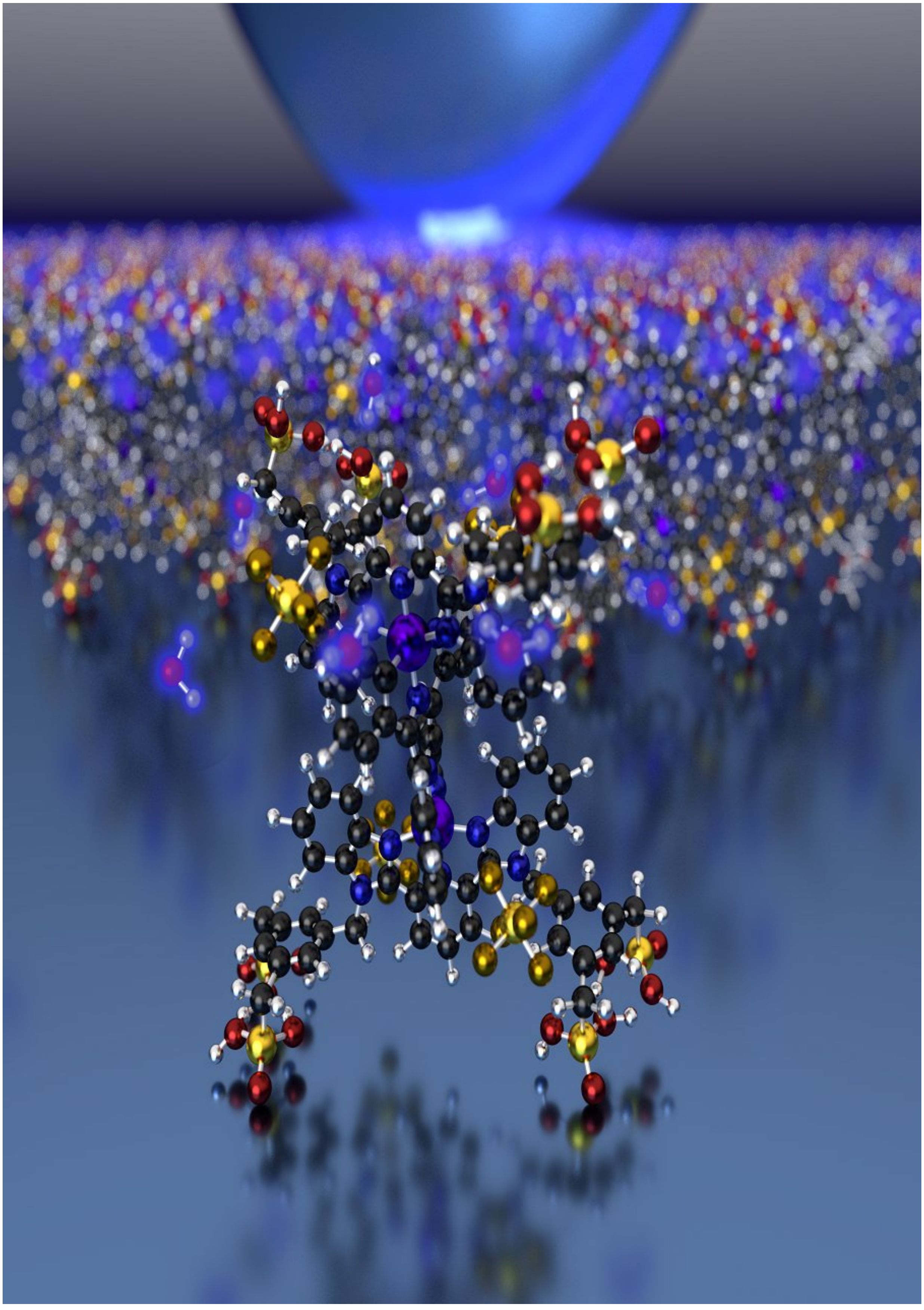
Humidity switches molecular diode off and on

