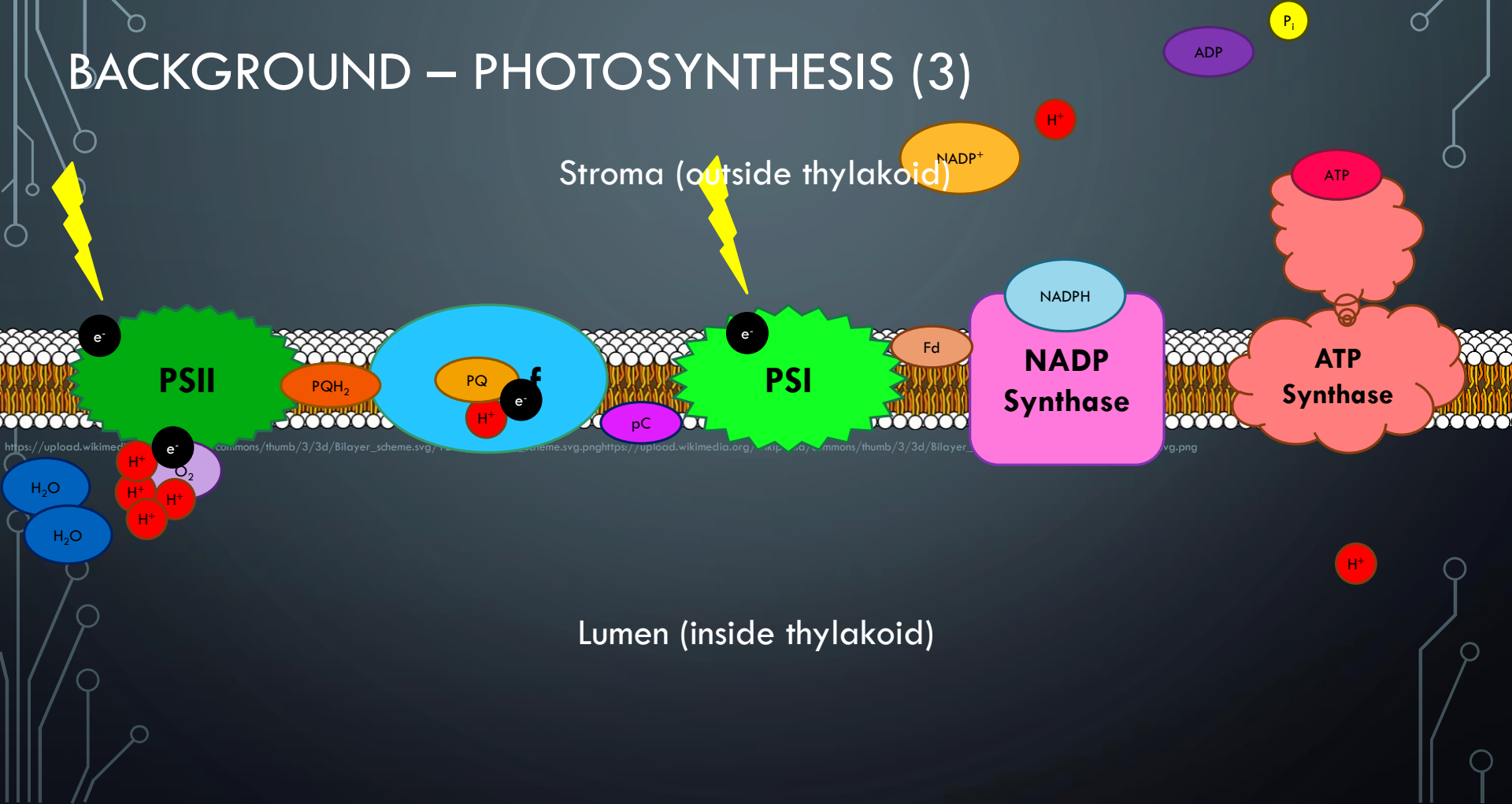


A COMBINED QUANTUM MECHANICS AND MOLECULAR MECHANICS SIMULATION OF ELECTRON TRANSFER IN PHOTOSYNTHESIS

ROBERT LESKE

BACKGROUND – PHOTOSYNTHESIS (3)



BACKGROUND

- Photosynthesis baffled scientists with its high efficiency (1,2,3)
- Reason for efficiency not fully understood (1,2,3)
 - Coherence: allows the electron to find the most efficient path (1)
 - Where does coherence originate



The background is a dark blue gradient. In the four corners, there are decorative white lines that resemble a circuit board or a neural network. These lines consist of straight segments connected by right-angle turns, ending in small white circles. The lines are more dense in the corners and become sparser towards the center.

