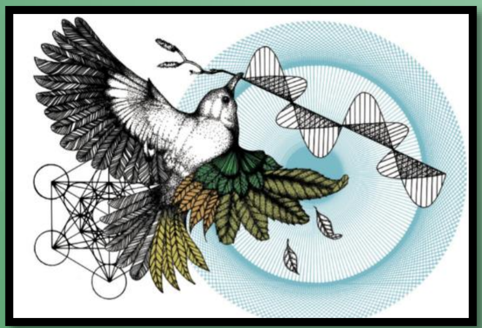
Significance

Quantum mechanics is the future of science and technology. Most modern mysteries in physics pertain to this field. As such, there is a lot of research that needs to go into understanding what is happening and how it can be harnessed.

It is understood that many natural phenomena employ quantum mechanics in ways that solve problems that are impossible with classical mechanics: high efficiency in photosynthesis, enzymes requiring less energy, and even birds using magnetism to fly. However, nature is hot, which means there is a lot of interaction with the environment in these systems. In our current usages of quantum mechanics (like the quantum computer), we have to cool things down to near to absolute zero (0K). If we can understand how biological systems use quantum mechanics we would be able to use it better ourselves.



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Technology is also being inspired by biological systems because of their efficiency. Researchers are looking into ways to use chlorophyll in photovoltaic cells (solar panels) because of their ease, abundance, and efficiency. Another major field of research is the research into using enzymes to turn carbon dioxide in the atmosphere into fuel because of the efficiency of enzymes

About Me

Robert Leske is a high school senior and science enthusiast. He takes on a rigorous academic course load and maintains a high GPA. He is highly involved in multiple clubs and honor societies and seeks to improve his community. He is also a world champion baton twirler with the Silver Starlites.

Robert Leske is a member of Pawling High School's Science Research Program. He is currently researching efficiency in photosynthesis under Dr. Raymond Kapral of the University of Toronto and Dr. Dennis Salahub of the University of Calgary

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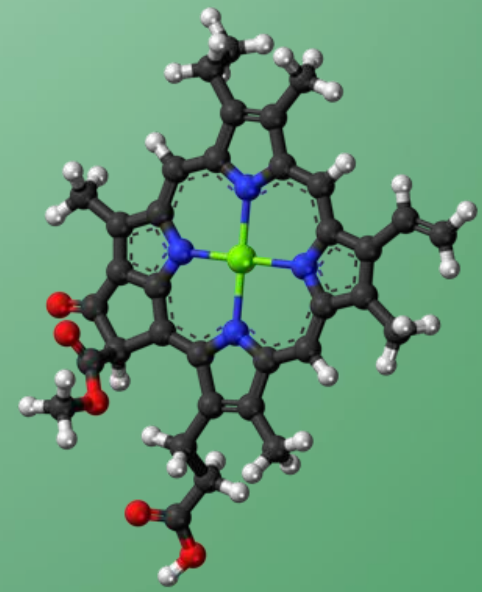
Efficiency in Photosynthesis

The Effect of Different Conditions on Efficiency in Photosynthesis



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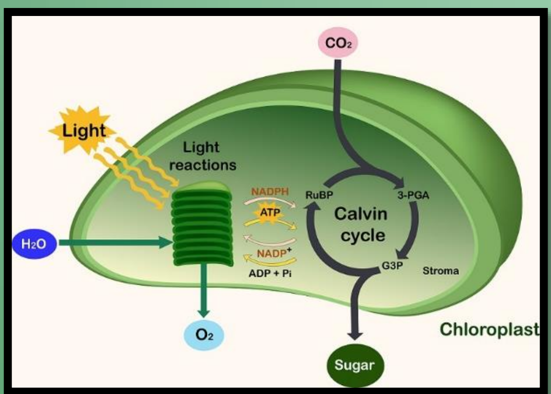
What is Photosynthesis?

Photosynthesis is the process whereby many plants, bacteria, and protest produce harness light to produce sugar.

This is a very complex process that involves many steps. First, light hits a pigment, such as chlorophyll, releasing an electron. This electron then travels through across the system to a reaction center, where it is used to produce the high energy molecules, NADPH and ATP. These are then used to provide energy for the production of other molecules, like sugars.



What is Meant by Efficiency?

Efficiency is a ratio of final energy to initial energy. This measures how much energy is lost during some process.

In photosynthesis, efficiency refers to how little energy is lost during the transport of the electrons from the chlorophyll until they are used. This process occurs with very high efficiency, which is impossible with normal, classical physics. However, quantum mechanics makes this more possible. Through quantum mechanics, an electron can travel multiple paths at a time.

Current Research:

The first paper in the field of photosynthesis through a lens of quantum biology studied a chlorophyll complex in bacteria experimentally. They observed quantum beats, which occurs when a wave function (a probabilistic function that governs quantum states) interferes with itself. This did not answer how the plant was able to maintain a quantum state, but only showed that it was able to.

Computational chemists attempted to solve this through simulations done with quantum mechanics. Previous research has studied how various factors affect photosynthesis individually.

Coherence
(quantum state)

Structure: The excited states present have different effects on electron localization (how tightly the nuclei hold onto electrons) in peridinin

Environment: In acetonitrile (a very polar solvent), electrons are more delocalized (shared between various nuclei) in peridinin than in the gas phase.

Orientation: Orientation of pigment (rotation) effects pigment-pigment interaction, which effects efficiency (studied chlorophyll-carotenoid interaction).

These studies, as with most computational chemistry studies, are limited. Quantum mechanics is complicated, so the computations used in the simulations take a long time, even for supercomputers. Some methods have been developed which make simplifications to increase the size of the simulation (such as Density Functional Theory), but accuracy is sacrificed.

The other main option is to use classical physics, but that is less accurate and is not able to include quantum phenomena that are important.

There are methods to combine the two types of simulation, but each method has its own limitations, usually because of error introduced when quantum mechanics and classical physics combine.

Current Research Continued:

The previous research has shown that individual factors can have drastic impacts on the ability of a photosynthetic system to maintain a state of coherence. However, there is very little research as to which factor affects it the most. This research aims to close that gap by studying which factors affect the ability of plants to maintain a state of quantum mechanics the most.

Vibrational effects: vibration within the molecule due to temperature

Electronic effects: the structure of the molecule (form of chlorophyll) and the solvation state (polarity of solvent if in solution) affecting the electronic interactions

Methodology:

This research predicts that the effects of temperature will outweigh the structural and solvent effects on efficiency. It has been shown through experimental studies that as the temperature decreases, the efficiency of photosynthesis decreases significantly. If the other factors were more important, then the decrease in efficiency would likely be lesser.

This research uses the deMon2k software for Density Functional Theory (DFT) which is a form of quantum mechanics simulation where electrons are not accounted for individually. Instead, they are treated like a cloud of different charge densities across the molecule. This makes computations faster, but still pretty accurate.

We varied the temperature on 10° C intervals from 253K to 313K (7 temperatures). There were 4 structures: Chlorophyll A with the attached chain, Chlorophyll A without the attached chain, Chlorophyll B with the attached chain, and Chlorophyll B without the attached chain. Each combination of variables was also done in no solution and in a solution of water.