Scientists get first look at how water 'lubricates' proteins

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Scientists are one step closer to understanding how proteins move when they perform functions essential for supporting life. For the first time, scientists have directly observed how water lubricates the movements of protein molecules to enable different functions to happen.

In a paper published in the online early edition of the *Proceedings of the National Academy of Sciences*, Ohio State University researchers report using ultra-fast light pulses to reveal how water molecules link up with proteins and enable them to move and function.

The finding could one day help researchers find new treatments for diseases such as Alzheimer's, Parkinson's, cataracts, cystic fibrosis, and diabetes.

Proteins are complex molecules that form the main support structure for plant and animal cells, and they also regulate biochemical reactions. The shape and movements of a protein molecule determine its function, and scientists have long known that proteins can't function unless they are immersed in water.

“Protein-water interactions are a central, long-standing, unsolved problem in protein science,” said Dongping Zhong, associate professor of physics at Ohio State and leader of the study. “We believe that we are making a major step to answer these fundamental questions, and the final results will be very important for many biological applications.”

For instance, scientists could better understand how proteins fold and mis-fold -- a key to understanding certain diseases. They could also design more effective drug molecules that link up with proteins in just the right way.

Molecules move fast, shape-shifting in mere fractions of a second, so the movements are hard to see.

This study marks the first time scientists have been able to map the movements of water molecules at different sites on a much larger protein molecule, and see how those movements influence the form and function of the protein.

Zhong and his team took laser “snapshots” of a single myoglobin protein -- the protein that carries oxygen inside muscle tissue -- immersed in water in the laboratory. They were able to measure how fast the water molecules were moving around the protein, and see how those movements related to characteristics of the protein at that moment -- the electrical charge at a particular site, for instance, or changes in the protein's shape.

Proteins can execute a movement in a few billionths of a second. Water normally moves a thousand times faster -- on the scale of a trillionth of a second. In previous work, the Ohio State researchers showed that water molecules slow down substantially as they gets close to a protein.

This new study shows that the water molecules slow even more once they reach the protein. The water forms a very thin layer -- only three molecules thick -- around the protein, and this layer is key to maintaining the protein's structure and flexibility, lubricating its movements.

Their findings challenge the conventional wisdom of theorists who try to

envision what is happening on these tiny scales. Because they can't directly see what's happening, scientists use simulations to fill the gap.

The simulation software has improved in recent years, Zhong said. But for two years his team has compared simulations to actual experiments, and found that the two don't match up.

“We are pretty confident at this point that the simulations need to change,” Zhong said. “Our experimental data provide a benchmark for testing and improving them.”

In the future, Zhong's team will study how water affects proteins interacting with each other, and with DNA.

“Our ultimate goal is to understand why water is so unique and important to life,” he said.

Source: Ohio State University