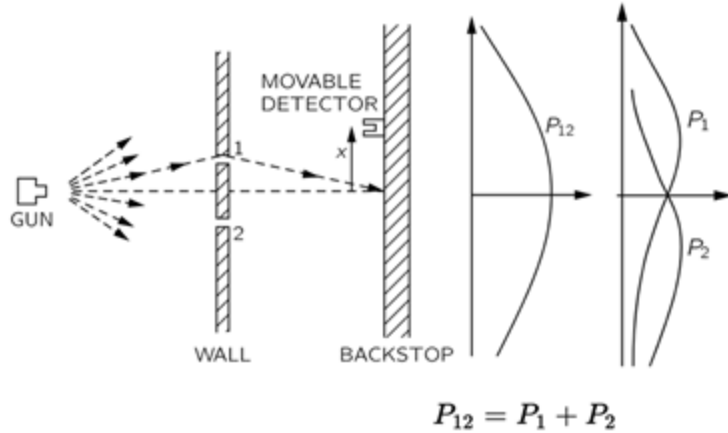


# **Basics of quantum computing and qubit implementation**

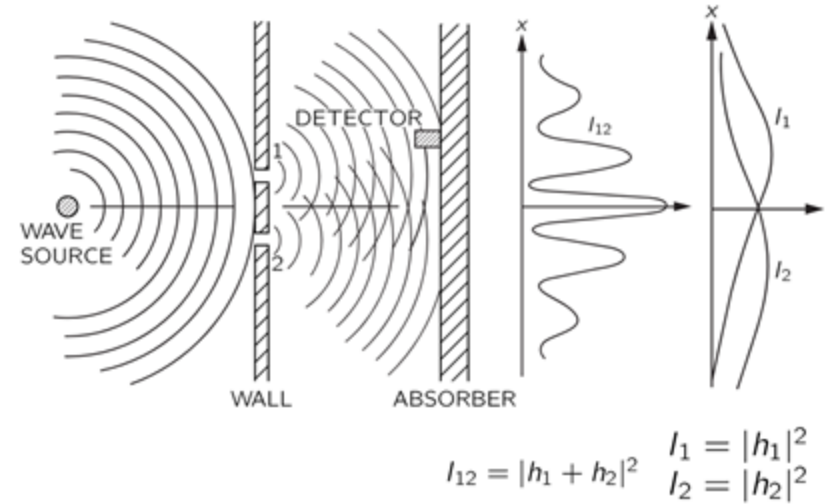
**Vishvendra S. Poonia**  
**Indian Institute of Technology Roorkee**

# Foundation: classical behavior

## Experiment with particles

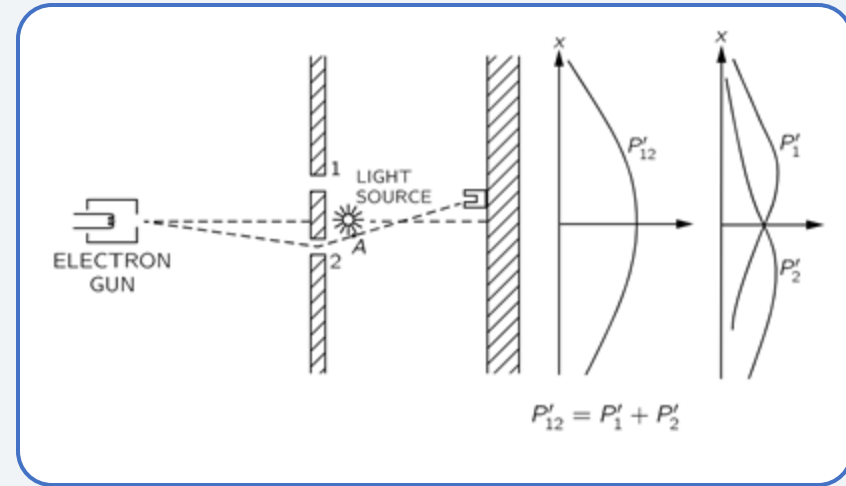
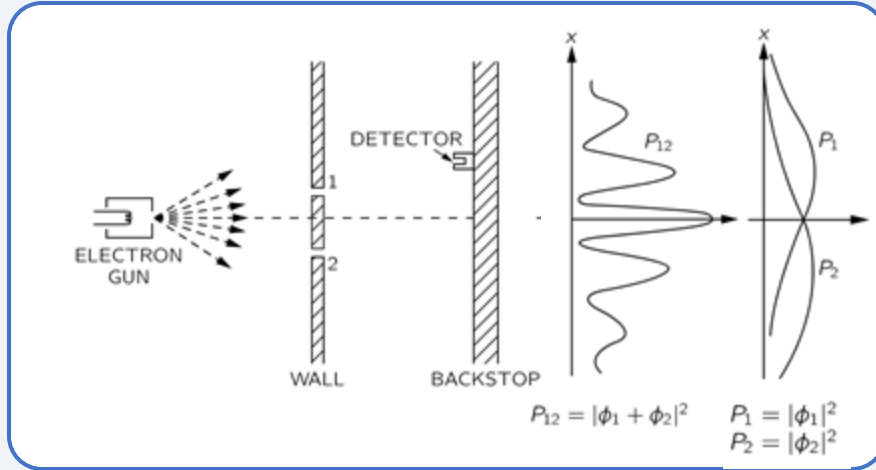


## Experiment with waves



# Foundation: quantum mechanical behavior

## Experiment with electrons



# Quantum Mechanics: Basics

- A system is represented by a wavefunction
  - Hilbert space
- Evolution is governed by Schrödinger equation
  - Hamiltonian
- Measurement
  - Hermitian operators
- Superposition
- Entanglement

# Quantum Computing: Qubits and Quantum Gates














## Qubit

A two level quantum system:  $|0\rangle$   $|1\rangle$

The qubit state:  $\alpha |0\rangle + \beta |1\rangle$

In real world, we don't want: decoherence.

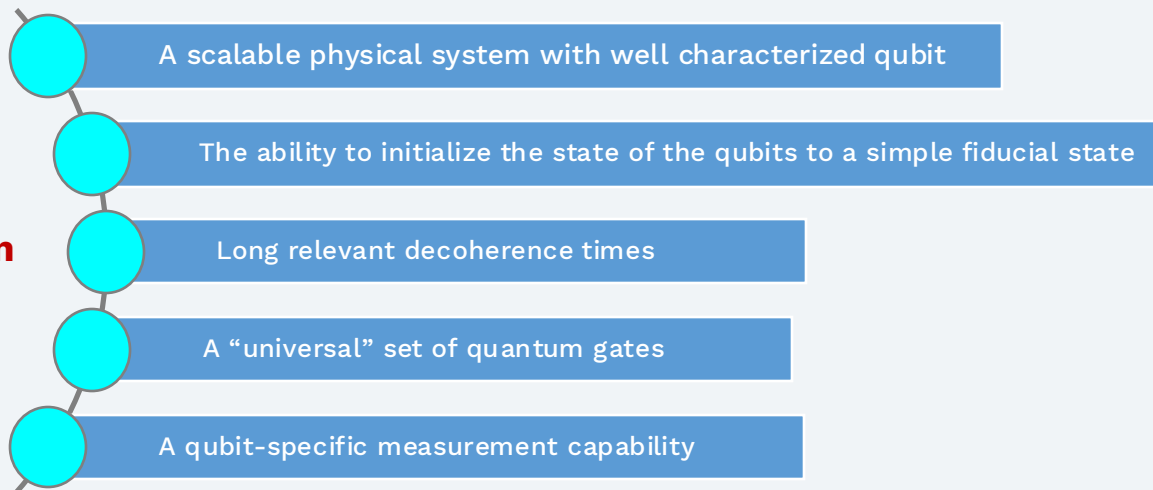
## Quantum Gates

Pauli-X (X)			$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)			$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)			$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)			$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)			$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)			$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$

