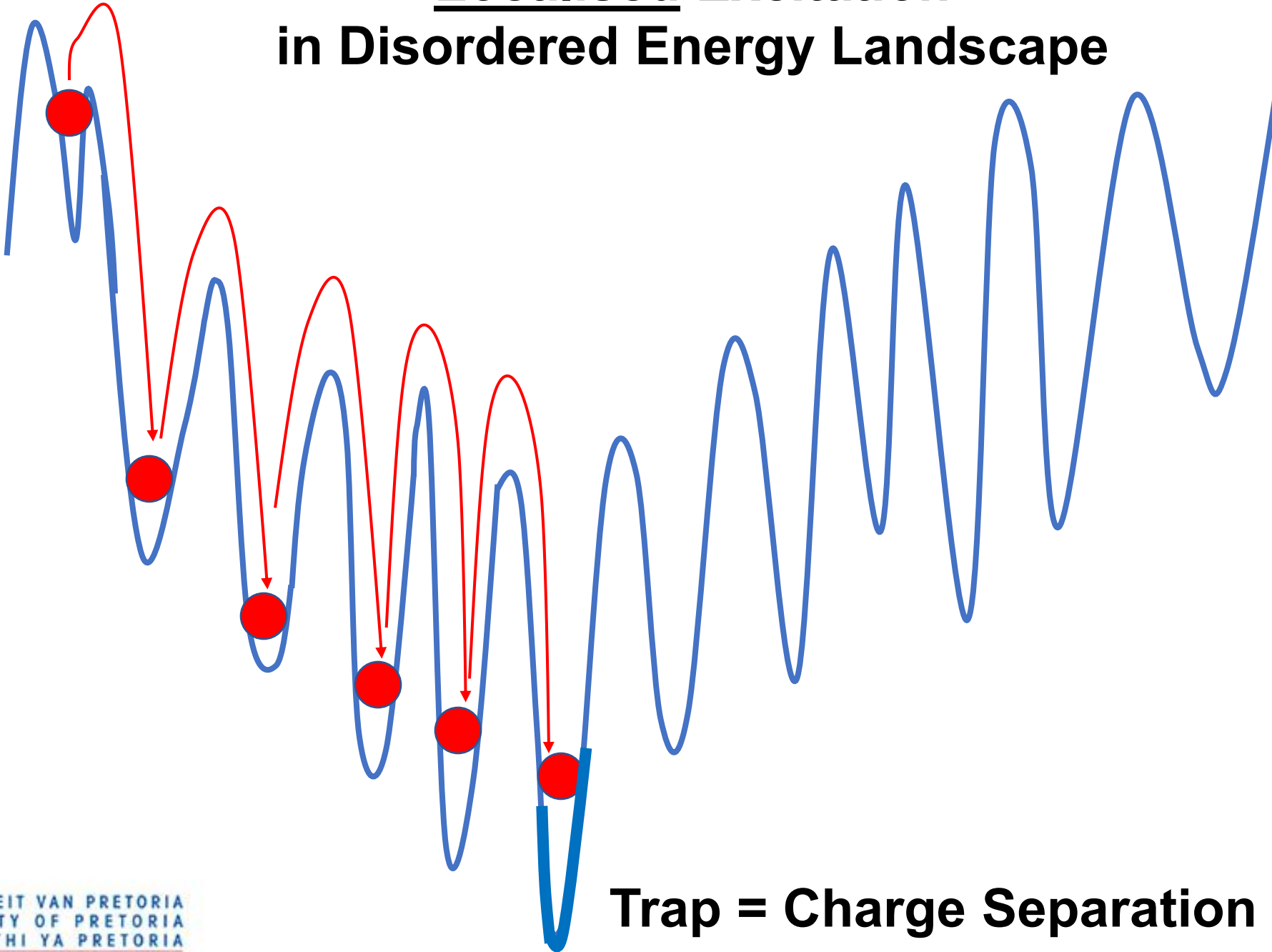
$$\Psi_{1,2} = \frac{1}{\sqrt{2}} (\phi_1^1 \phi_2^0 \pm \phi_1^0 \phi_2^1)$$



Physiological benefits:

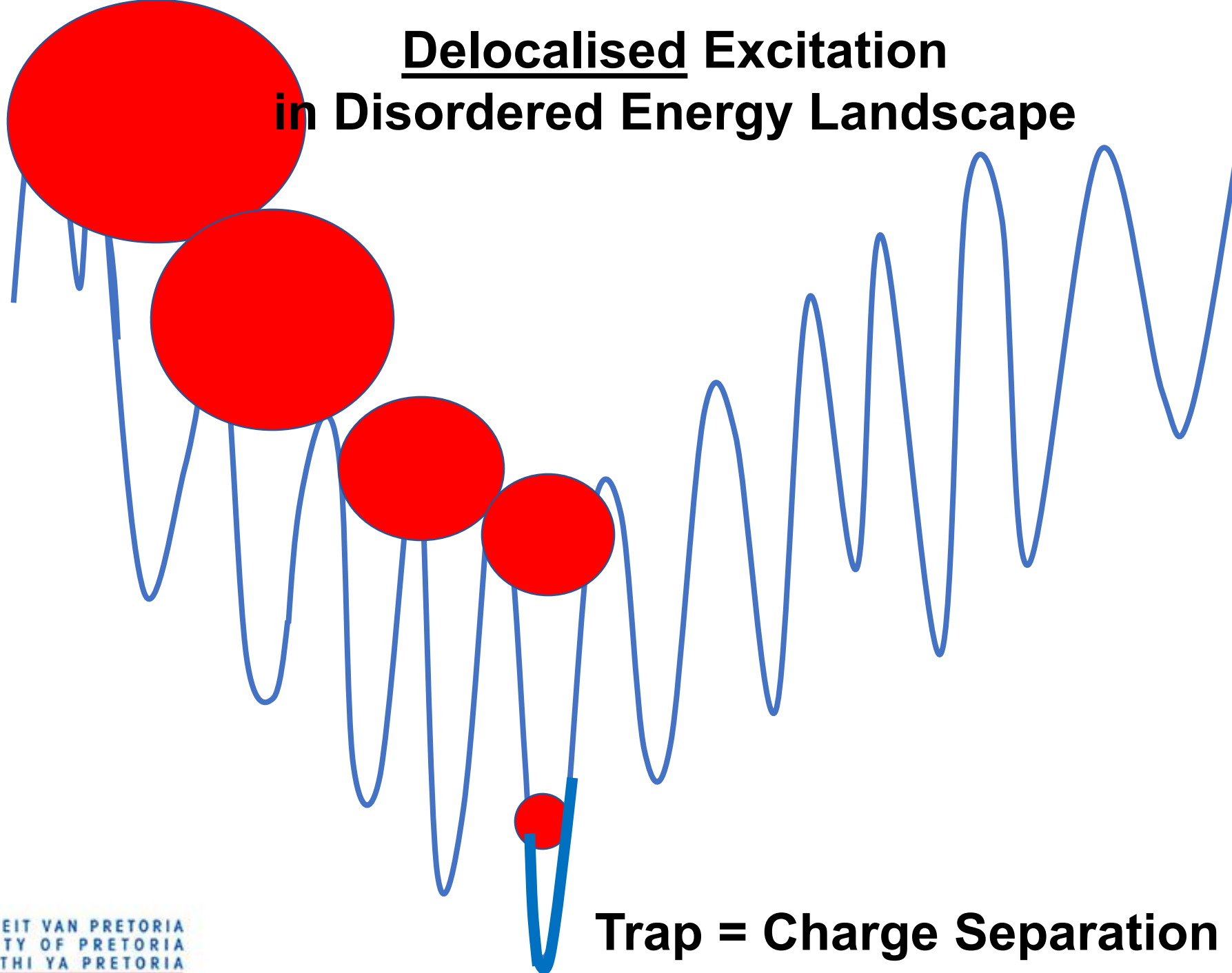
1. Enhanced light absorption
2. Enhanced energy funnelling
3. Enhanced energy transfer: >10x
4. Less trapping and energy loss in antennas
5. Faster charge separation in reaction centres