How can plants avoid decoherence?

And

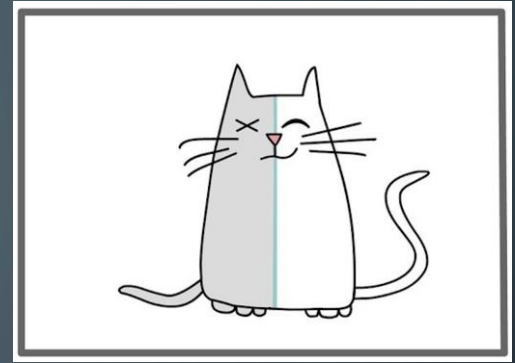
What can we learn from them?

BACKGROUND

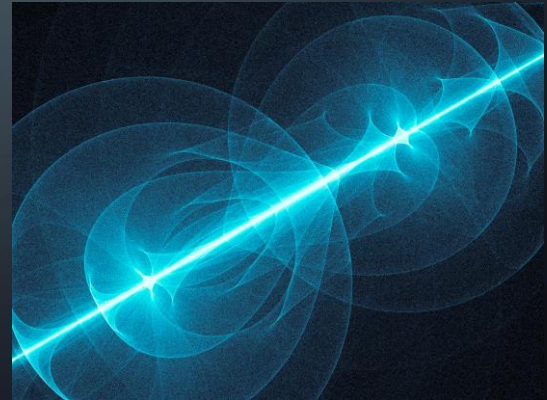
- Plants make use of:
 - Superposition
 - Wave-particle duality



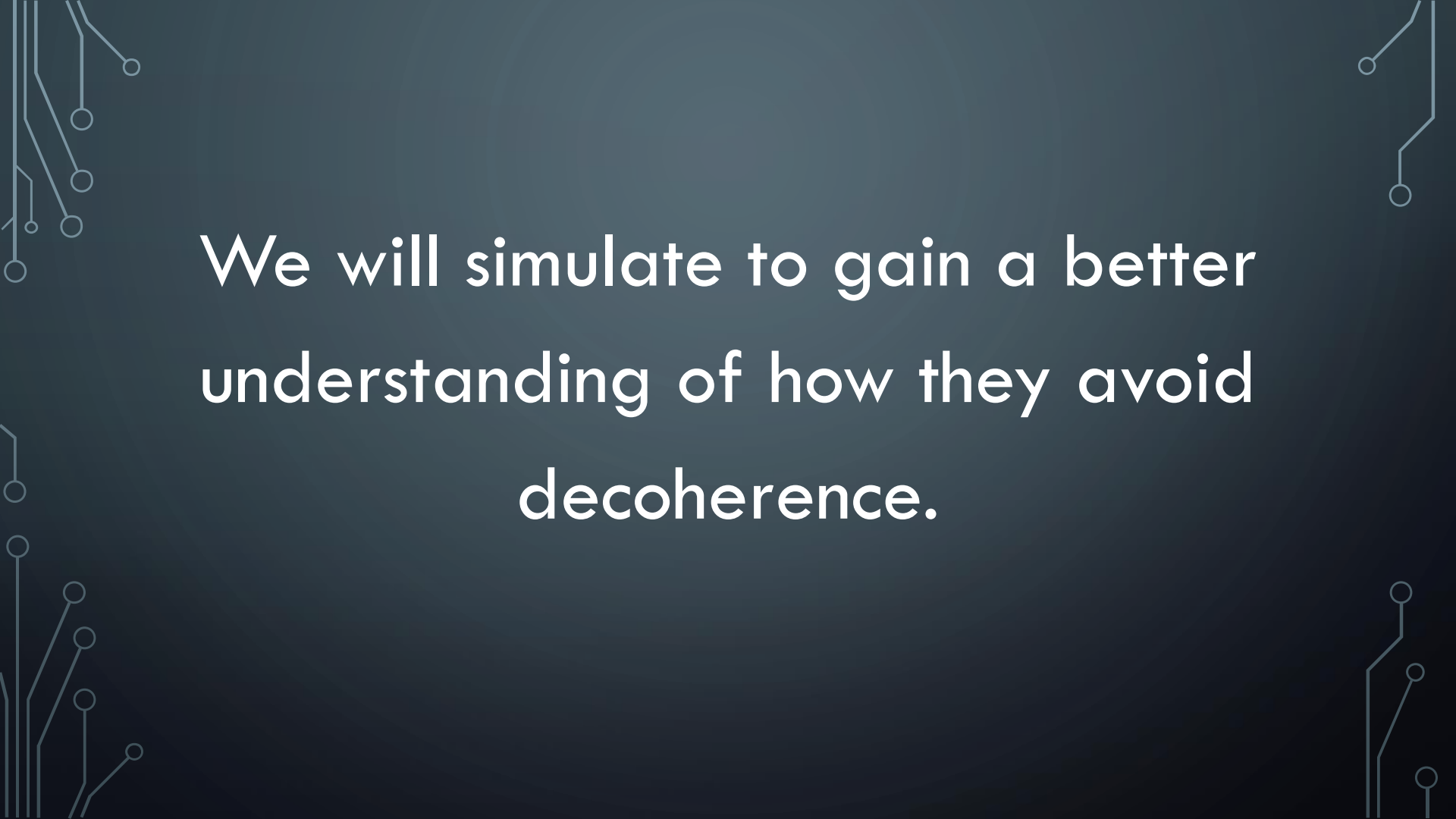
Environment can interact
causing decoherence