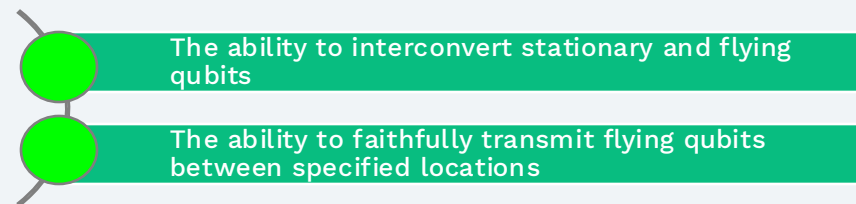
Universal set of gates (CNOT, H, S and T gates)

# DiVincenzo's criteria

## Quantum Computation



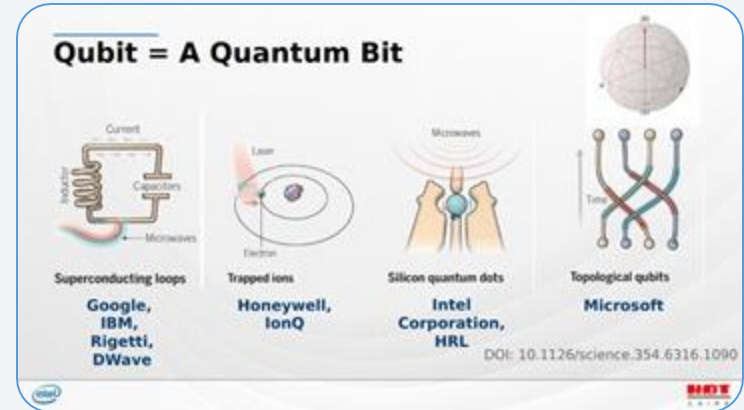
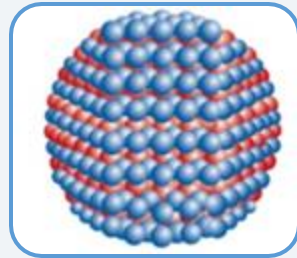
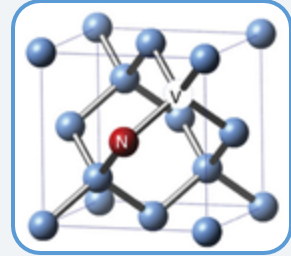
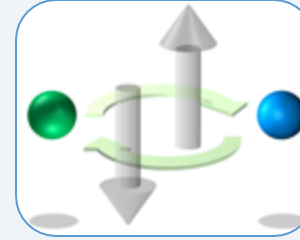
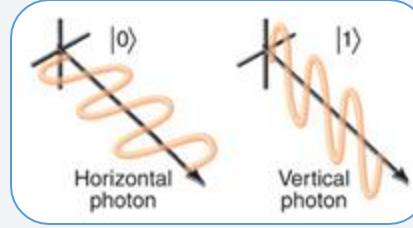
## Quantum Communication/Internet



# Ways of realizing a qubit

A two level quantum system  $|0\rangle$   $|1\rangle$

The qubit state:  $\alpha |0\rangle + \beta |1\rangle$



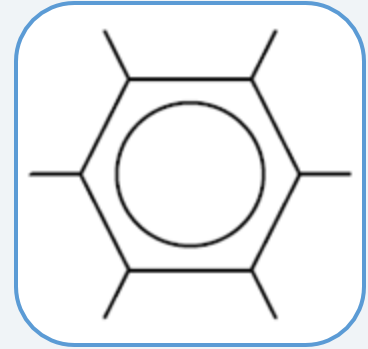
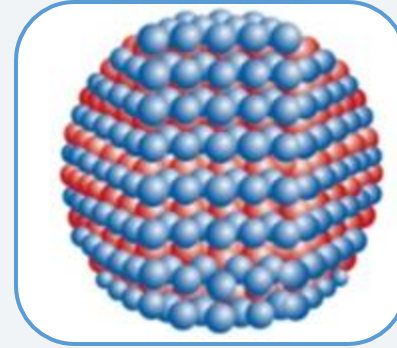
Courtesy: Brian King, MacMaster University

<https://medium.com/quantumcomputingindia/qubits-implementation-quantum-hardware-102-ec55e645f9eb>

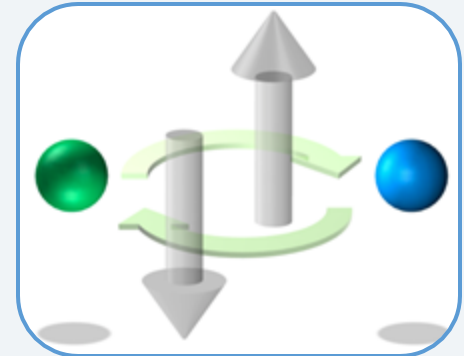
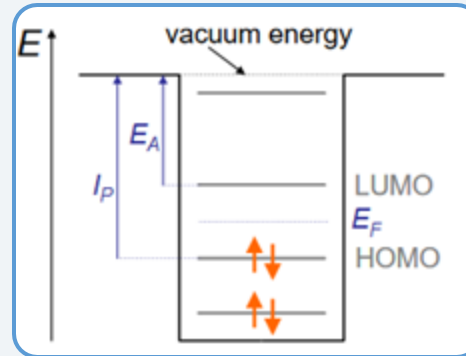
<https://physicsworld.com/a/physicists-break-distance-record-for-electron-spin-state-transmission-in-spin-qubits/>

# Quantum dots – 0 D conductor

- Electrons confined in all directions.
- Discrete energy levels
- Like big molecule

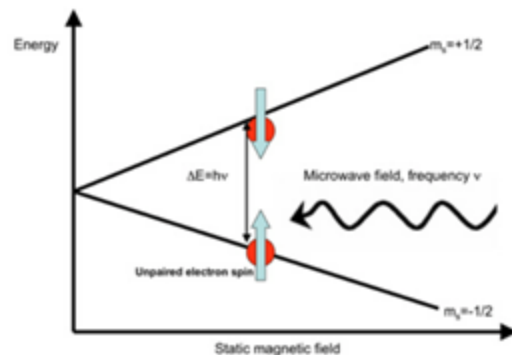
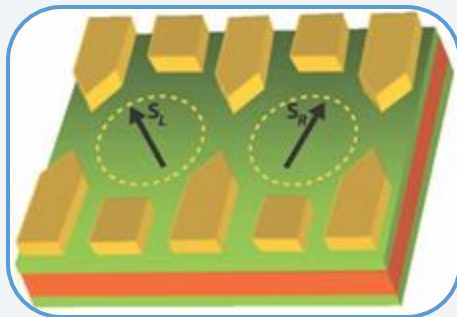
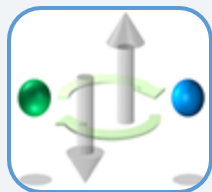


Growth (an example): when InGaAs is grown on GaAs islands form spontaneously, due to the mismatch in the lattice constants.



