Argonne scientists develop techniques for creating molecular movies

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They may never win an Oscar, but scientists at the U.S. Department of Energy's (DOE) Argonne National Laboratory have developed techniques for creating accurate movies of biological and chemical molecules, a feat only theorized up until now.

Biological and organic molecules in solution are far more complex than the standard crystalline structures of salt or metals since they are constantly moving and changing over time. These motions have not yet been seen directly, but scientists using the high intensity x-rays at the Advanced Photon Source have measured images that are "blurred" by these motions and have used them to create more accurate movies of molecular motions.

Computer simulations are currently the only way to visualize molecular motions in solution, but researchers have not had a means to check the accuracy of these simulations for complex molecules. For the first time, scientists can see the movements first hand and compare them to their theoretical counterparts.

"The blurring that we see in our solution x-ray patterns are remarkably sensitive to the type of the molecular motion," senior chemist David Tiede said. "For the first time, we are able to test the accuracy of the simulation and change it to fit data better. Without it, we had no way of knowing how accurate the models were."

Tiede hopes an improved accuracy in molecular modeling will give

insights into the structure and behavior of the molecules. Collaborators at the National Institutes of Health have used this approach to help determine structures of important biological molecules.

Tiede and his collaborators also plan to examine how a structure reacts to an outside stimulus. By using a laser to excite the atoms, he will create a movie that shows how the molecule reacts to the initial laser pulse and also how it returns to a stable condition.

“We hope to establish between ‘good’ and ‘bad’ molecular actors in important chemical processes like photosynthesis, solar energy and catalysts,” Tiede said. “Once we see that, we can make these processes work better.”

Source: Argonne National Laboratory