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<https://www.google.com/url?sa=i&url=https%3A%2F%2Fwww.thoughtco.com%2Fdefinition-of-wave-particle-duality-605947&psig=AOvVaw33eP2y05Q3ne-plys4t2ZY&ust=159047391989000&source=images&cd=vfe&ved=DCAIQJRxqFwoTCKDlvfmuzakCFQAAAAAdAAAAABAD>

The image features a dark blue background with white, stylized circuit board traces in the corners. These traces consist of lines and small circles, resembling electronic components or connections. The text is centered in a clean, white, sans-serif font.

We will simulate to gain a better understanding of how they avoid decoherence.

BACKGROUND

Quantum Mechanics (4, 5, 8, 9)

- Based in Quantum Physics
- Extremely accurate
- Requires high computational effort

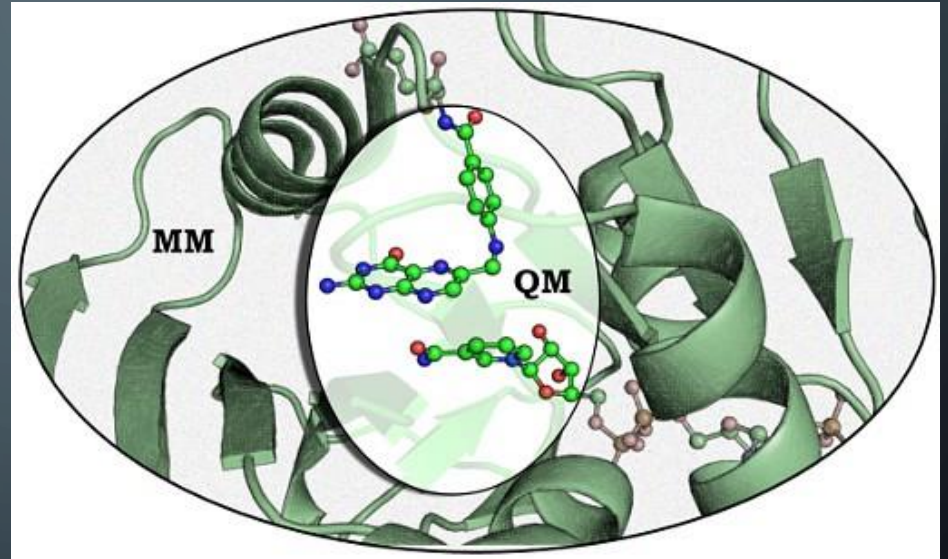
Molecular Mechanics (4, 5, 8, 9)