Localised Excitation in Disordered Energy Landscape

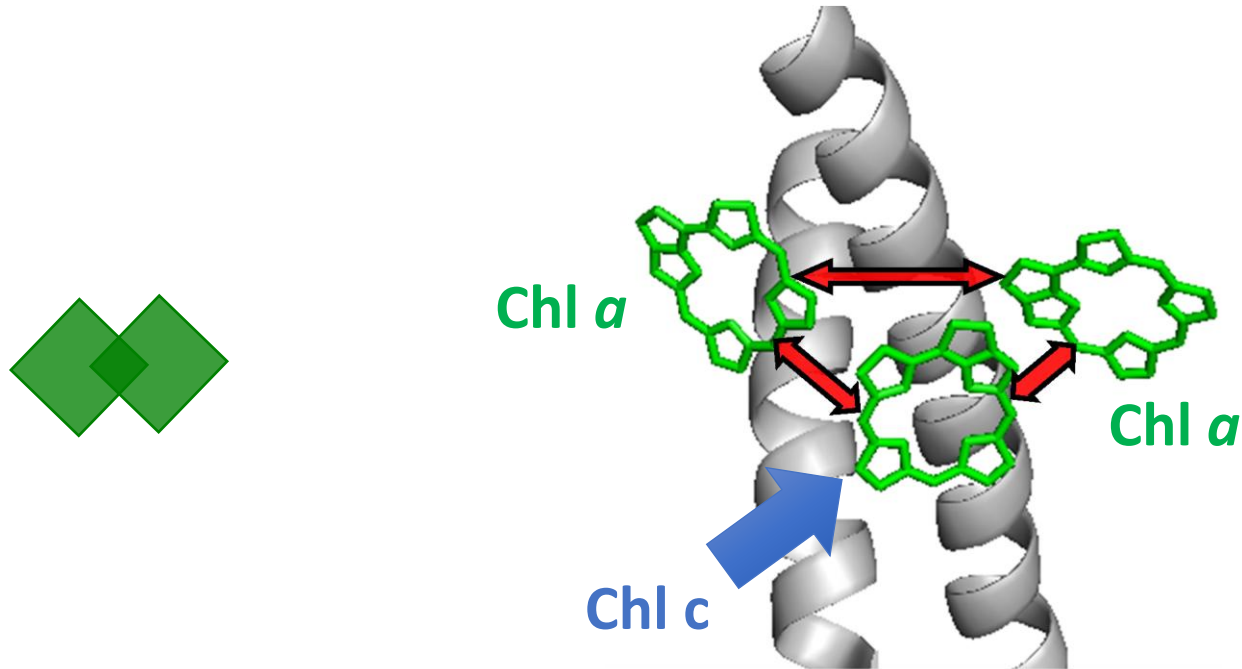


Trap = Charge Separation

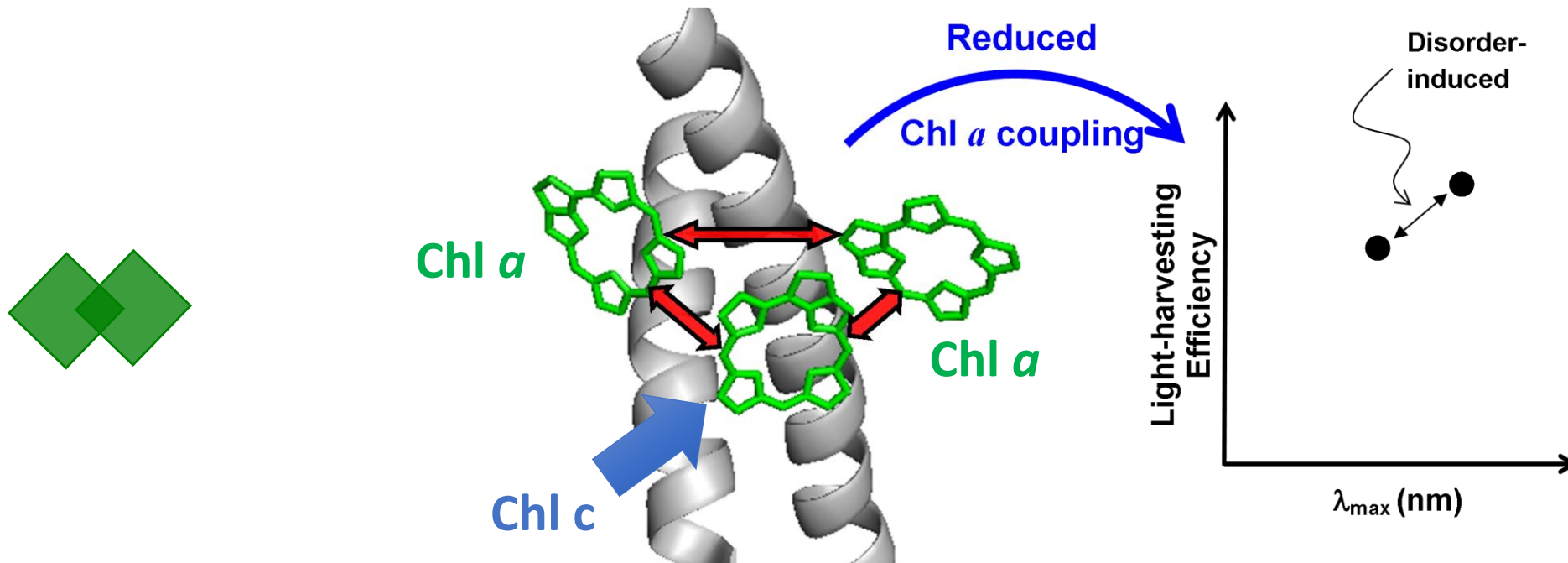
Delocalised Excitation in Disordered Energy Landscape