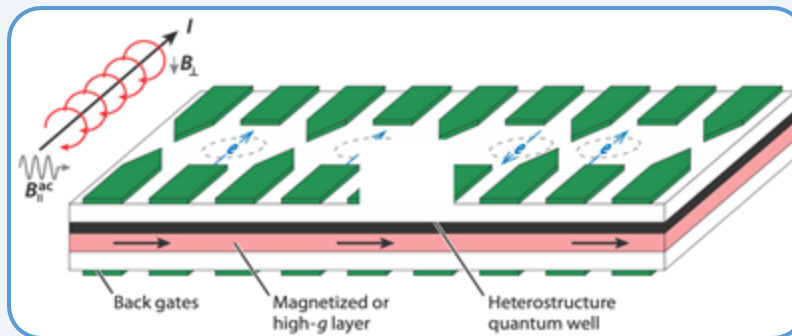


# Quantum Dot Qubits

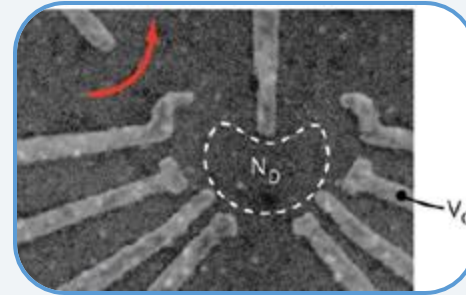


$$\Delta E = \mu_B B m_\ell$$

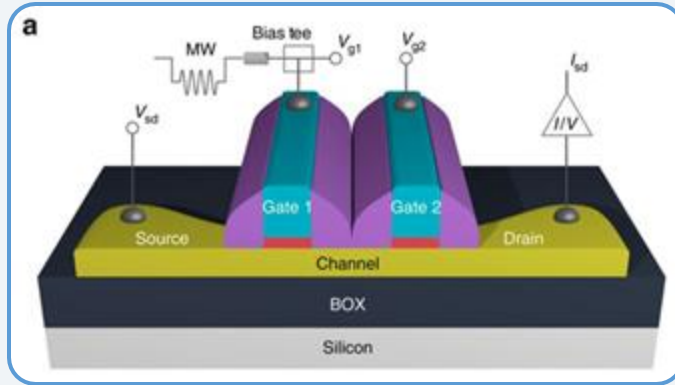
With electric and magnetic fields – both charge and spin degrees of freedom are controlled.



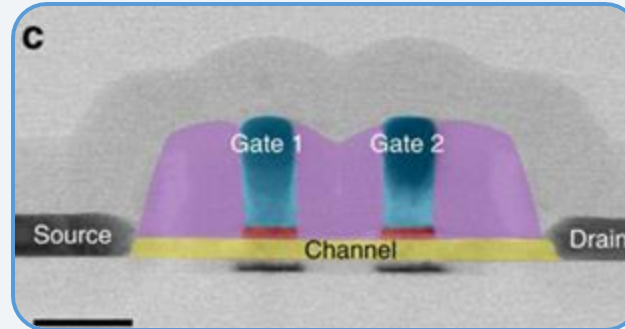
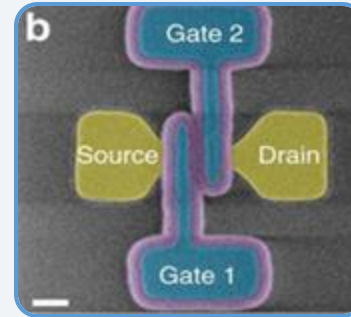
# A quantum dot qubit system



# Quantum Dot Qubits: CMOS Platform

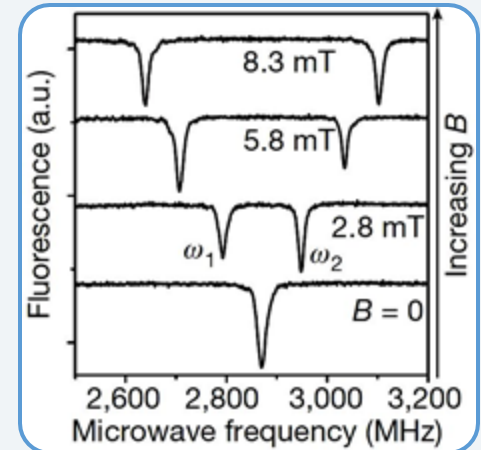
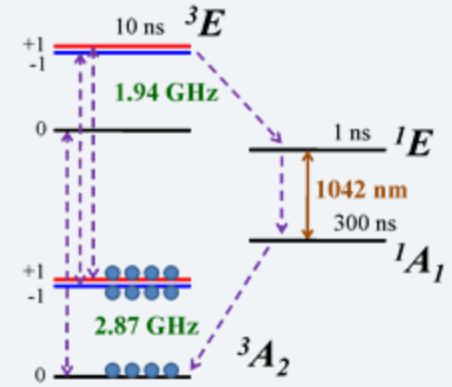
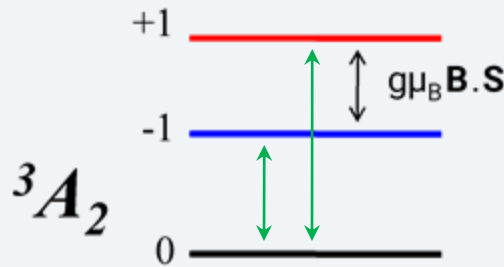
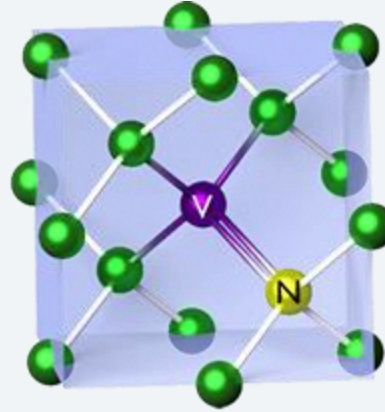


Qubit on the standard CMOS platform



# NV Center qubits

- Ground and excited triplet states
- Intermediate singlet states
- Long coherence time (upto ms) at 300K



# **Quantum Effects in Biological Systems and Biomimetic Devices**

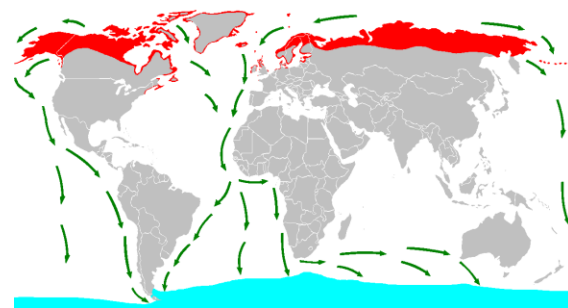


**Bar-tailed Godwit**

- **Alaska to New Zealand/Australia**
  - ~ 11,000 km
  - ~ 60 km hr<sup>-1</sup>
  - ~ 8 days



**Arctic Tern**



**Pole to Pole (50k – 70k km Roundtrip)**

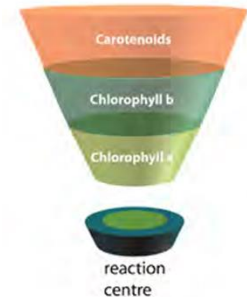
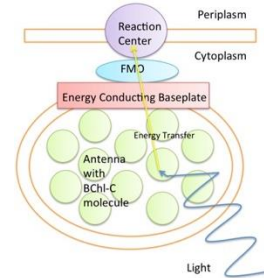
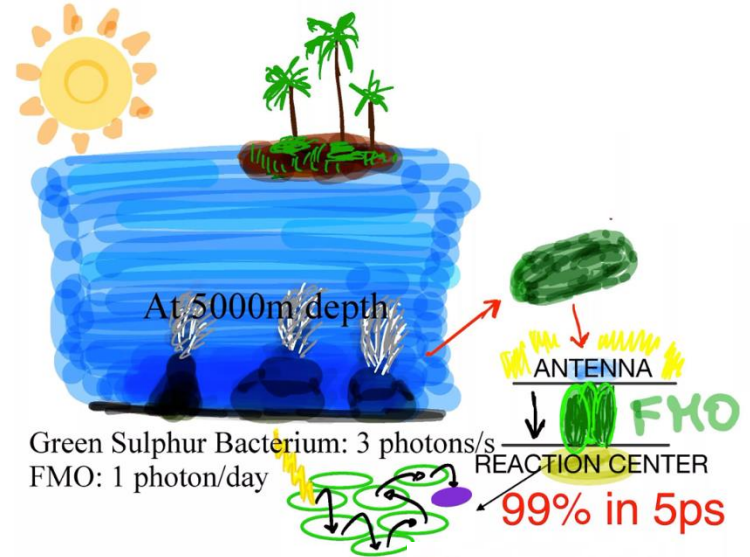