- Based in Classical Physics
- Less accurate
- Requires less computational effort

BACKGROUND

QM/MM uses both (4, 5)

- QM in places where more accuracy is needed (PS)
- MM everywhere else (SS)

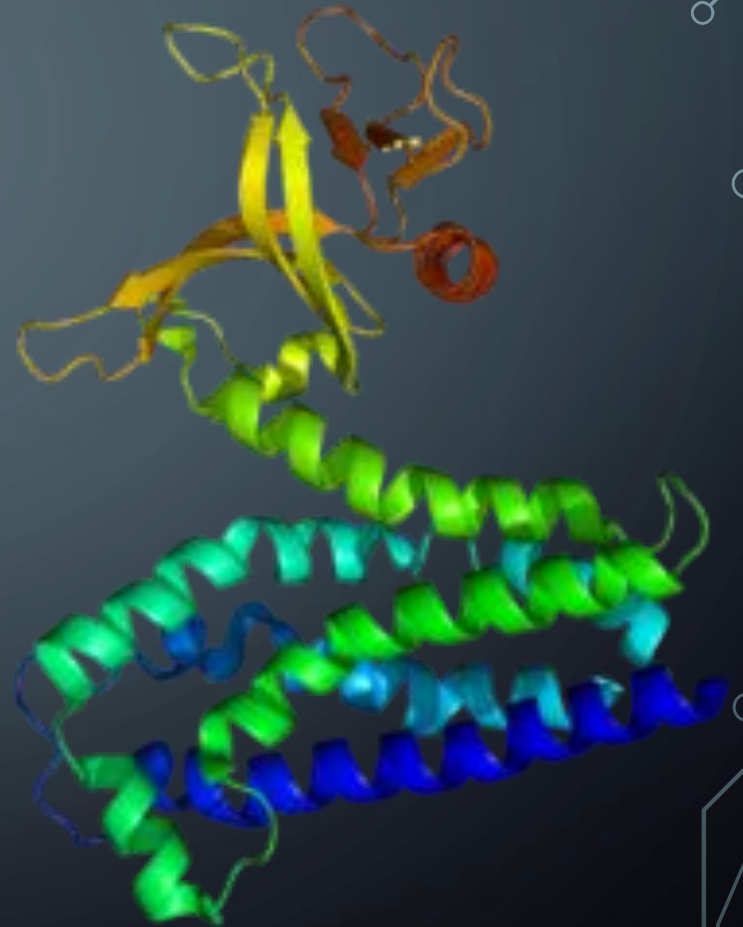


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BACKGROUND

By simulating system:

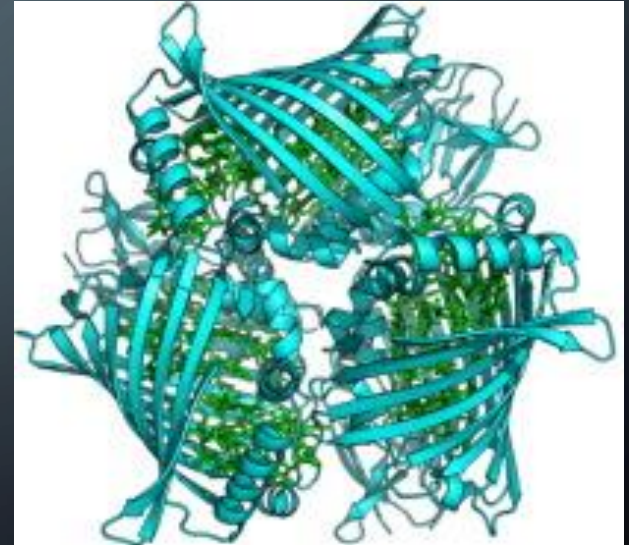
- Understand phenomena better (4, 5, 6)
- Check accuracy/efficiency of models
- Apply these for predictions (7)



LIT REVIEW

Seminal paper for chlorophyll in quantum biology (Engel et al.) (1)

- Previous studies of FMO complex ignored QM
- QM effects were predicted
- Direct observation of beats
- Shows that coherence was responsible for efficiency
- Does not explain origins of coherence