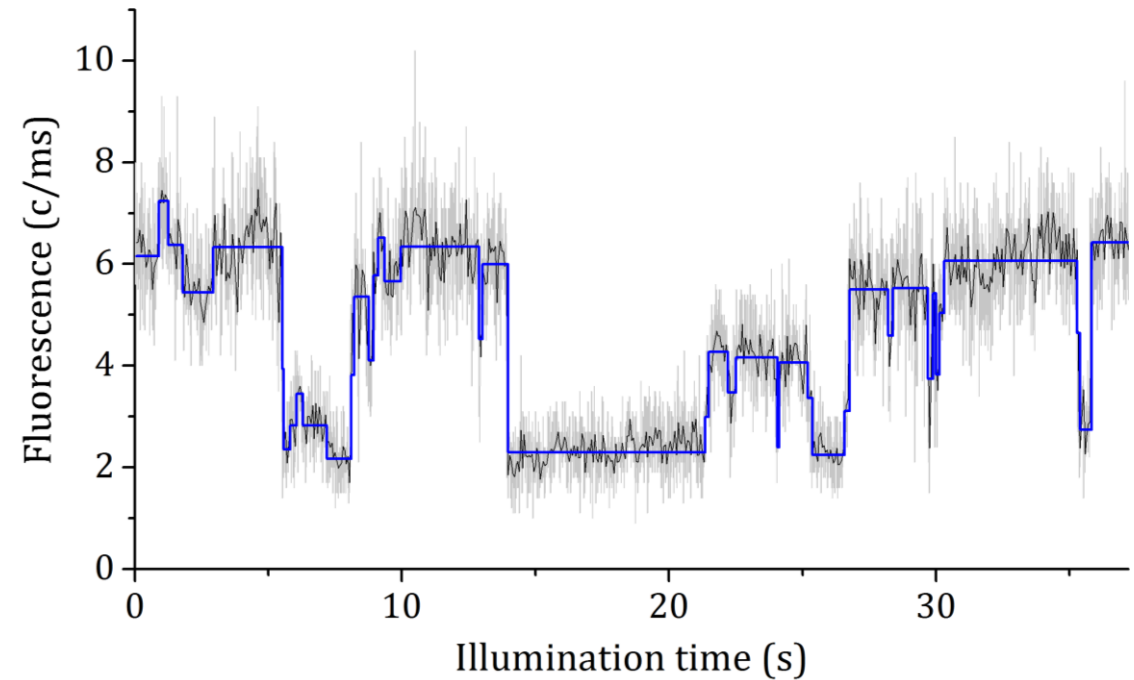
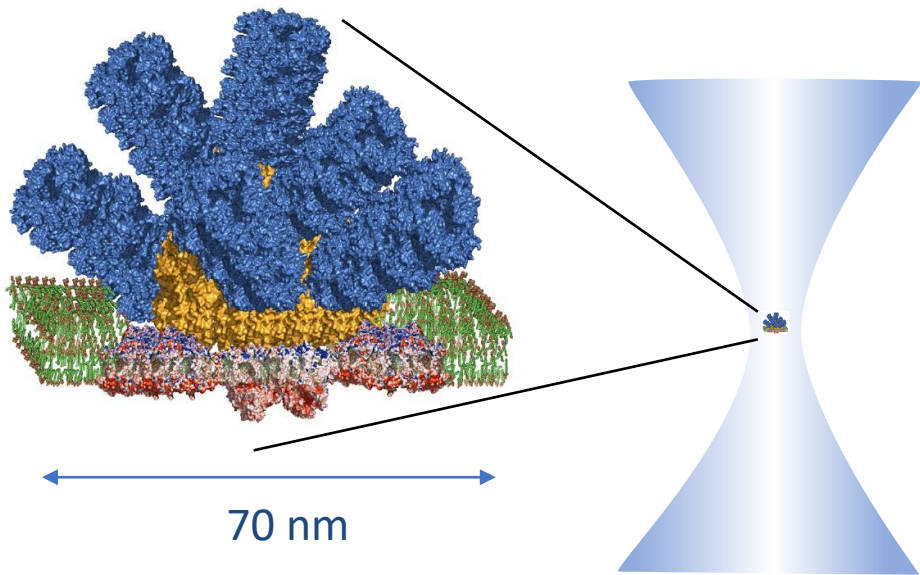
Example: How diatoms tune their quantumness