**Bar-tailed godwit**

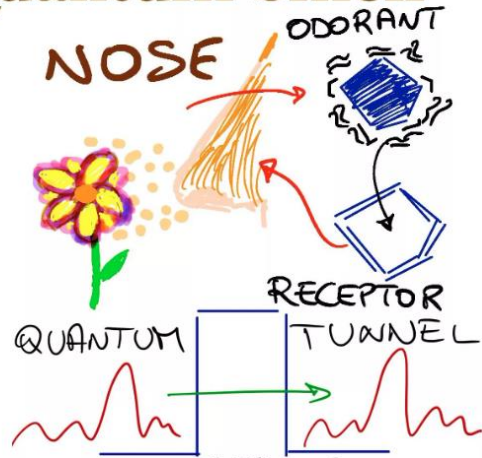
- **Alaska to New Zealand**

- ~11,000 km
- ~60 km hr<sup>-1</sup>
- ~8 days

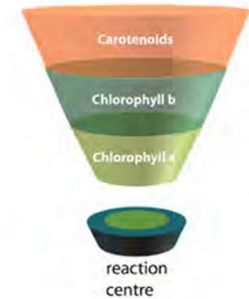
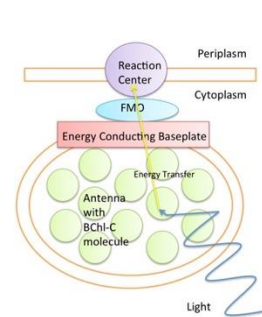
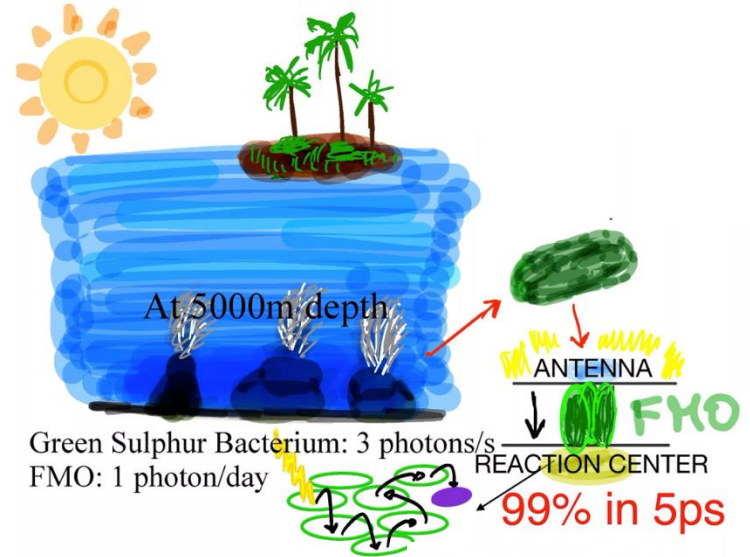
## Light Harvesting



# Quantum Smell

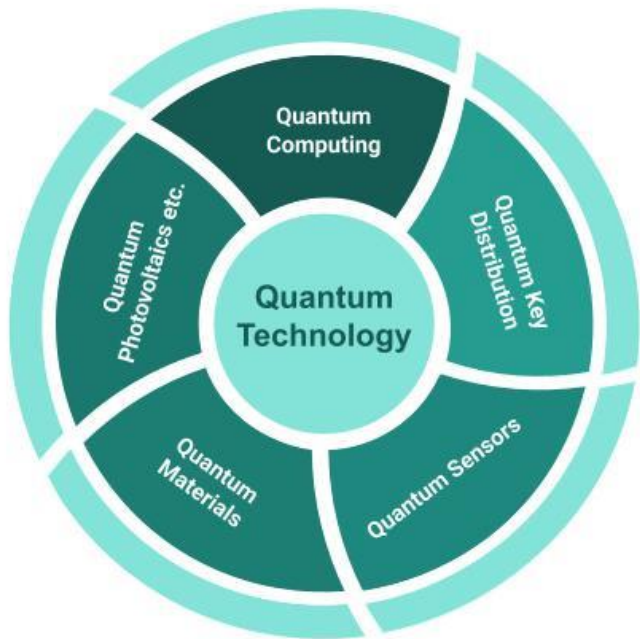


# Light Harvesting





# Quantum Technology



## Quantum Coherence

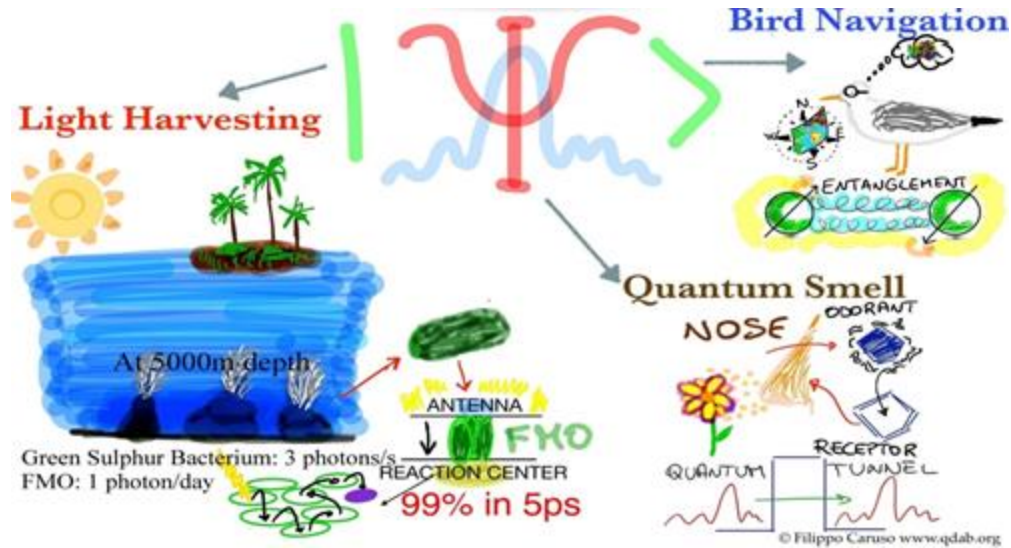
- 'Quantum' superposition
- Responsible for interference effect



## Quantum Entanglement

- 'Spooky' action at a distance
- A valuable 'quantum' resource

# “Quantum” Biology



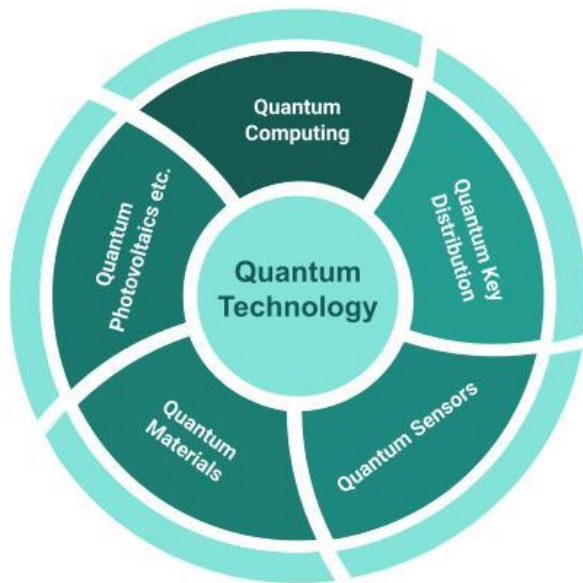
Quantum Coherence

Quantum Entanglement

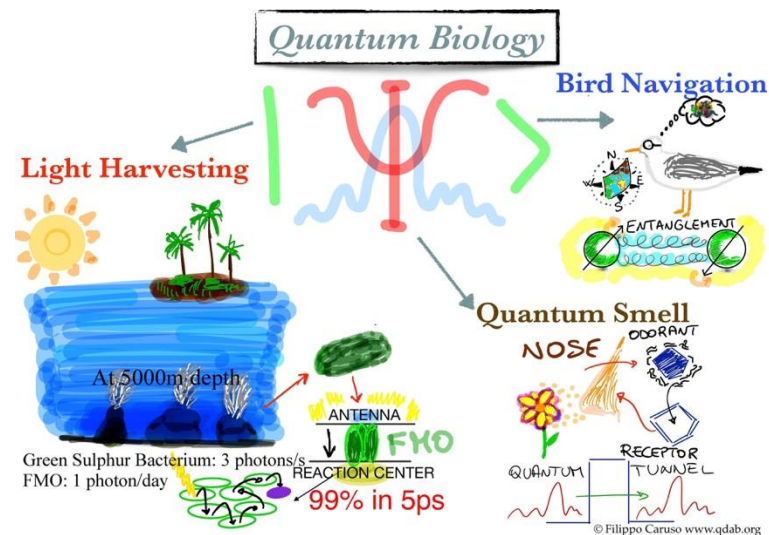
Quantum Tunneling

Biological systems seem to have figured out a way to sustain and utilize 'quantum' effects