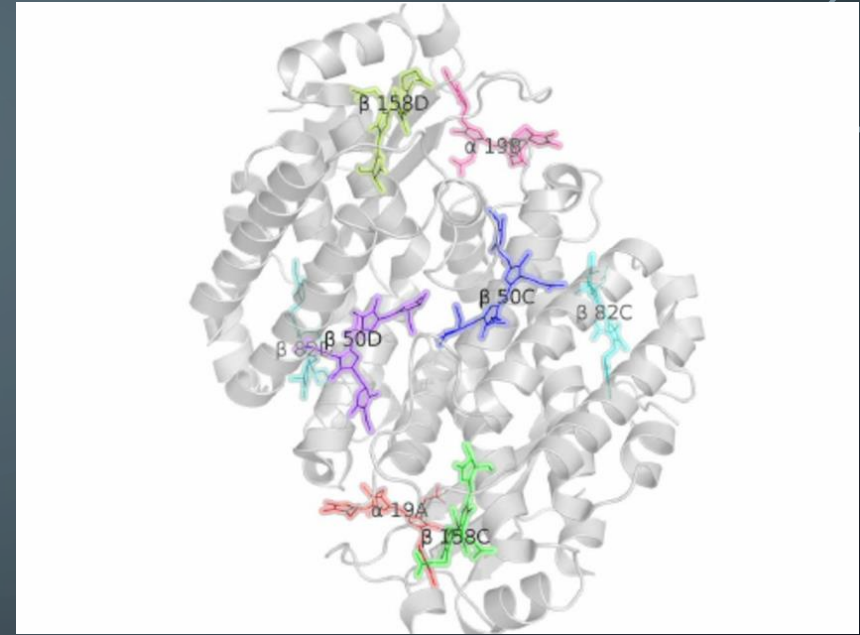


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LIT REVIEW

Recent study (Tong et al.) (2)

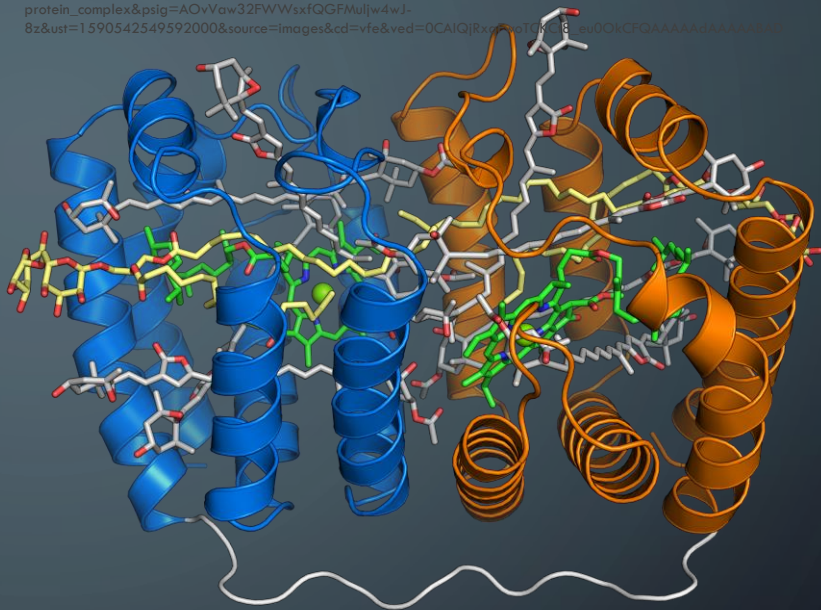
- Studies secondary pigment (PE545 is red)
- MD-QM/MM
- Accurate qualitatively (energy, absorption spectra)
- Did not distinguish between vibrational, electronic, and vibronic



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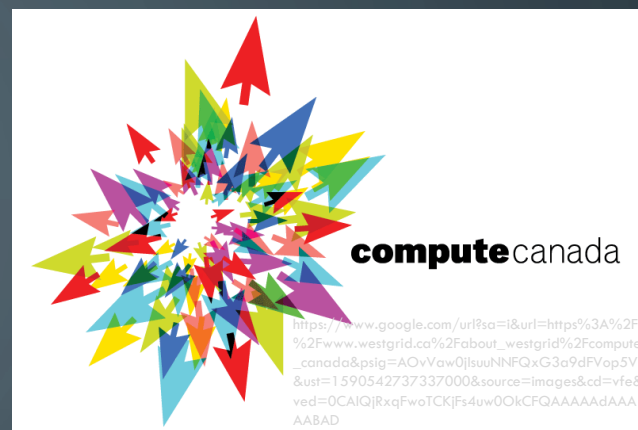
METHODS

