On-surface chemistry leads to novel products

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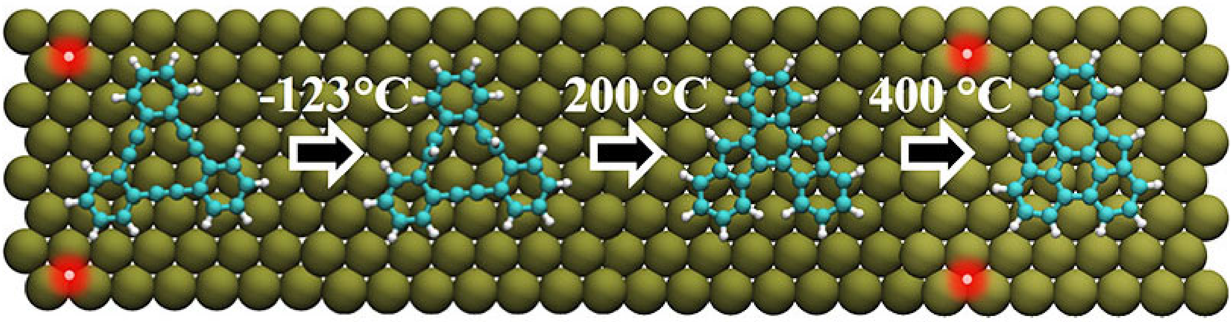

Catalyzed by the copper atoms of the surface, the precursor molecule alters its structure and spatial arrangement when heated gradually. The researchers were able to monitor the synthesis of the end product, which has not been synthesized yet by solution chemistry, with the aid of an ultra-high-resolution atomic force microscope. Credit: University of Basel, Department of Physics

On-surface chemical reactions can lead to novel chemical compounds not yet synthesized by solution chemistry. The first-step, second-step, and third-step products can be analyzed in detail using a high-resolution atomic force microscope, as demonstrated in *Nature Communications* by scientists from the Swiss Nanoscience Institute and the Department of Physics at Basel University and their colleagues from Japan and Finland.

In numerous nanotechnology applications, individual molecules are placed on surfaces to fulfill specific functions - such as conducting an electrical current or emitting a light signal. Ideally, scientists will synthetize these sometimes extremely complex chemical compounds directly on the surface. The on-surface chemical reactions can be followed step by step with the aid of ultra-high-resolution atomic force microscopes. The data obtained also enables them to calculate the precise molecular structure and the energetics along the path.

For their experiments, colleagues of Professor Ernst Meyer from the University of Basel selected a molecule consisting of three benzene rings joined by a triple bond. When the researchers apply this molecule to a silver surface, the molecules arrange themselves in a consistent pattern—but there is no chemical reaction.

Copper as a catalyst

On a copper surface, however, the molecules react already at a temperature of -123 °C. Catalyzed by the copper atoms, the precursor molecule incorporates two hydrogen atoms thereby altering its structure and spatial arrangement. When the sample is heated to 200 °C, a further reaction step takes place in which two pentagonal rings are formed. A further increase in temperature to 400 °C causes a cleaving of hydrogen atoms and forms a further carbon-carbon bond. The final two reaction steps lead to aromatic hydrocarbon compounds, which had previously not been synthetized in solution chemistry.

The researchers conducted these experiments in ultra-high vacuum conditions and were able to monitor the synthesis using a high-resolution atomic force microscope with a carbon monoxide terminated tip. Comparative computer calculations generated the precise molecular structure, which perfectly matched the microscope images.

Tailored nanostructures

Through their experiments, the international research team has shown that on-surface chemistry can lead to novel products. "This extremely pure form of chemistry provides us with tailored on-surface nanostructures that can be used in a variety of ways," says Meyer, commenting on the work largely performed by Dr. Shigeki Kawai. In the example presented, the copper surface functions as a catalyst; the chemical reaction of the precursor molecules is controlled by adding heat and can be monitored via atomic force microscopy.

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Provided by University of Basel

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