# Quantum Technology and Quantum Biology



- Quantum Coherence
- Quantum Entanglement
- Quantum Tunneling



# Quantum Biology: History

- 1943: Erwin Schrödinger – “*What is Life*”
  - Genetic structure and stability is determined by quantum nature of molecular energy levels
  - “... quantum indeterminacy plays no biologically relevant role...”
  - No consideration of
    - Coherence
    - Entanglement

**Non-trivial  
quantum  
effects**

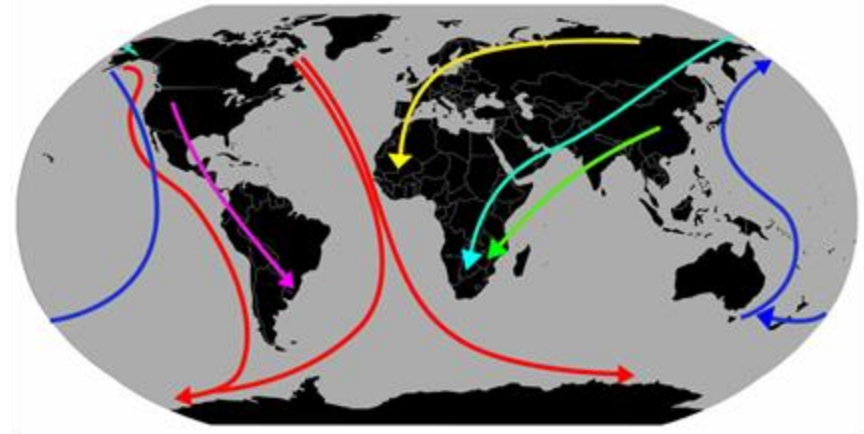
- **Experiments:**

- 2007: Fleming et al.: excitonic coherence in EET during light harvesting
- 2010: Engel et al., Scholes et al.: quantum coherence of EET in LHCs at ambient temperatures

- **Other ‘quantum’ biology proposals**

- 1996 Turin: inelastic electron tunneling in olfaction
- 1998: Schulten et al.: radical pair mechanism of bird navigation
- 1995: Hameroff, Penrose: quantum coherence in brain microtubules – consciousness?

# Avian Magnetoreception



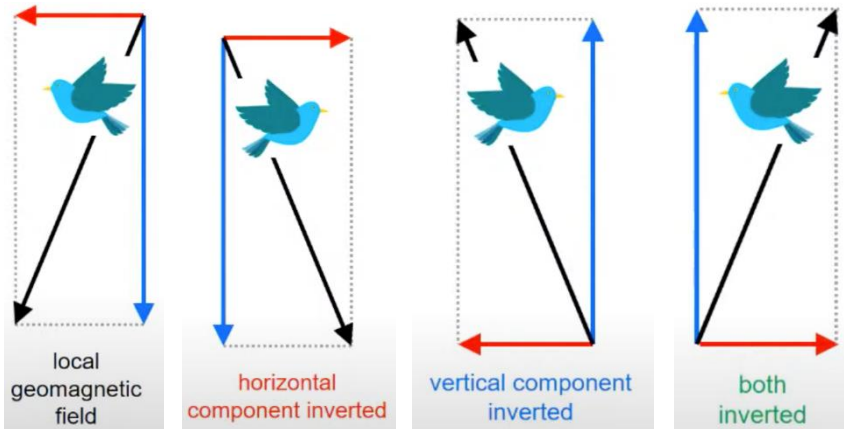
<i>Oenanthe oenanthe</i>	<span style="color: cyan;">—</span> Northern Wheatear
<i>Sterna paradisaea</i>	<span style="color: red;">—</span> Arctic Tern
<i>Falco amurensis</i>	<span style="color: green;">—</span> Amur Falcon
<i>Puffinus tenuirostris</i>	<span style="color: blue;">—</span> Short-tailed Shearwater
<i>Philomachus pugnax</i>	<span style="color: yellow;">—</span> Ruff
<i>Buteo swainsoni</i>	<span style="color: magenta;">—</span> Swainson's Hawk

# The avian compass: behavioral characteristics

Experiments @ Frankfurt on European Robin:  
local geomagnetic field = 46  $\mu\text{T}$

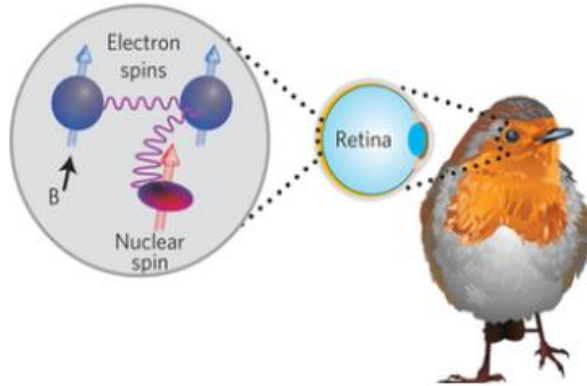


## Behavioral characteristics

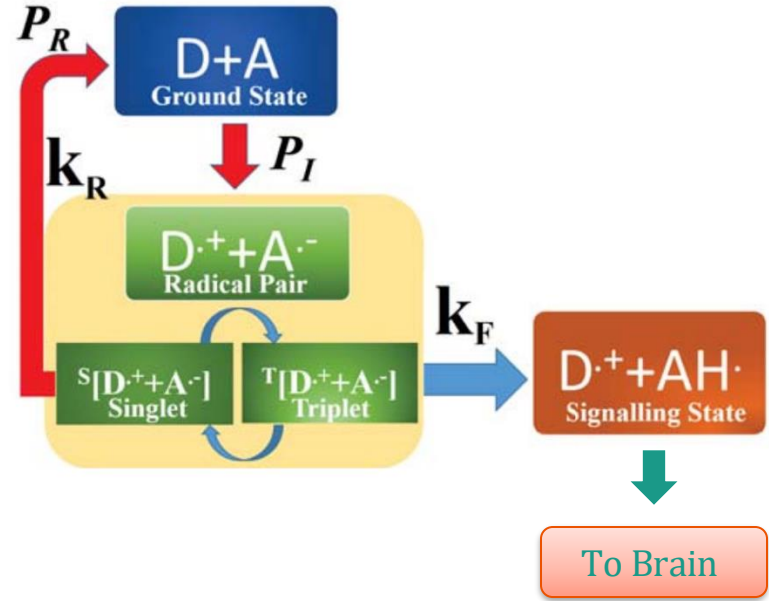
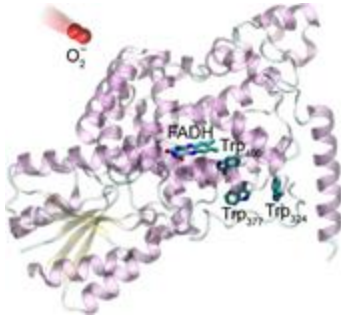


- ☐ **Inclination compass only**
  - No North-South distinction
- ☐ **Operational in some optical frequency range**
- ☐ **RF disruption**
  - Small (50nT) field transverse RF field (specific frequency 1.315 MHz) destroys compass action
- ☐ **Adaptive functional window**
  - Dynamic range:  $\pm 30\%$  of local geomagnetic field