- Larger plant chlorophyll complex
- QM/MM simulations
 - Chlorophyll and some extended area in PS
- Try to look for causes of coherence (vibrational, electronic, vibronic) (2)



METHODS

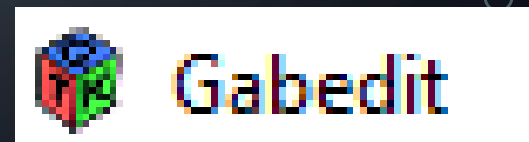
- Using deMon2k for QM/MM
 - ADFT
 - CHARMM or CUBY
- On Compute Canada computers
- Gabedit: pre-processing
- Molden: post-processing



deMon2k

density of Montréal

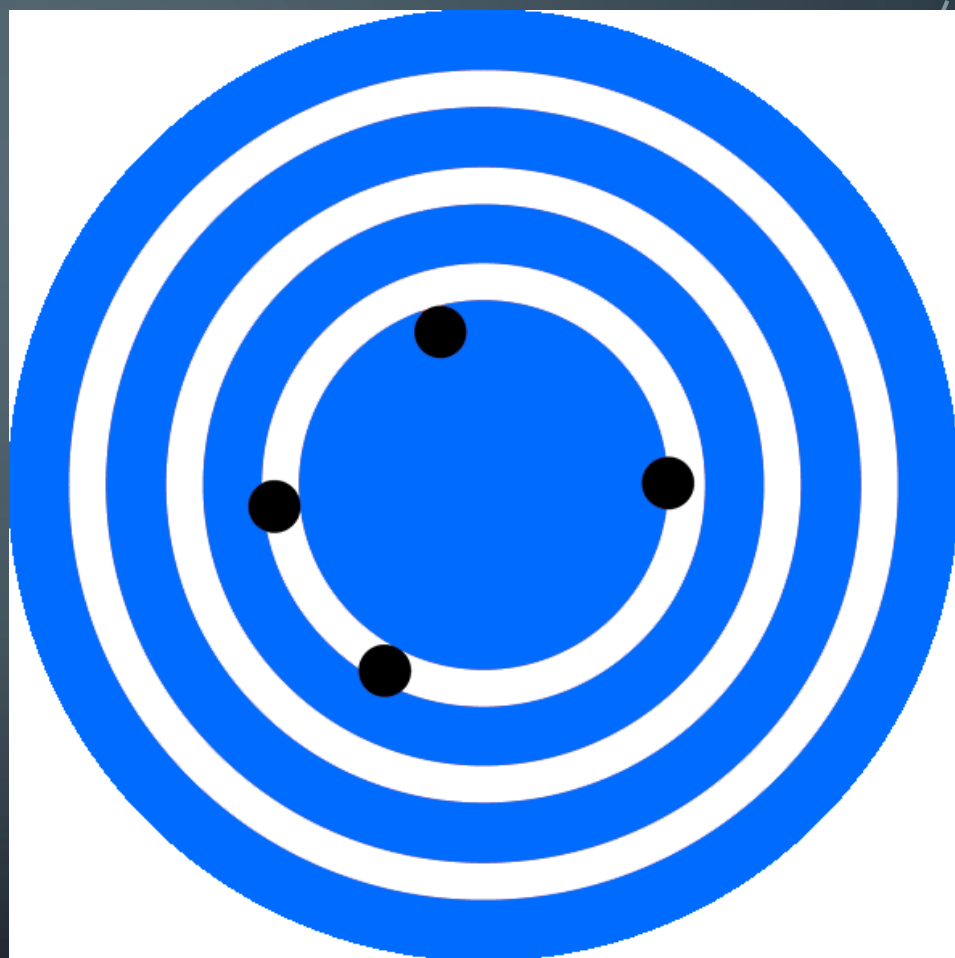
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METHODS

Looking for:

