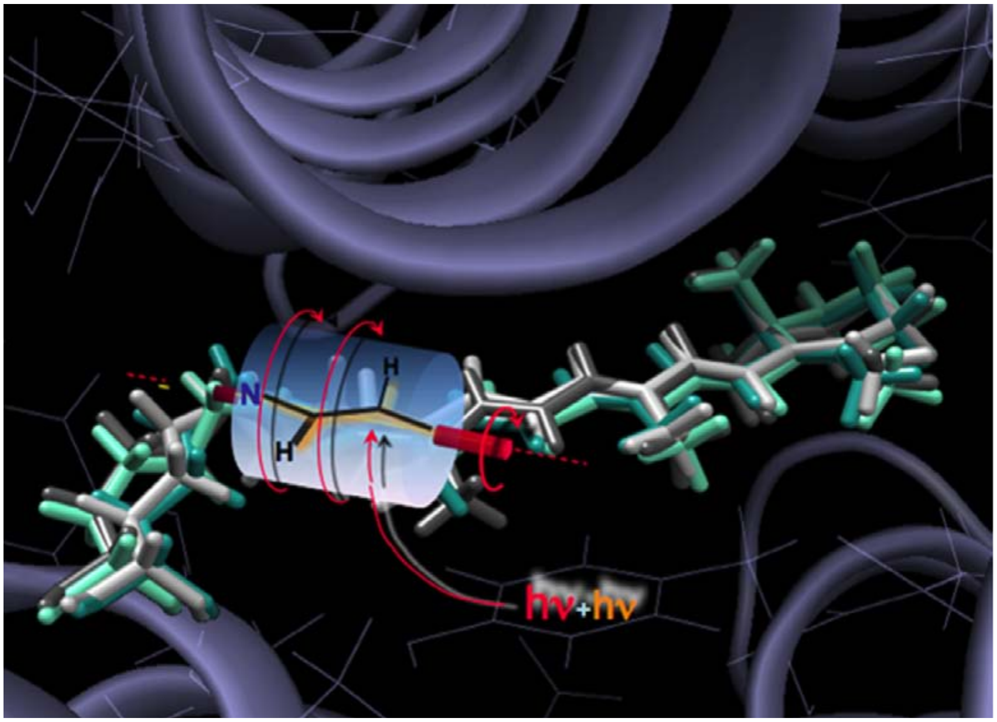

left: In a simulation created at the Ohio Supercomputer Center by Bowling Green's Massimo Olivucci, a short fragment of the long retinal chromophore backbone of Anabaena Sensory Rhodopsin undergoes a complete clockwise rotation powered by the energy carried by two photons.

Olivucci assesses potential, **implications of bacterial photoreceptors**

Blue-green algae are causing havoc in Midwestern lakes saturated with agricultural run-off, but in a northwest Ohio lab, researchers are studying how to harness the positive properties of a closely related strain of bacteria – *Anabaena*.

"An in-depth understanding of light sensing, harvesting and energy conversion in Anabaena may allow us to engineer this and related organisms to thrive in diverse illumination conditions," said Massimo Olivucci, Ph.D., a research professor of chemistry at Bowling Green State University. *"Such new properties would contribute to the field of alternative energy via the microbial conversion of water and light to oxygen and hydrogen. Biophysical studies of the bacterial photoreceptor and its underlying molecular mechanisms can help us to understand its biotechnological potentials and the associated environmental implications."*

Olivucci's research focuses on a sensory protein found in the Anabaena sensory rhodopsin (ASR) bacteria. ASR senses light of two different colors and behaves like the "eye" of Anabaena, which serves as a model for cyanobacteria, the scientific term for freshwater blue-green algae. Cyanobacteria use sunlight as an energy source, and ASR controls sensing green light to activate a cascade of light-sensitive reactions.

"We are constructing quantum-mechanical and molecular-mechanical models on Ohio Supercomputer Center systems," Olivucci explained. *"Past simulations have revealed that light induces a molecular-level rotary motion in the protein interior. Now, the same computer models will be used to engineer hundreds of mutants that display programmed spectroscopic, photochemical and photobiological properties and identify which mutants should be prepared in the laboratory. This new approach constitutes a unique opportunity for developing computational tools useful for understanding the molecular factors that control the spectra of proteins and their photo-responsive properties in general."*

Olivucci noted that protein mutants displaying properties, such as high-binding affinities and novel catalytic activities, have been designed using computational tools based on molecular mechanics. He pointed out, however, that the design of mutants with specific responses to light represents a more complex problem. In these cases, he employs ab initio complete-active-space self-consistent-field method and multi-configurational second-order perturbation theory computations – quantum chemical methods capable of describing both ground and electronically excited states of the ASR.

Olivucci's research will lead to an unprecedented tool by which hundreds to thousands of mutant models can be screened for wanted properties, such as color, excited state lifetime or photochemical transformations. This will provide tailored genetic materials for generating organisms that, for instance, can thrive under alternative light conditions and modulate biomass production or be used in engineering applications. ■

Project lead: Massimo Olivucci, Bowling Green State University

Research title: Computational engineering and predictions of excited state properties of bacterial photoreceptor mutants

Funding sources: Ohio Board of Regents, Bowling Green State University

Web site: www.bgsu.edu/departments/photochem/people/molivuc.html