December 4 2017

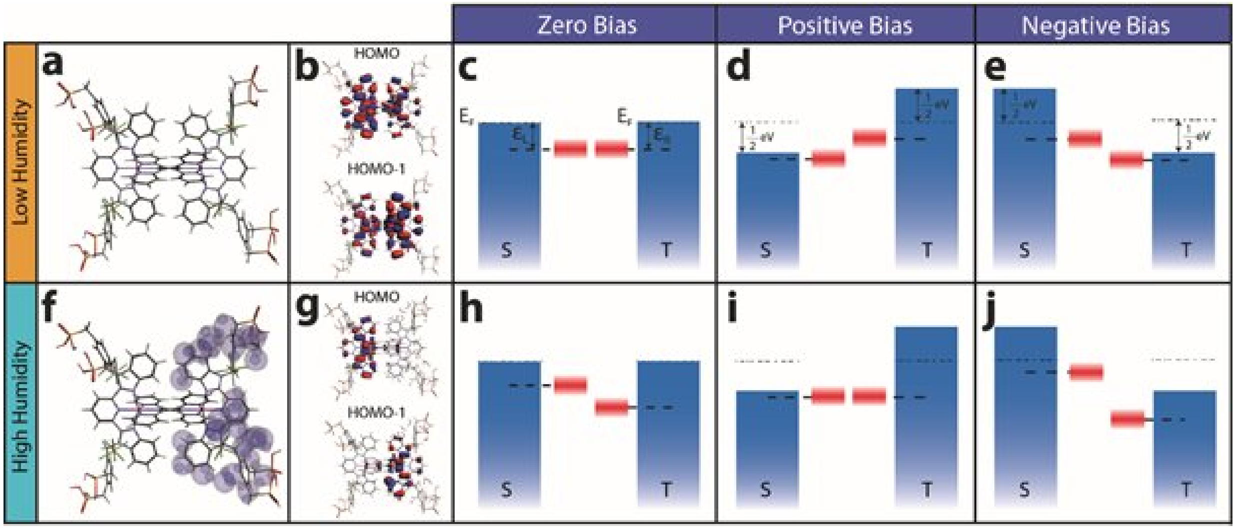


Credit: Leiden Institute of Physics

An international group of scientists from Leiden, Delft, Bern and Chuo has developed the first switchable molecular diode, which can be turned on and off through humidity. It also functions as a humidity sensor at the nanoscale. The study has been published in *Nature Nanotechnology*.

In 2016, Feringa, Stoddard and Sauvage received the Nobel Prize for developing molecular motors. Their work provides a spectacular example of a broader research area in which scientists study molecules with a chemically programmed function. Apart from motors, they also work on molecular diodes, switches and transistors, all with a typical length of a nanometer, and thus represent the ultimate miniaturization. Leiden physicists Sense Jan van der Molen and Huseyin Atesci, together with Delft, Bern and Chuo (Japan), have now demonstrated the first switchable molecular diode.

The scientists discovered that the electric conductivity of the molecule 2-Ru-N depends on humidity. In dry conditions, the same amount of current flows through the molecule under positive or negative voltage. This changes dramatically in a humid environment. In that case, only a positive voltage induces a current. The researchers have created a molecular circuit that works as a unique combination of a switch and a diode—a switchable molecular diode turned on and off with humidity. The molecule also functions as a humidity sensor based on the structure of a specific molecule.



Top: Low humidity. At zero voltage (c), the energy levels of the left and right side of the symmetric molecule (a) are equal. Now if we apply a voltage, the energy levels will shift with respect to each other. The distance between the levels is independent of positive (d) or negative (e) voltage. Therefore, an equally large current will flow for positive and negative voltage. Bottom: High humidity. Because the water resides on one side of the molecule, the symmetry between the energy levels breaks already at zero voltage (h). At positive voltage (i), the energy levels get closer together, so a significant current can flow. However, a negative voltage (j) enlarges the difference between both levels, so the current is blocked. Credit: Leiden Institute of Physics

The tiny diode works by means of an asymmetry caused by water molecules. At around 60 percent humidity, they lump together at the right side of the molecular layer (see figure f). This causes an imbalance between the energy levels on both sides (h), which strongly limits the flow of electrons. A positive voltage across the molecule lifts the energy level of the right side (i), so the levels' alignment is restored and current flows again. A negative voltage on the other hand creates an even larger asymmetry (j) and leading to a very low current. Under dry circumstances, the molecule's symmetry doesn't break and the diode behavior disappears.

Principle

"The whole principle is based on symmetry, so it doesn't exclusively apply to water," says Van der Molen. "In theory this concept also works with for alcohol or toxic gases, for example." This means the discovery does not just relate to measuring moisture in the air. If scientists find a suitable molecule in the future consisting of two symmetric halves, just as 2-Ru-N," the principle enables other sensors too, like a molecular alcohol test or carbon monoxide detector.

More information: Huseyin Atesci, Veerabhadrarao Kaliginedi, Jose A. Celis Gil, Hiroaki Ozawa, Joseph M. Thijssen, Peter Broekmann, Masa-aki Haga, Sense Jan van der Molen, 'Humidity-controlled rectification of ruthenium-complex molecular junctions', *Nature Nanotechnology*, nature.com/articles/doi:10.1038/s41565-017-0016-8

Provided by Leiden Institute of Physics

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