# The radical pair mechanism



Cryptochrome

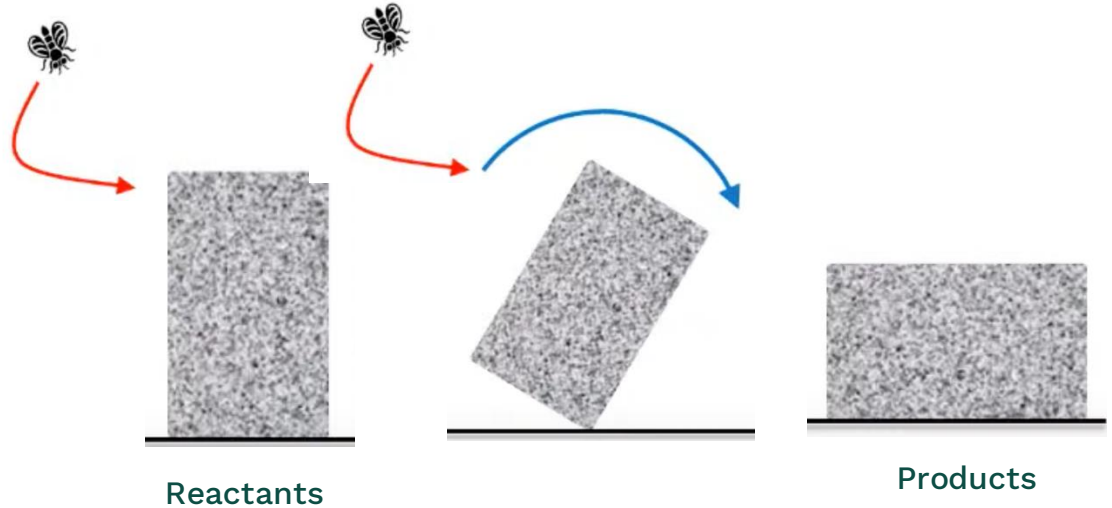
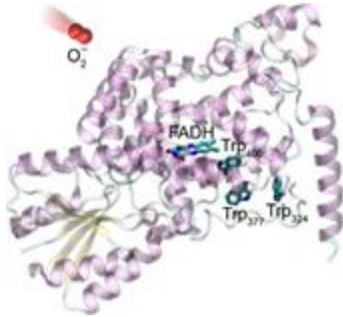
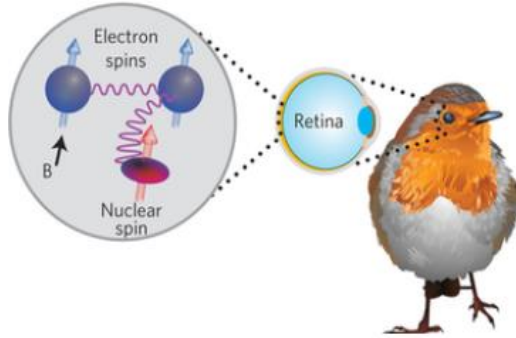


**Compass** action can be quantified by:

- **Singlet yield:** fraction of the singlet products
- **Triplet yield**
- **Protonated Signaling state**



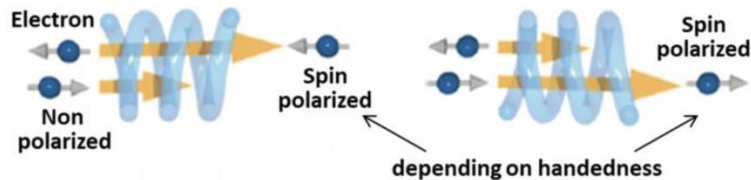
# The radical pair mechanism: energetics





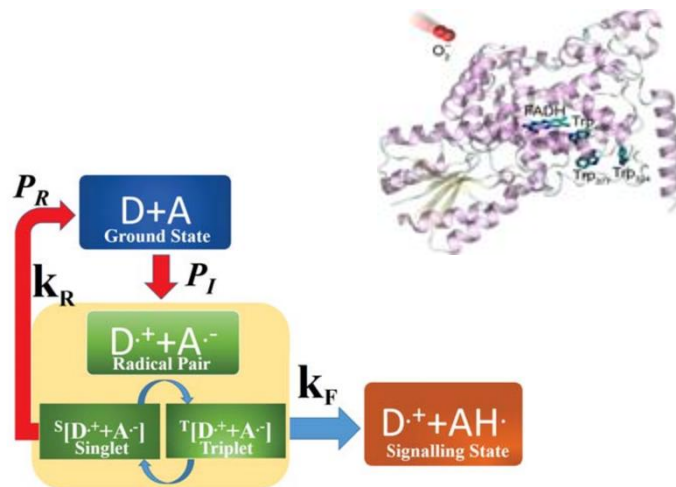
# Chirality-induced spin selectivity (CISS) and the RP model

- ❖ **Preferential transmission of electrons parallel or anti-parallel to the direction of motion** – based on chirality of the molecule



- ❖ CISS has been experimentally observed in different contexts:

- **Electron Transmission**
- **Electron Transport**
- **Electron transfer/rearrangement in chemical reactions**



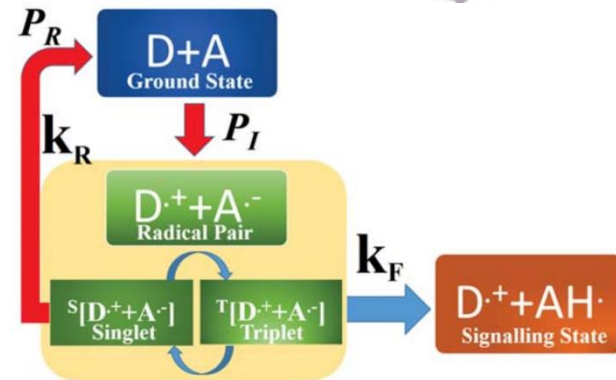
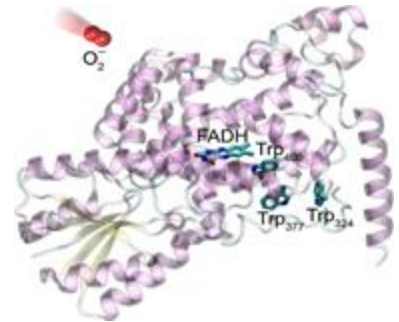
# Inclusion of CISS in the RP model

$$\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H}, \hat{\rho}(t)]_- - \frac{1}{2}k_R[\hat{P}^R, \hat{\rho}(t)]_+ - k_F\hat{\rho}(t)$$