Example: How diatoms tune their quantumness

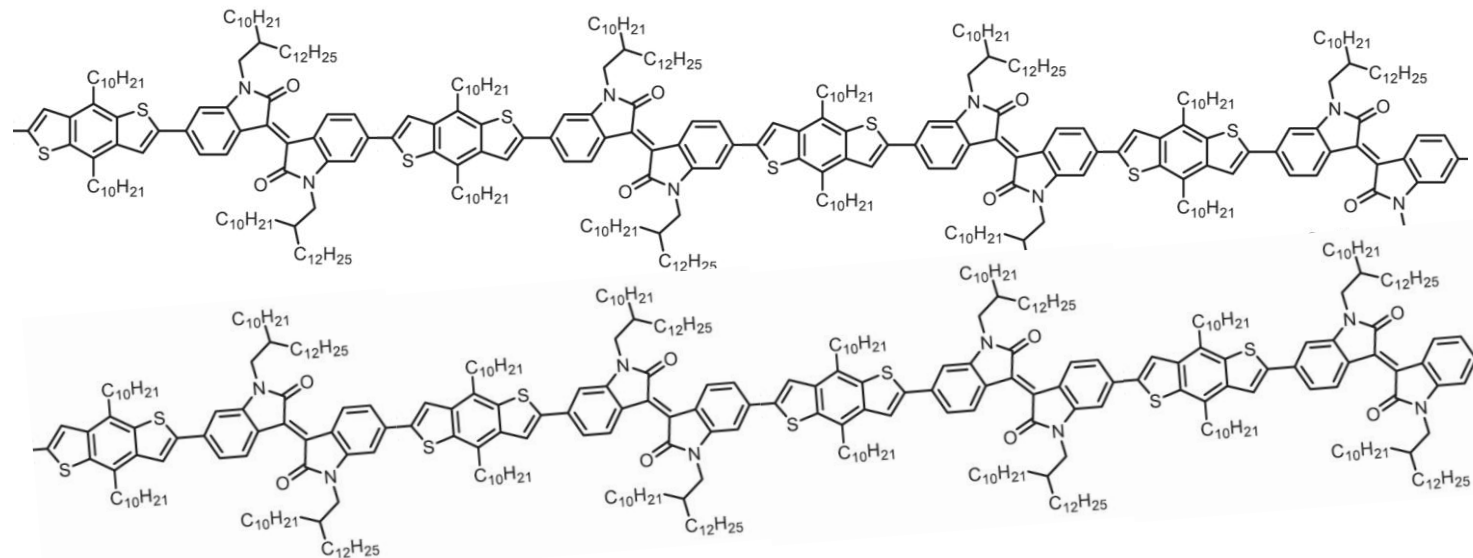


Example: How cyanobacteria tune their quantumness

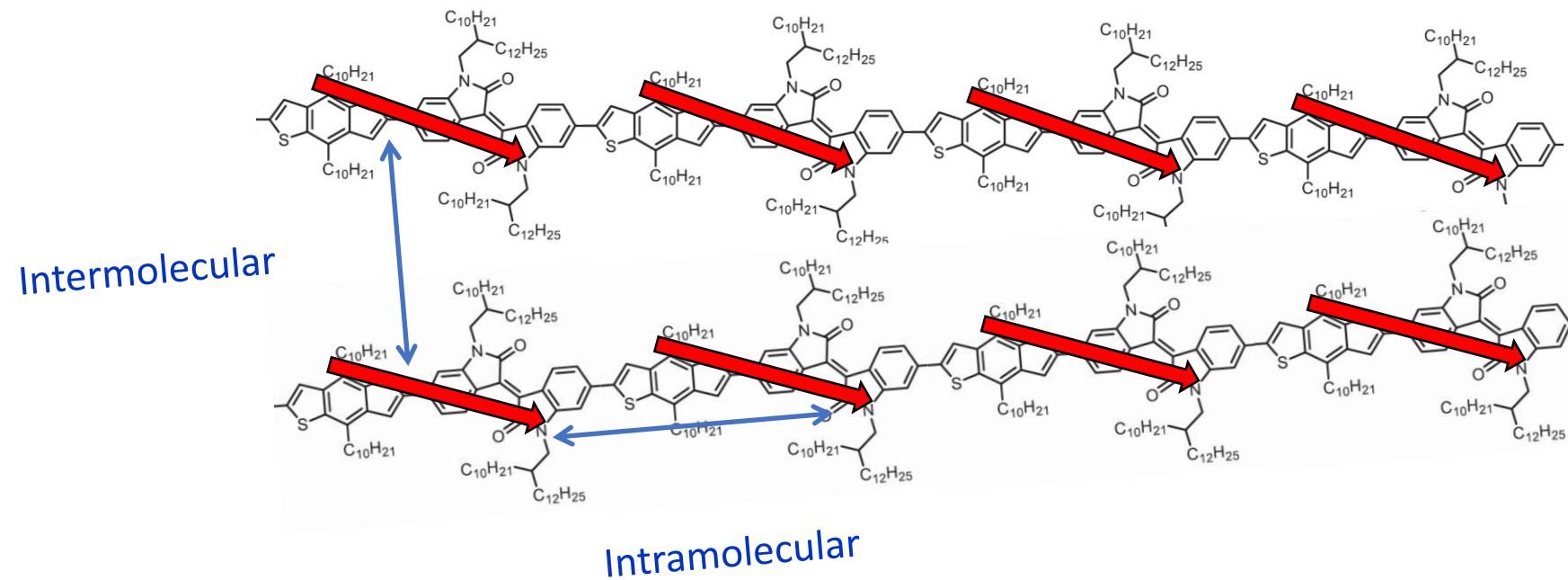


The photosynthetic activity is rapidly switched on and off!

