# Scientists model molecular switch

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Michigan Technological University physicist Ranjit Pati and his team have developed a model to explain the mechanism behind computing's elusive Holy Grail, the single molecular switch.

If born out experimentally, his work could help explode Moore's Law and could revolutionize computing technology.

Moore's Law predicts that the number of transistors that can be economically placed on an integrated circuit will double about every two years. But by 2020, Moore's Law is expected to hit a brick wall, as manufacturing costs rise and transistors shrink beyond the reach of the laws of classical physics.

A solution lies in the fabled molecular switch. If molecules could replace the current generation of transistors, you could fit more than a trillion switches onto a centimeter-square chip. In 1999, a team of researchers at Yale University published a description of the first such switch, but scientists have been unable to replicate their discovery or explain how it worked. Now, Pati believes he and his team may have found the mechanism behind the switch.

Applying quantum physics, he and his group developed a computer model of an organometallic molecule firmly bound between two gold electrodes. Then he turned on the juice.

As the laws of physics would suggest, the current increased along with the voltage, until it rose to a miniscule 142 microamps. Then suddenly, and counterintuitively, it dropped, a mysterious phenomenon known as negative differential resistance, or NDR. Pati was astonished at what his analysis of the NDR revealed.

Up until the 142-microamp tipping point, the molecule's cloud of electrons had been whizzing about the nucleus in equilibrium, like planets orbiting the sun. But under the bombardment of the higher voltage, that steady state fell apart, and the electrons were forced into a different equilibrium, a process known as "quantum phase transition."

"I never thought this would happen," Pati said. "I was really excited to see this beautiful result."

Why is this important? A molecule that can exhibit two different phases when subjected to electric fields has promise as a switch: one phase is the "zero" and the other the "one," which form the foundation of digital electronics.

Pati is working with other scientists to test the model experimentally. His results appear in the article "Origin of Negative Differential Resistance in a Strongly Coupled Single Molecule-metal Junction Device," published June 16 in *Physical Review Letters*.

Source: Michigan Technological University