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Chemists take closer look at useful xenon gas

Xenon, the gas that produces that bright blue-white headlight glow on many luxury cars, has other potential uses, including as an anesthetic.

Because its atoms can nestle in nano-sized pockets of protein molecules, some scientists think it may have use as a marker for imaging tissues, if its behavior in proteins could be better understood.

New research by chemists at UIC and the Steacie Institute for Molecular Sciences at Canada's National Research Council in Ottawa may help advance that understanding.

Working independently, the Chicago and Ottawa scientists studied xenon in dipeptide crystals, whose structure at the atomic level is precisely known. A dipeptide is a small version of a protein, having only two amino acid units instead of hundreds or thousands.

The dipeptide crystals used for this experiment could be electronically assembled and manipulated in a computer. The idea was to track the behavior of xenon atoms and changes in the dipeptide crystal as the atoms filled tiny nooks, crannies and channels.

Cynthia Jameson, professor of chemistry at UIC, and former doctoral student Devin Sears, worked in Chicago. Igor Moudrakovski, Dmitriy Soldatov and John Ripmeester worked in Ottawa.

The Canadian team did an experiment with actual xenon and dipeptides in a laboratory. Jameson and Sears predicted the xenon behavior in the dipeptide entirely by a computer simulation program run in Chicago.

Both teams were blind to each other's information or data. But the results characterizing the xenon's behavior proved remarkably similar.

"They were amazed," said Jameson of the Canadian team's reaction.

“This is a real example of the predictive power of theoretical calculations.”

Jameson and Sears wrote a computer program that took into account what is known about xenon’s behavior in the environment of other atoms and employed a coin-toss probability technique called “grand canonical Monte Carlo simulations” — named for the famed gambling haven — to beat the odds and predict how xenon would behave elsewhere within the narrow confines of the dipeptide crystal.

For Jameson, the dual studies via laboratory and computer experiments underscore the power and value of theoretical calculations.

“When I say that I understand something, as a physical chemist, it means that I can duplicate the experiment by calculation.

“Then I truly understand it, because I have put into my calculation the essence of what actually exists in nature,” she said.

“The main goal is to be able to go into proteins. What will be the ability of xenon to go into particular protein sites? Will it go in, or not? Wouldn’t it be nice to predict how strong or weak the binding will be?” said Jameson.

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