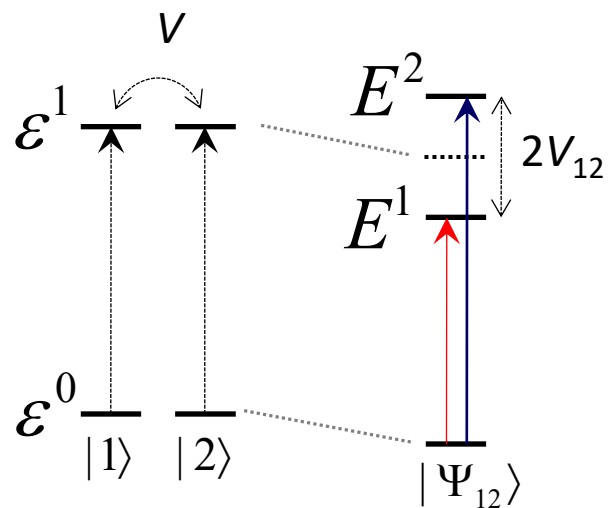
Application to organic solar cells



Application to organic solar cells



Molecular excitons: quantum coherence

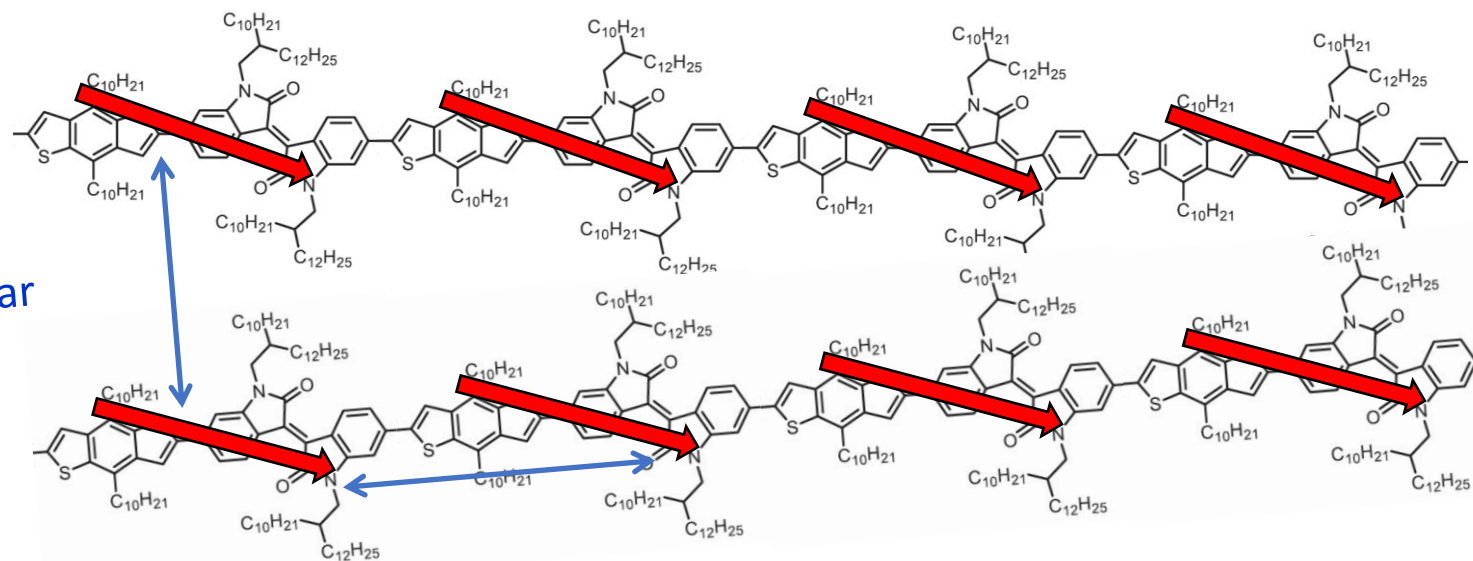


monomers

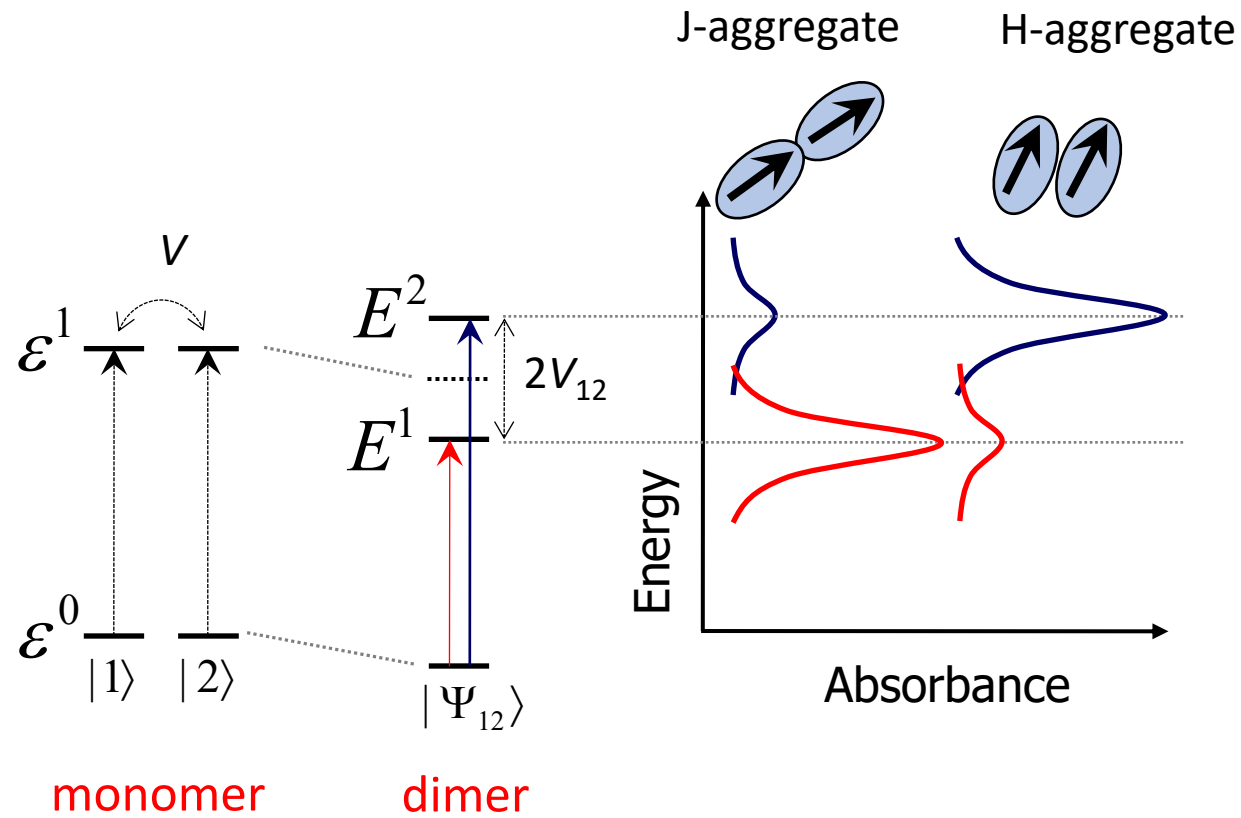
dimer

Intermolecular

Intramolecular



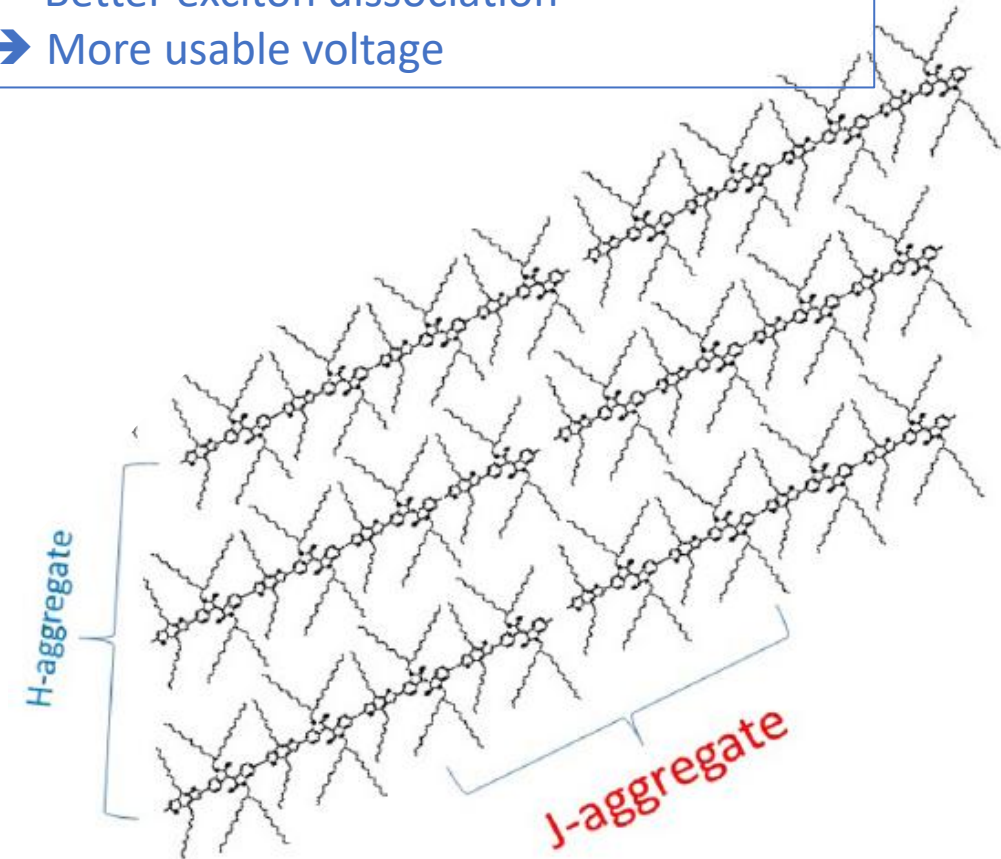
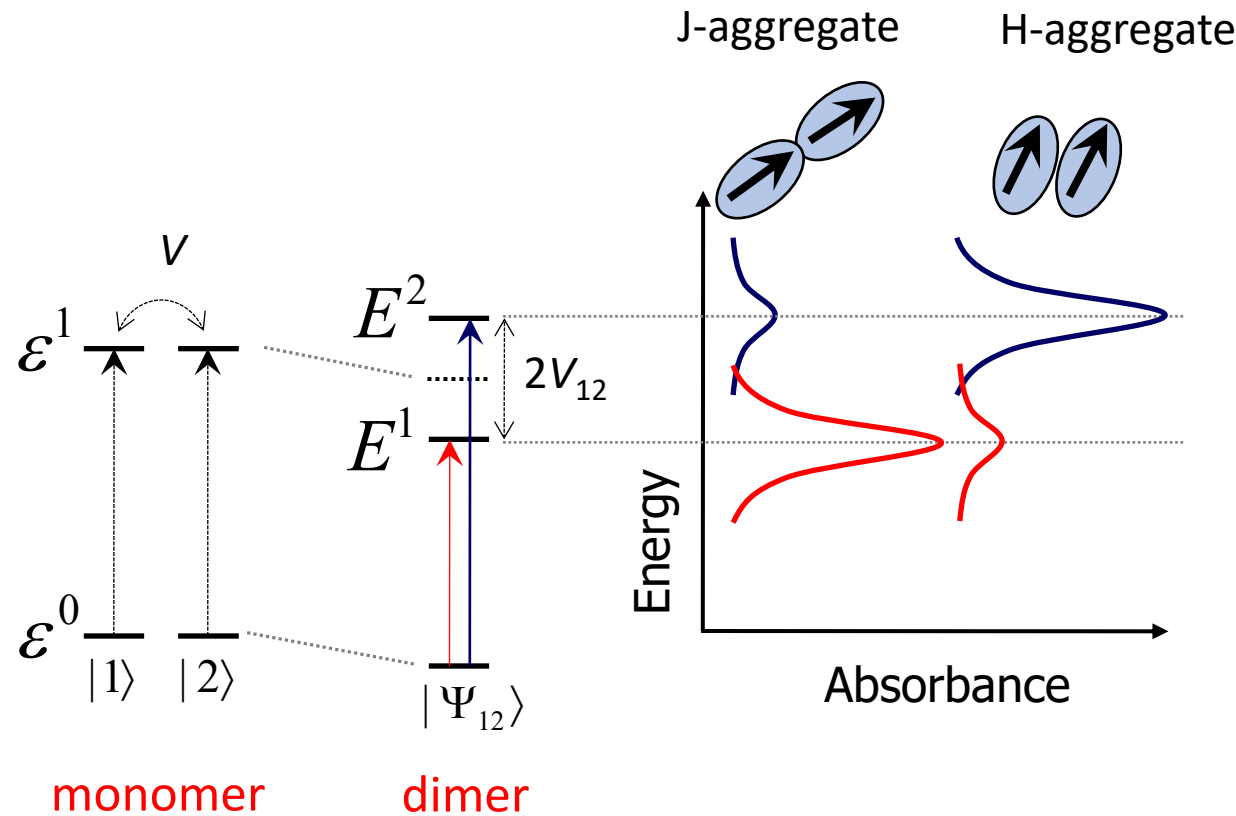