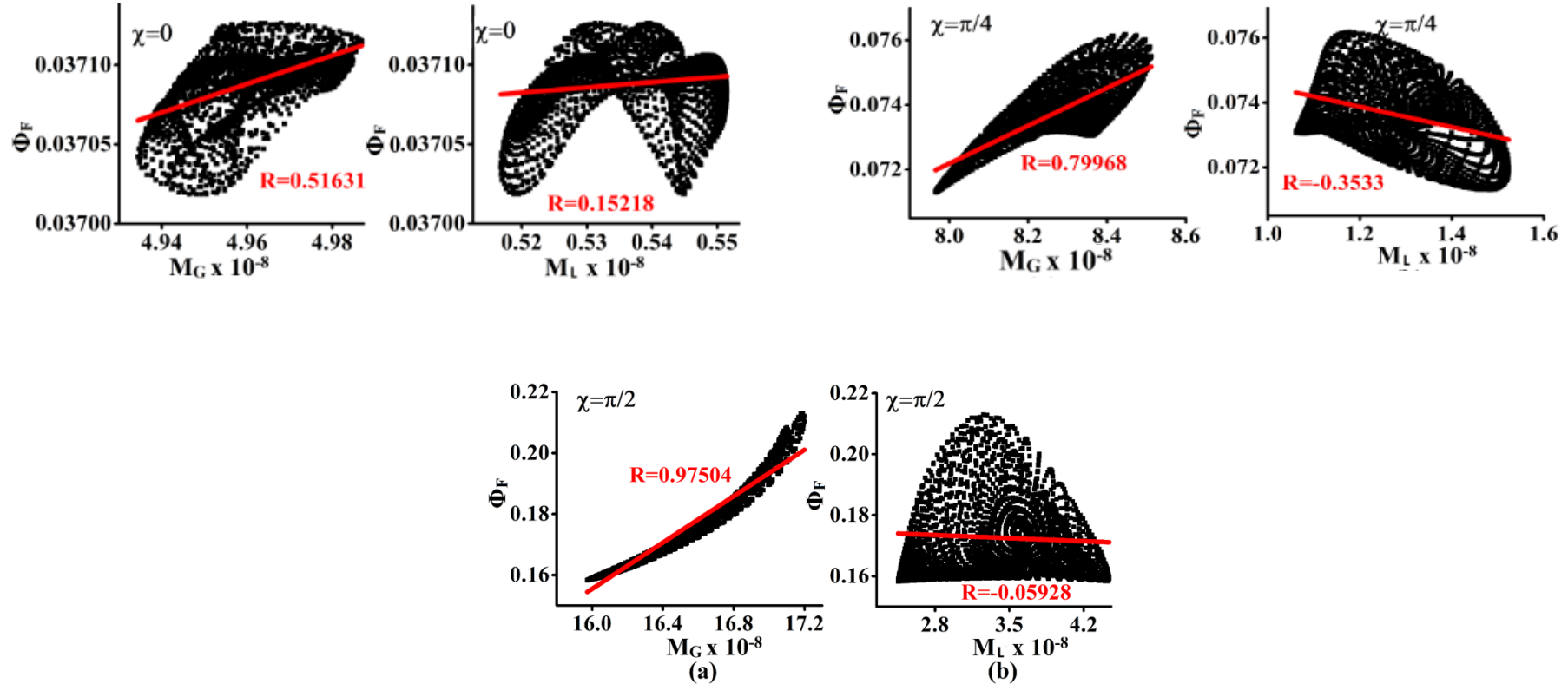
## In full CISS case

Only one spin polarity electrons can travel in one direction

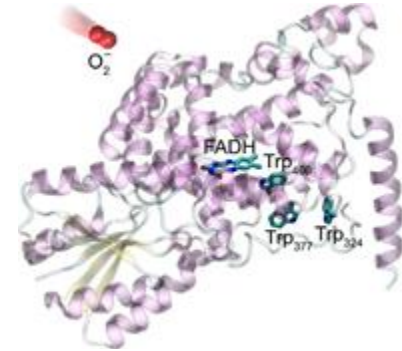
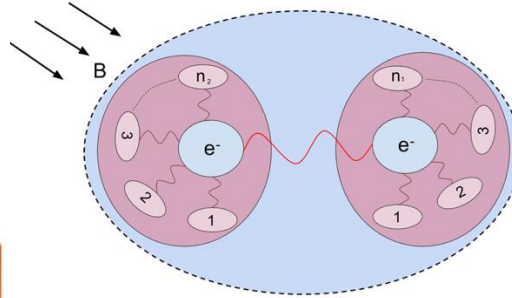
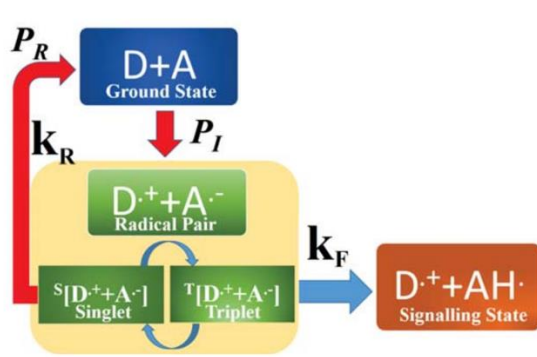
Opposite polarity electrons would travel in the opposite direction



# The radical pair model with CISS: Coherence and Signaling State Yield



# Radical Pair Mechanism: In conclusion



**CISS enhances compass sensitivity and coherence (both local and global)**

**Global coherence shows strong correlation with signaling state yield**

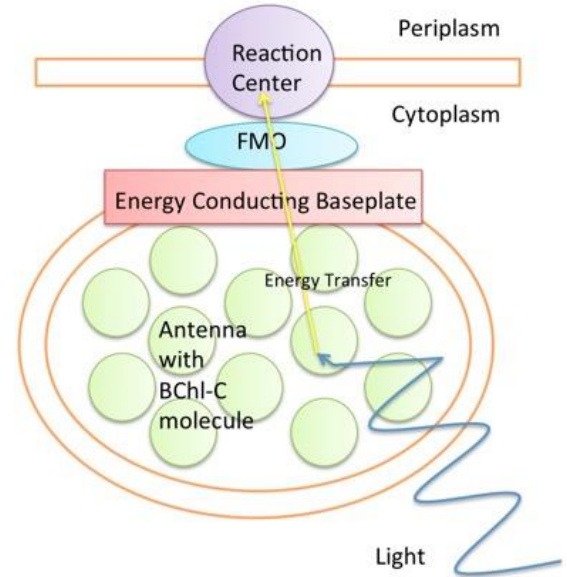
**Functional Window?**

**RF Disruption?**

**Emulation of RP Mechanism –  
Quantum Sensor for navigation**

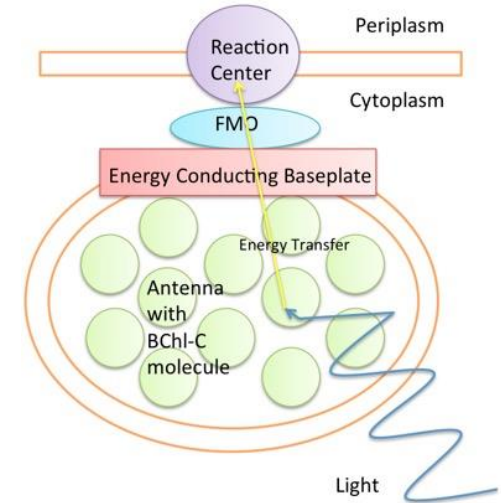
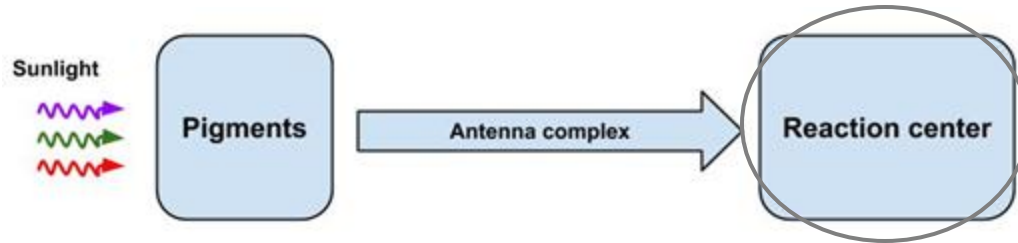
**CISS for Quantum Technologies**

# Photosynthetic Apparatus



# The Photosynthetic Apparatus: Excitonic Transport and Charge Separation

- ❑ **Photosynthesis:** Synthesis of carbohydrates from  $\text{CO}_2$  and water in presence of sunlight
- ❑ **Steps:**
  - **Pigments:** Captured photons create excitons
  - **Antenna:** Excitonic transport from pigments to the reaction center
  - **Reaction center:** Charge separation



