Quantum strangeness gives rise to new electronics

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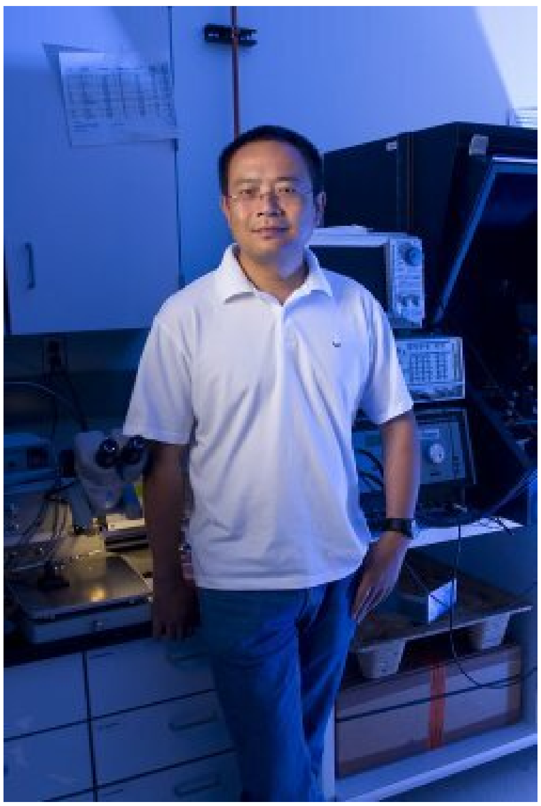

Nongjian 'NJ' Tao, Ph.D., is the director of the Center for Bioelectronics and Biosensors at the Biodesign Institute and is a professor in the Ira A. Fulton Schools of Engineering at Arizona State University. Credit: The Biodesign Institute at Arizona State University

Noting the startling advances in semiconductor technology, Intel co-founder Gordon Moore proposed that the number of transistors on a chip will double each year, an observation that has been born out since he made the claim in 1965. Still, it's unlikely Moore could have foreseen the extent of the electronics revolution currently underway.

Today, a new breed of devices, bearing unique properties, is being developed. As ultra-miniaturization continues apace, researchers have begun to explore the intersection of physical and chemical properties occurring at the molecular scale.

Advances in this fast-paced domain could improve devices for data storage and information processing and aid in the development of molecular switches, among other innovations.

Nongjian "NJ" Tao and his collaborators recently described a series of studies into electrical conductance through single molecules. Creating electronics at this infinitesimal scale presents many challenges. In the world of the ultra-tiny, the peculiar properties of the quantum world hold sway. Here, electrons flowing as current behave like waves and are subject to a phenomenon known as quantum interference. The ability to manipulate this quantum phenomenon could help open the door to new nanoelectronic devices with unusual properties.

"We are interested in not only measuring quantum phenomena in single molecules, but also controlling them. This allows us to understand the basic charge transport in molecular systems and study new device functions," Tao says.

Tao is the director of the Biodesign Center for Bioelectronics and Biosensors. In research appearing in the journal *Nature Materials*, Tao and colleagues from Japan, China and the UK outline experiments in which a single organic molecule is suspended between a pair of electrodes as a current is passed through the tiny structure.

The researchers explore the charge transport properties through the molecules. They demonstrated that a ghostly wavelike property of electrons—known as quantum interference— can be precisely modulated in two different configurations of the molecule, known as Para and Meta.

It turns out that quantum interference effects can cause substantial variation in the conductance properties of molecule-scale devices. By controlling the quantum interference, the group showed that electrical conductance of a single molecule can be fine-tuned over two orders of magnitude. Precisely and continuously controlling quantum interference is seen as a key ingredient in the future development of wide-ranging molecular-scale electronics, operating at high speed and low power.

Such single-molecule devices could potentially act as transistors, wires, rectifiers, switches or logic gates and may find their way into futuristic applications including superconducting quantum interference devices (SQUID), quantum cryptography, and quantum computing.

For the current study, the molecules—ring-shaped hydrocarbons that can appear in different configurations—were used, as they are among the simplest and most versatile candidates for modeling the behavior of molecular electronics and are ideal for observing quantum interference effects at the nanoscale.

In order to probe the way charge moves through a single molecule, so-called break junction measurements were made. The tests involve the use of a scanning tunneling microscope or STM. The molecule under study is poised between a gold substrate and gold tip of the STM device. The tip of the STM is repeatedly brought in and out of contact with the molecule, breaking and reforming the junction while the current passes through each terminal.

Thousands of conductance versus distance traces were recorded, with the particular molecular properties of the two molecules used for the experiments altering the electron flow through the junction. Molecules in the 'Para' configuration showed higher conductance values than molecules of the 'Meta' form, indicating constructive vs destructive quantum interference in the molecules.

Using a technique known as electrochemical gating, the researchers were able to continuously control the conductance over two orders of magnitude. In the past, altering quantum interference properties required modifications to the charge-carrying molecule used for the device. The current study marks the first occasion of conductance regulation in a single molecule.

As the authors note, conductance at the molecular scale is sensitively affected by quantum interference involving the electron orbitals of the molecule. Specifically, interference between the highest occupied molecular orbital or HOMO and lowest unoccupied molecular orbital or LUMO appears to be the dominant determinant of conductance in single molecules. Using an electrochemical gate voltage, quantum interference in the molecules could be delicately tuned.

The researchers were able to demonstrate good agreement between theoretical calculations and experimental results, indicating that the HOMO and LUMO contributions to the conductance were additive for Para molecules, resulting in constructive interference, and subtractive for Meta, leading to destructive interference, much as waves in water can combine to form a larger wave or cancel one another out, depending on their phase.

While previous theoretical calculations of charge transport through single molecules had been carried out, experimental verification has had to wait for a number of advances in nanotechnology, scanning probe microscopy, and methods to form electrically functional connections of molecules to metal surfaces. Now, with the ability to subtly alter conductance through the manipulation of quantum interference, the field of molecular electronics is open to a broad range of innovations.

More information: Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport, DOI: 10.1038/s41563-018-0280-5 , www.nature.com/articles/s41563-018-0280-5

Provided by Arizona State University

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