Molecular excitons: quantum coherence



Molecular excitons: quantum coherence

- ✓ Better exciton generation
- ➔ Higher current

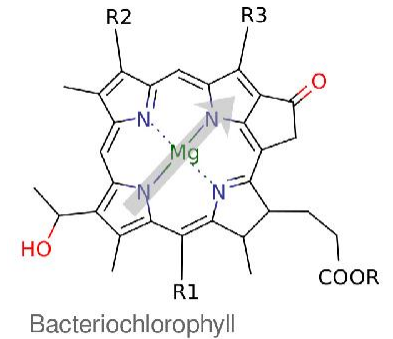
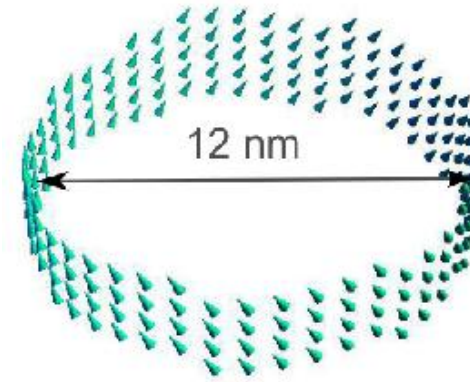
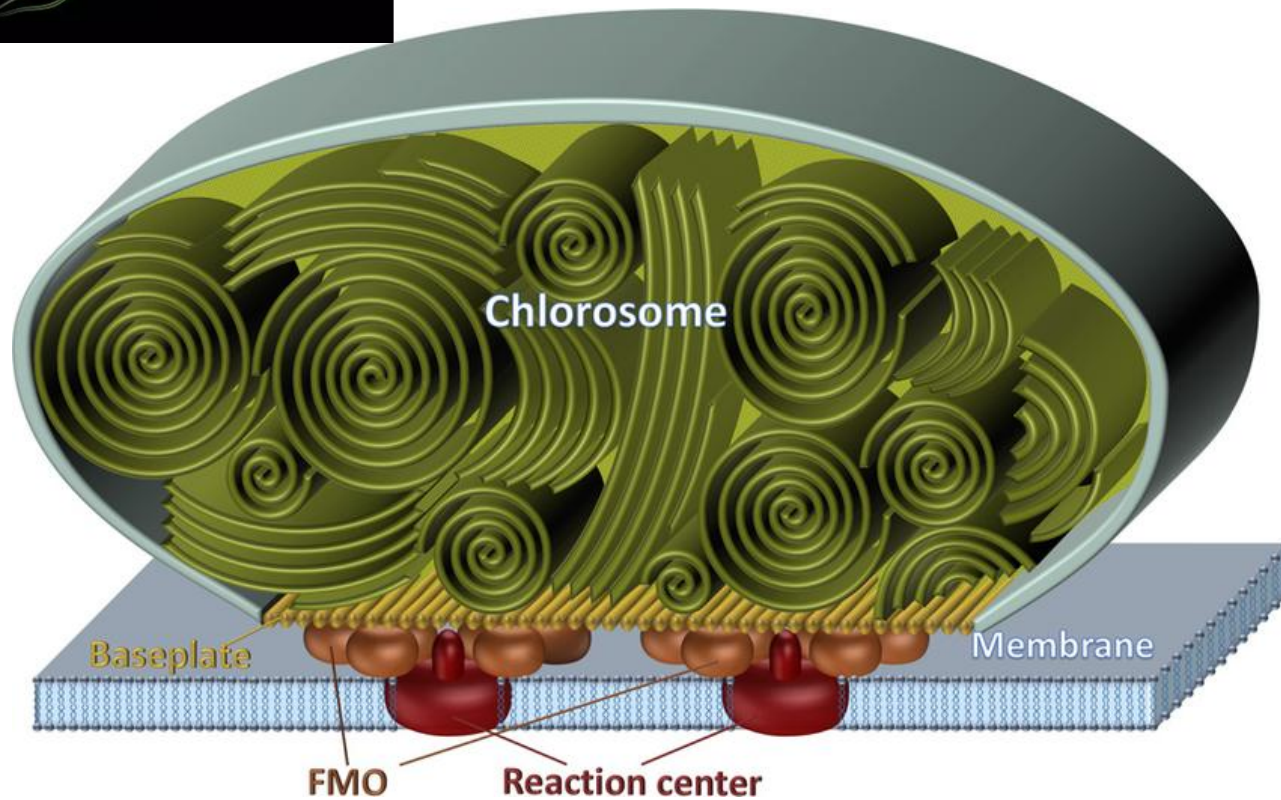
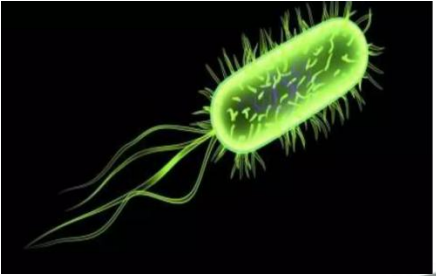
- ✓ Better exciton dissociation
- ➔ More usable voltage