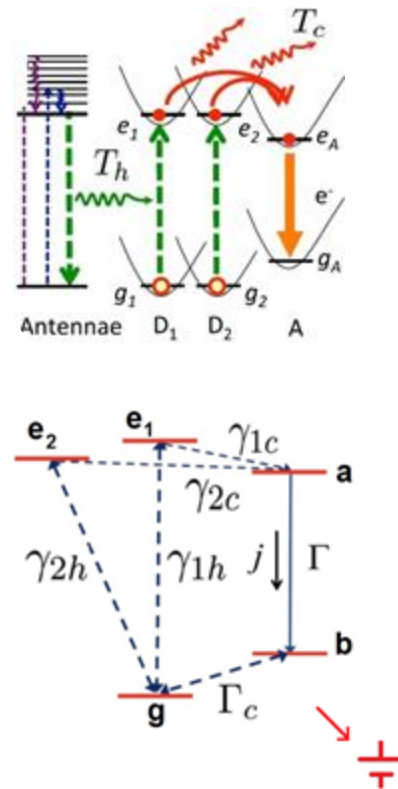
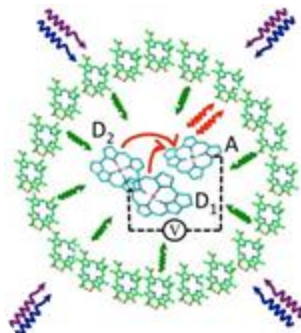
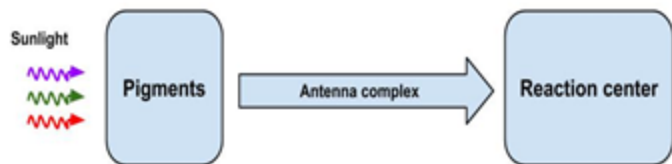
## Two crucial steps in photosynthesis

- Excitonic transport through molecular complex
- Charge separation at the reaction center

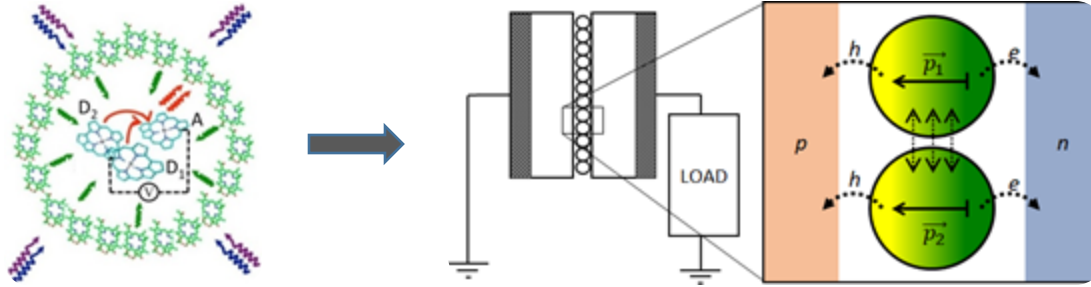
# The Reaction Center

## Structure

- Two donors, one acceptor

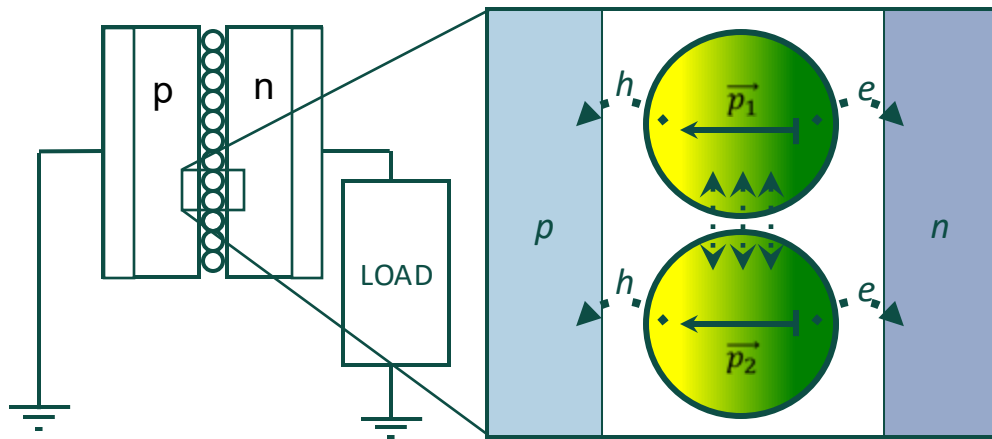


# Reaction center emulation



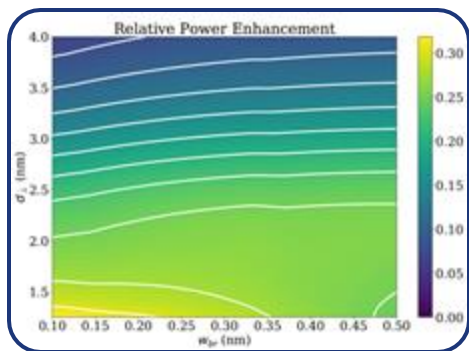
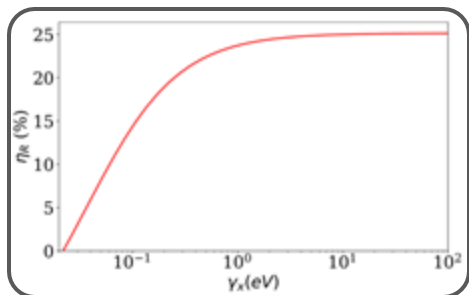


# RC Emulation: A Quantum Photocell



- Inspired from photosynthetic reaction center  
And builds on Marlan O. Scully's idea of a quantum photocell.
- Strong built-in electric fields – excitonic dipole-dipole coupling between adjacent dots
- Helps in breaking the detailed balance.
- The photovoltaic cell exhibits enhanced photo-voltage and photocurrent (~25%).

# Results (contd...)



- Relative power enhancement

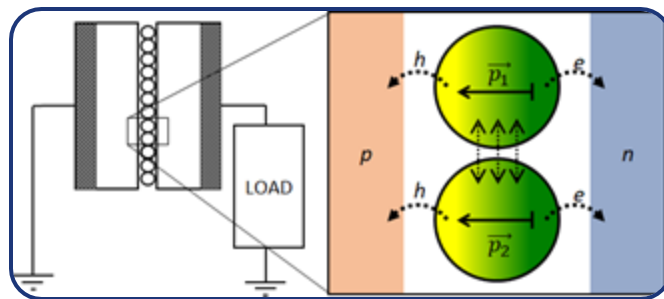
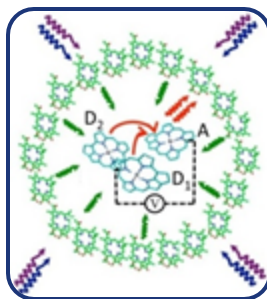
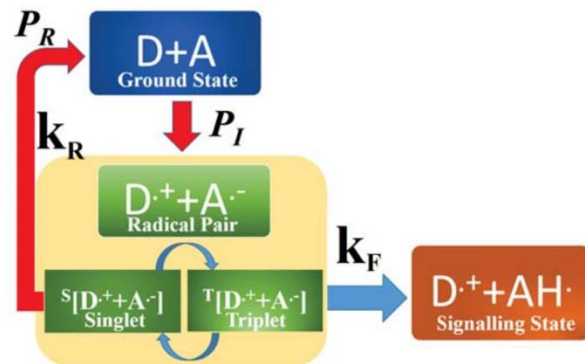
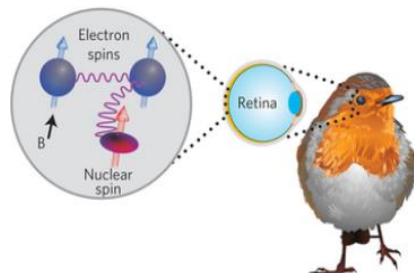
$$\eta_R = \frac{\tilde{p}_{out}^{max} - p_{out}^{max}}{p_{out}^{max}}$$

- Power enhancement upto 25% is observed due to excitonic delocalization.

## Some observations:

- Greater spacing between dots leads to poorer coupling and reduces efficiency.
- Another mechanism of charge carrier extraction must be found to augment the low tunnelling rates.
  - Phonon mediated transfers could be the key to this.
- The phonon spectrum of GaN quantum dots needs to be studied in detail
  - This and variation of the geometry of the photocell may be done through DFT/tight-binding methods.

# In summary



**THANK YOU**