Organic semiconductors get weird at the edge

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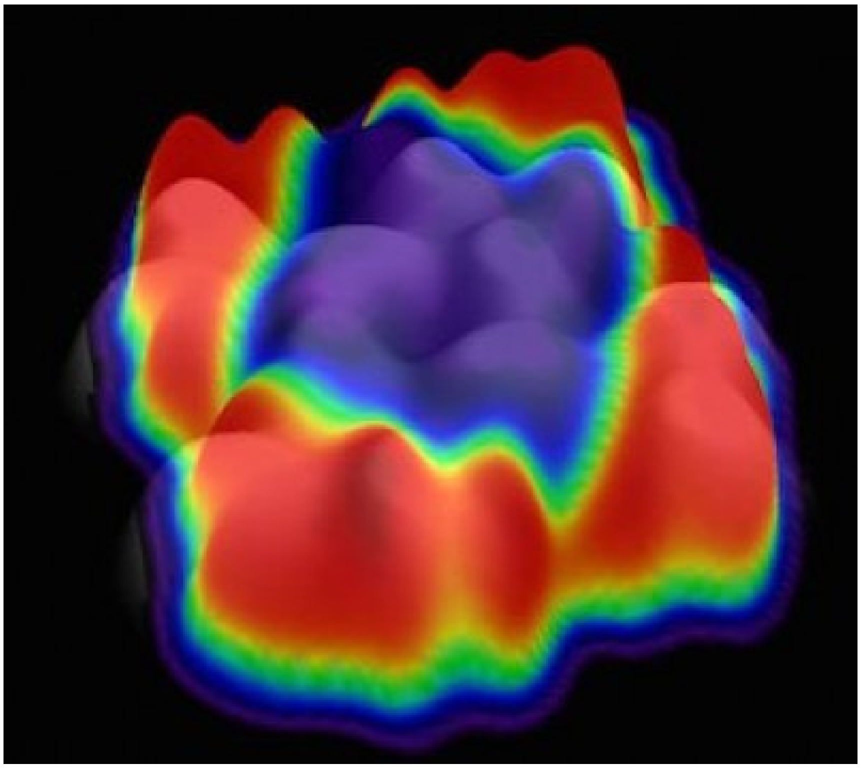

Composite image shows the difference in electronic states at the edge of the material compared to molecules in the centre.

As the push for tinier and faster electronics continues, a new finding by scientists at the University of British Columbia (UBC) and Monash University could help inform the design of the next generation of cheaper, more efficient devices.

The work, published this week in *Nature Communications*, details how electronic properties at the edges of organic molecular systems differ from the rest of the material. All of the research was carried out at UBC's Quantum Matter Institute.

Organic materials—plastics—are of great interest for use in solar panels, light emitting diodes and transistors. They're low-cost, light, and take less energy to produce than silicon. Interfaces—where one type of material meets another—play a key role in the functionality of all these devices.

"We found that the polarization-induced energy level shifts from the edge of these materials to the interior are significant, and can't be neglected when designing components," said UBC PhD researcher Katherine Cochrane, lead author of the paper.

Co-author Dr Agustin Schiffrin, from UBC and Monash points out at the relevance of the research, which shows that subtle variations of the nanoscale structure of an interface can significantly influence the electronic properties of the material.

"The functionality of electronic devices is dictated by the electronic processes that occur at their interfaces. Our work demonstrates that – in order to achieve optimal efficiency of such systems – it is crucial to control how atoms and molecules are arranged at the boundaries of the active materials, and do this with exquisite precision", Dr Schiffrin said.

'While we were expecting some differences, we were surprised by the size of the effect and that it occurred on the scale of a single molecule," added Professor Sarah Burke from UBC, an expert on nanoscale electronic and optoelectronic materials and Chief Investigator of the study.

The researchers looked at 'nano-islands' of clustered organic molecules.

The molecules were deposited on a silver crystal coated with an ultra-thin layer of salt only two atoms deep. The salt is an insulator and prevents electrons in the organic molecules from interacting with those in the silver—the researchers wanted to isolate the interactions of the molecules.

Not only did the molecules at the edge of the nano-islands have very different properties than in the middle, the variation in properties depended on the position and orientation of other molecules nearby.

The research team used a simple, analytical model to explain the differences which can be extended to predict interface properties in much more complex systems, like those encountered in a real device.

"Herbert Kroemer said in his Nobel Lecture that 'The interface is the device' and it's equally true for organic materials," said Burke.

"The differences we've seen at the edges of molecular clusters highlights one effect that we'll need to consider as we design new materials for these devices, but likely there are many more surprises waiting to be discovered."

The research team plans to keep looking at what happens at interfaces in these materials and to work with materials chemists to guide the design rules for the structure and electronic properties of future devices.

Methods

The experiment was performed at UBC's state-of-the-art Laboratory for Atomic Imaging Research, which features three specially designed ultra-quiet rooms that allow the instruments to sit in complete silence, totally still, to perform their delicate measurements. This allowed the researchers to take dense data sets with a tool called a scanning tunnelling microscope (STM) that showed them the energy levels in real-space on the scale of single atoms.

Provided by Monash University