It's incredibly difficult to predict the exact arrangement of self-assembled organic aggregates

Self-assembled pigment aggregates

High quantum efficiency means robustness to static disorder



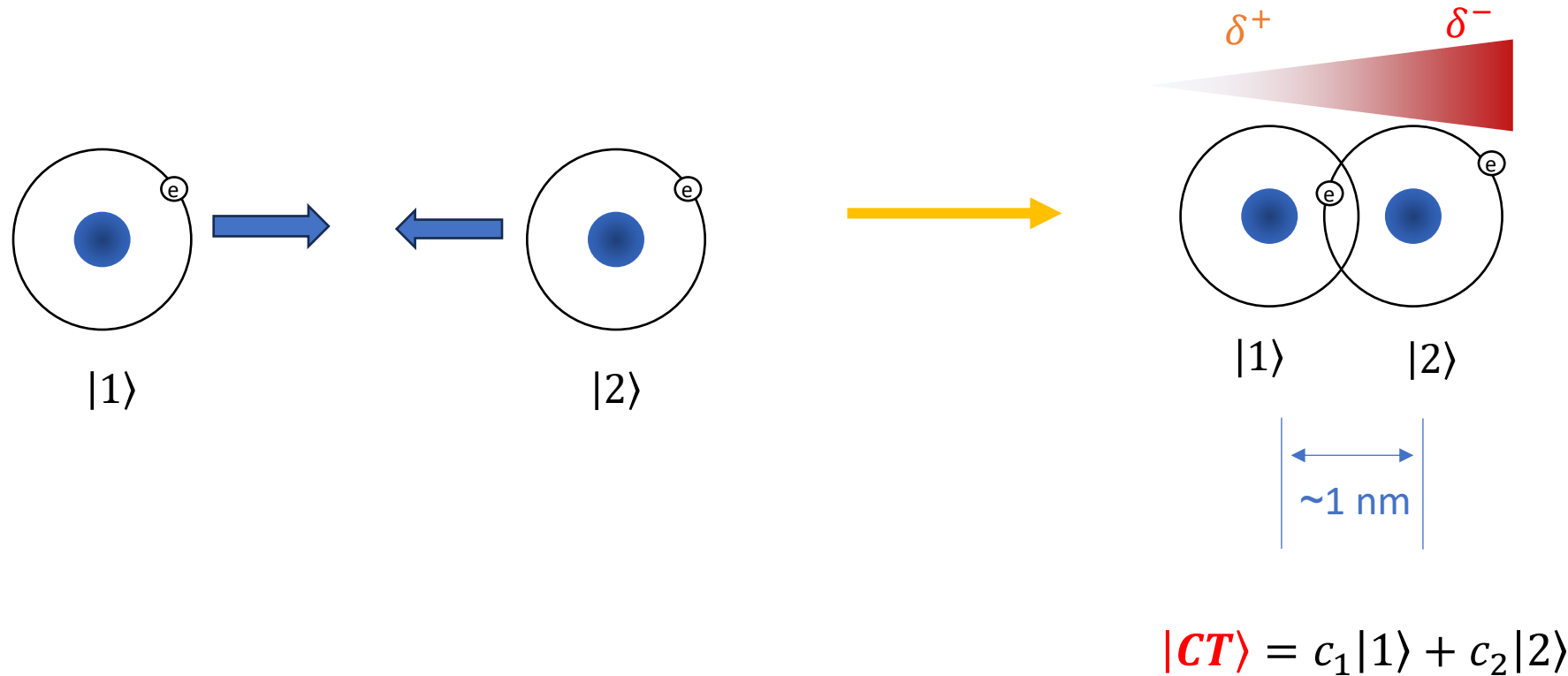
perfect molecular crystals!

Quantum biology: inspiration from nature

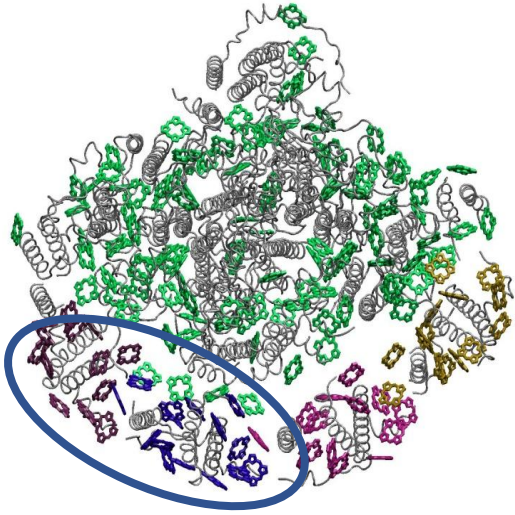
Various EU Key Enabling Technologies are based on quantum-mechanical phenomena and find examples in nature.

