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Electrons 'tunnel' through water molecules between nestled proteins

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Duke University theoretical chemists who spend much of their time calculating how the exotic rules of quantum mechanics govern electrons motion between and through biological molecules have garnered surprising results when they add water to their models.

They have discovered that a scant handful of water molecules positioned in the nearly infinitesimal gap between two "docking" proteins creates unexpectedly favorable conditions for electrons to "tunnel" from one protein to another. The researchers, chemistry professor David Beratan and postdoctoral researchers Jianping Lin and Ilya Balabin, revealed their findings in a paper to be published in the Nov. 25, 2005, issue of the journal *Science*.

Their work, supported by the National Institutes of Health, delves into puzzling guidelines of physics that Beratan said nature has to follow in order to harness energy and avoid disease.

"Electrons have dual characteristics, sometimes acting like billiard balls and sometimes like waves on a pond," Beratan said in an interview. "As a consequence, electrons do very peculiar things. One thing they can do is tunnel through barriers forbidden to them under the 'classical' rules of physics.

"Biology has to move electrons through proteins in order to trap energy from the sun, capture energy from our food, and control damage to living systems," he added. "So biology has had to come to terms with this duality. Although electrons have the ability to tunnel, it's very costly for them. But one thing that proteins seem to do is to guide such electrons from place to place."

Scientists have already deduced that electron movements are enhanced when proteins fold into complex three-dimensional shapes in their active forms. "It is much easier for electrons to tunnel quantum mechanically through a folded protein than it is for them to penetrate empty space," he said.

Beratan said he and other Duke chemists have spent years studying proteins' roles in electron transport. But only recently has his group addressed how water between protein molecules affects electron movement.

For instance, whenever two proteins that transfer electrons interact strongly -- or "dock" -- they must exchange electrons in a watery medium. What scientists didn't understand was the role of water at this interface, he said.

According to Beratan, electrons cannot simply hop over the very small half billionths of a meter gaps that separate such docking proteins. Quantum mechanics requires that those electrons instead follow pathways or conduits that are heavily influenced by the positions of nearby atoms and gaps between atoms.

"What our study was about was probing how that tunneling process changes if we begin pulling two proteins apart and the gap between them fills with water," he said.

"What we show is that at the shortest separations electrons take advantage of the proteins in tunneling between those two molecules. But there is an intermediate distance where the proteins are beyond contact and the water molecules start moving into this interface.

"In this intermediate distance before the proteins are too far apart, the water plays a very special role in mediating the electron tunneling more strongly than might have been expected."

An illustration in their Science paper, derived from massive computer studies by the authors, shows how a mere handful of those water molecules can form an organized cluster under the influence of the protein molecules on either side of the gap. This cluster aids the electron transfer process, he said.

Electrons can then tunnel between "donor" atoms at the tip of one protein to "acceptor" atoms on the other protein. Along the way, the electrons follow multiple pathways through these water molecules that facilitate the transport more strongly than expected.

"Before our study, expectations for electron tunneling were that interactions between the electron donor and acceptor through water would drop exponentially as a function of the distance," Beratan said.

"What we found was that water is a better mediator for electron transfer at intermediate distances than anybody had expected. Another finding was that the water-mediated tunneling drops only very slightly as a function of distance within this intermediate length."

The Duke team's computations show tunneling initially dropping off very rapidly when the proteins first start separating -- just like scientists originally expected. But at intermediate distances of a few tenths of a billionths of a meter "the rates of tunneling don't change very much," he said. "Then, when the proteins are separated somewhat further, the rates again drop exponentially again as a function of their separation distance," he added.

Experiments in the Netherlands as well as at the University of California, Berkeley also suggest a special role for water in promoting electron transfers between proteins, he said.

"You could think about the structure of the proteins as well as the water as guiding or shepherding the electrons," Beratan said. "So evolution has had to come to terms with physics in the way protein and water direct electrons through complex structures."

The study was the final Ph.D. project for Lin, Beratan's former graduate student, who is first author of the Science paper. Co-author Balabin helped the group calculate how the naturally occurring motion of atoms in the protein might further influence the electron transfer.

"We see pictures of proteins in fixed positions, but in reality we should think of their atoms as wiggling all over the place," Beratan said.

Source: Duke University