

Quantum physics predict chemical reactions

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Purdue University scientists say chemists trying to predict how complex biological molecules react with others may soon get help from quantum physics.

Using supercomputers to analyze the interplay of electrons around such molecules, physicists led by Purdue's Jorge Rodriguez have found the quantum property of electrons called "spin" must be considered to obtain a complete picture of how many biochemical reactions take place.

In particular, a class of metal-based proteins -- including hemoglobin and chlorophyll -- and their reactions in plants and animals, can be better understood with the technique.

Rodriguez said the discovery could help scientists with a number of practical problems, such as selecting the best potential new drug compounds from a vast group of candidates, a process that can cost pharmaceutical companies years of work and millions of dollars.

"Whereas we have had to be satisfied with observing the chemistry in living things and describing it afterward without complete understanding, we are developing computational tools that can predict what will happen between molecules before they meet in the test tube," said Rodriguez, an assistant professor of physics.

Two papers on the subject appear in this week's issue of the Journal of Biological Chemistry.

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