Key Enabling Quantum Technology	Research field	Examples in nature
Single-photon detection in a noisy, low-voltage electrochemical environment at room temperature	Photonics	• Eye • Photoreceptors • Light-harvesting complexes
N ₂ fixation at room temperature and pressure	Nanotechnology	Certain bacteria
Chemically powered transport of ions and electrons across nanometres with low dissipation	Nanoelectronics	Transmembrane ion transport across basically every (sub)cellular membrane
H ₂ from H ⁺ without noble metals at 0 V SHE	Advanced Materials	Many organisms, e.g. cyanobacteria
Photo-induced charge separation with near-unity quantum efficiency in a noisy environment at room temperature	Photovoltaics	Photosynthetic photosystems

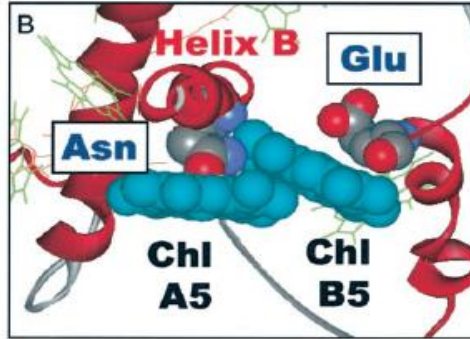
Charge-transfer states: strong charge gradient



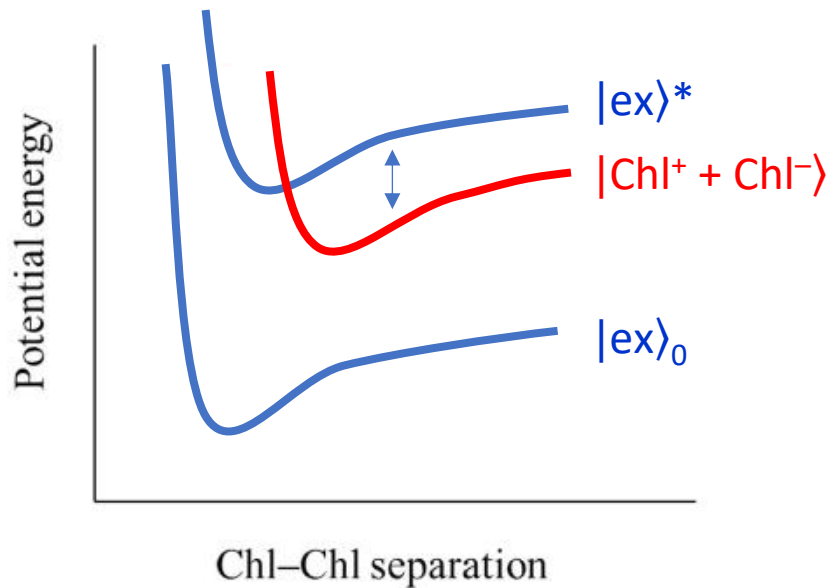
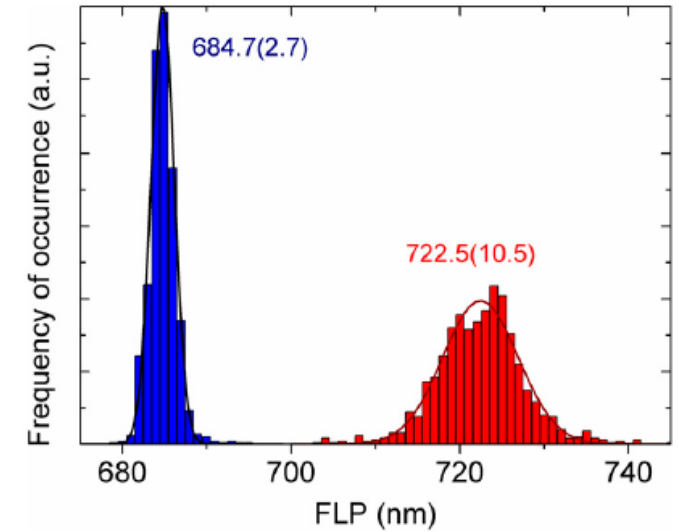
LHCs are strain sensors: sub-Å sensitivity



Lhca1/4



$$\Delta \sim 0.7 - 0.8 \text{ \AA}$$



$$\hat{H}_{mix} = \epsilon_{ex}|ex\rangle\langle ex| + \epsilon_{CT}|CT\rangle\langle CT| + V(|ex\rangle\langle CT| + |CT\rangle\langle ex|)$$

$$E_{mix}^{\pm} = \frac{\epsilon_{ex} + \epsilon_{CT}}{2} \pm \sqrt{\frac{(\epsilon_{ex} - \epsilon_{CT})^2}{4} + V^2}$$

Take-home messages

- Nature is a rich source of inspiration, even for quantum tech
- Photosynthetic LHCs exploit and finely control quantum phenomena to enhance their biological function in several ways:
 - ✓ super-efficient organic solar cells can be created through “programmable” self-assembled molecules
 - ✓ highly sensitive strain sensors
 - ✓ biological single-photon emitters: can they be tuned to deliver on-demand photons for biotech applications?



A portrait of Steve Jobs, co-founder of Apple, wearing his signature round glasses and a dark turtleneck. He is holding a white iPhone in his right hand, displaying the iOS home screen with various app icons. The background is a solid dark blue.

Steve Jobs

“I think the biggest innovations of the 21st century will be at the intersection of biology and technology. A new era is beginning.”

Biophysics @ UP

Social media

<https://biophysicsup.netlify.app>

<https://x.com/TjaartKrueger>

<https://www.linkedin.com/company/103670300/admin/dashboard>

<https://www.instagram.com/biophysics.up/#>

<https://www.youtube.com/@biophysicsattheuniversityo7970>

Funding



Science and
Technology
Facilities Council



South African
Quantum
Technology
Initiative



National Research
Foundation

RISA

Research and Innovation
Support and Advanceme



science
& technology

Department:
Science and Technology
REPUBLIC OF SOUTH AFRICA



FULBRIGHT



UNIVERSITEIT VAN PRETORIA
UNIVERSITY OF PRETORIA
YUNIBESITHI YA PRETORIA



african laser centre

NITheCS

National Institute for
Theoretical and Computational Sciences



CSIR
Touching lives through innovation



Deutscher Akademischer Austauschdienst
German Academic Exchange Service

OPIT
OPPENHEIMER
MEMORIAL TRUST



Biophysics
Research Group