- Accurate energies
- Short computation time
- Rate constants from QM phenomena



METHODS

Still figuring out details

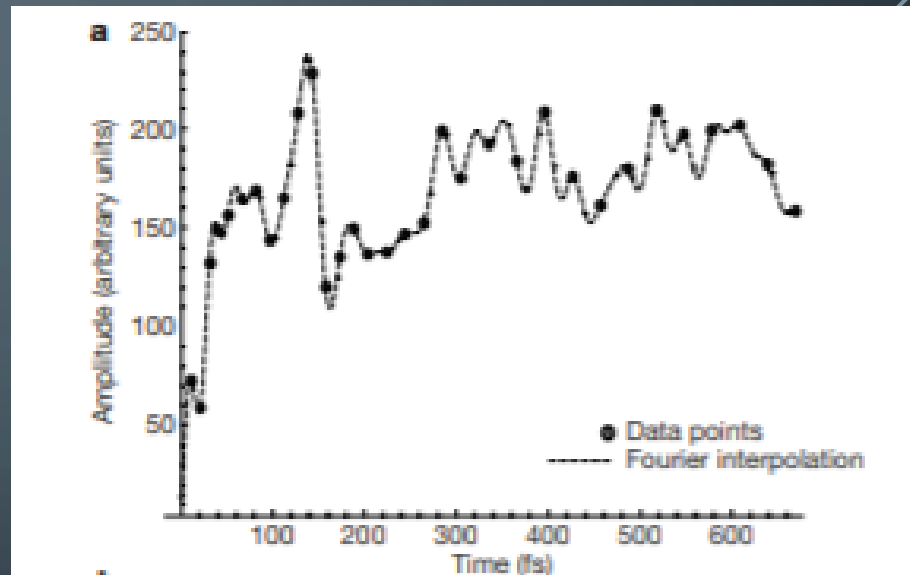
- Many different structures
- pH (3)
- Lesser studied section



ANTICIPATED RESULTS

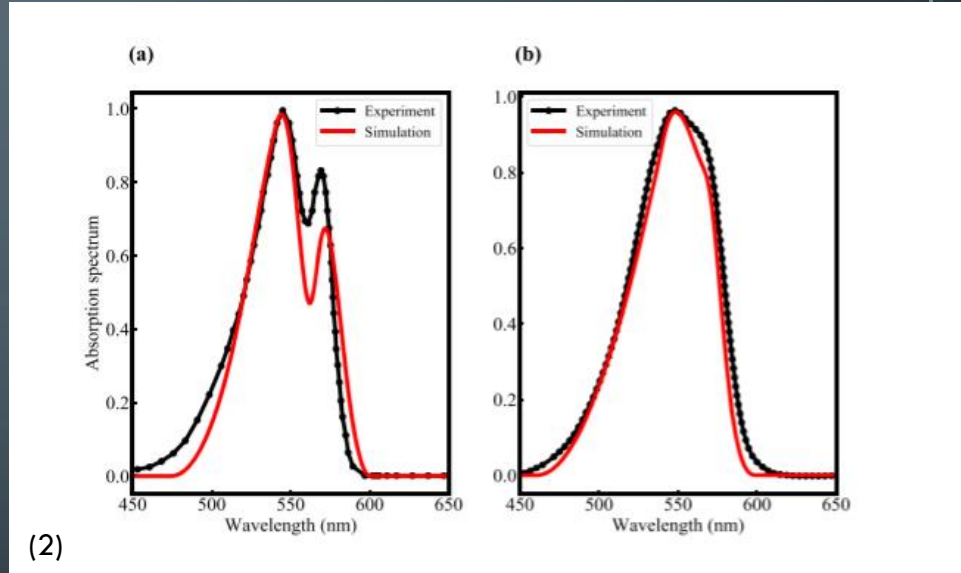
I anticipate:

- Accurate energy
- Accurate rate constants
- Compared to experimental results
- More data and factors accounted for



PREVIOUS RESULTS

- Accuracy (energy and rate constants)
(2)
- Still mystery about avoiding decoherence (1, 2, 3)
 - Think the whole system is superposition-like
 - More data needed to support/refute this idea



SIGNIFICANCE

- Deeper understanding of QM
- Better ideas of how to avoid decoherence
 - Application to quantum computers
- Better understanding of biology and chemistry
 - Better predictions and optimizations
- Accuracy of deMon and DFT




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- Friends and Peers
- Family

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