Photosynthesis uses vibrations as 'traffic signals'

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Researchers have discovered a new role for protein vibrations in controlling the transformation of sunshine into useful energy. The study illuminates a mechanism that could help design better solar materials.

The research was conducted in CIFAR Senior Fellow Alan Aspuru-

Guzik's lab at Harvard University by CIFAR Postdoctoral Fellow Doran Bennett, Samuel Blau and Christoph Kreisbeck in collaboration with CIFAR Senior Fellow Gregory Scholes at Princeton University. Their findings were published in the *Proceedings of the National Academy of Sciences* on March 27.

Plants and algae soak up sunlight and transfer the energy using proteins holding colored pigments. A pigment energized by a photon can pass that excitation energy to another nearby pigment—like passing the baton between runners in a relay. By repeating this process the photon's energy is carried to the reaction center where it is used to produce oxygen and power plant growth.

Scientists have long wondered how plants move this energy so quickly and efficiently across the large collections of pigments surrounding each reaction center.

In this study, researchers focused on one photosynthetic protein known as PC645. Using computer simulations and experimental data, they found that PC645 controls where energy goes by tuning the vibrations of pigments to enhance energy transport along specific routes.

"You can imagine these proteins using the vibrations of different pigments like traffic signals that send excitations in one direction or another," explains Bennett, who was in Toronto for the CIFAR Bio-inspired Solar Energy program meeting.

For example, when a 'blue' pigment is excited it could pass the excitation to a number of different neighboring pigments with similar energies. By controlling the vibrations, proteins can direct the 'blue' pigment to pass the excitation to a specific 'red' pigment thereby skipping over pigments with intermediate colours.

"The weird thing is that when you run the experiments, the excitation doesn't step down an energy ladder. It jumps from the very highest rung to the very lowest rung and never touches anything in the middle. It makes you wonder—why? And more importantly, how?" says Bennett.

Previously, researchers thought this could only be explained by quantum effects like entanglement. Vibronic coherence—the entanglement between electron and vibrational motion—was thought to be necessary for the fast jumps between very different energy levels. However, this new research suggests that what is needed is not vibronic coherence, but a large band of vibrations that bridge the energy gap between two pigments.

"From a material perspective, this kind of classical mechanism is more useful because it's robust to reasonable levels of disorder that current synthetic techniques can achieve," Bennett says.

Bennett and his colleagues are pursuing further research in several directions, including continuing to study how photosynthetic proteins can control and enhance the energy transport necessary for efficient photosynthesis. They are also interested in using these natural design principles to help develop new solar energy materials.

"One of the key challenges is that we need better tools," Bennett explains, "this simulation required 10 million CPU hours and more than two years of human time to study one protein. In the future we hope to speed this up, possibly by borrowing techniques from the field of machine learning."

More information: Samuel M. Blau et al, Local protein solvation drives direct down-conversion in phycobiliprotein PC645 via incoherent vibronic transport, *Proceedings of the National Academy of Sciences* (2018). DOI: 10.1073/pnas.1800370115

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