# Researchers develop new methods for studying materials at the smallest possible scale

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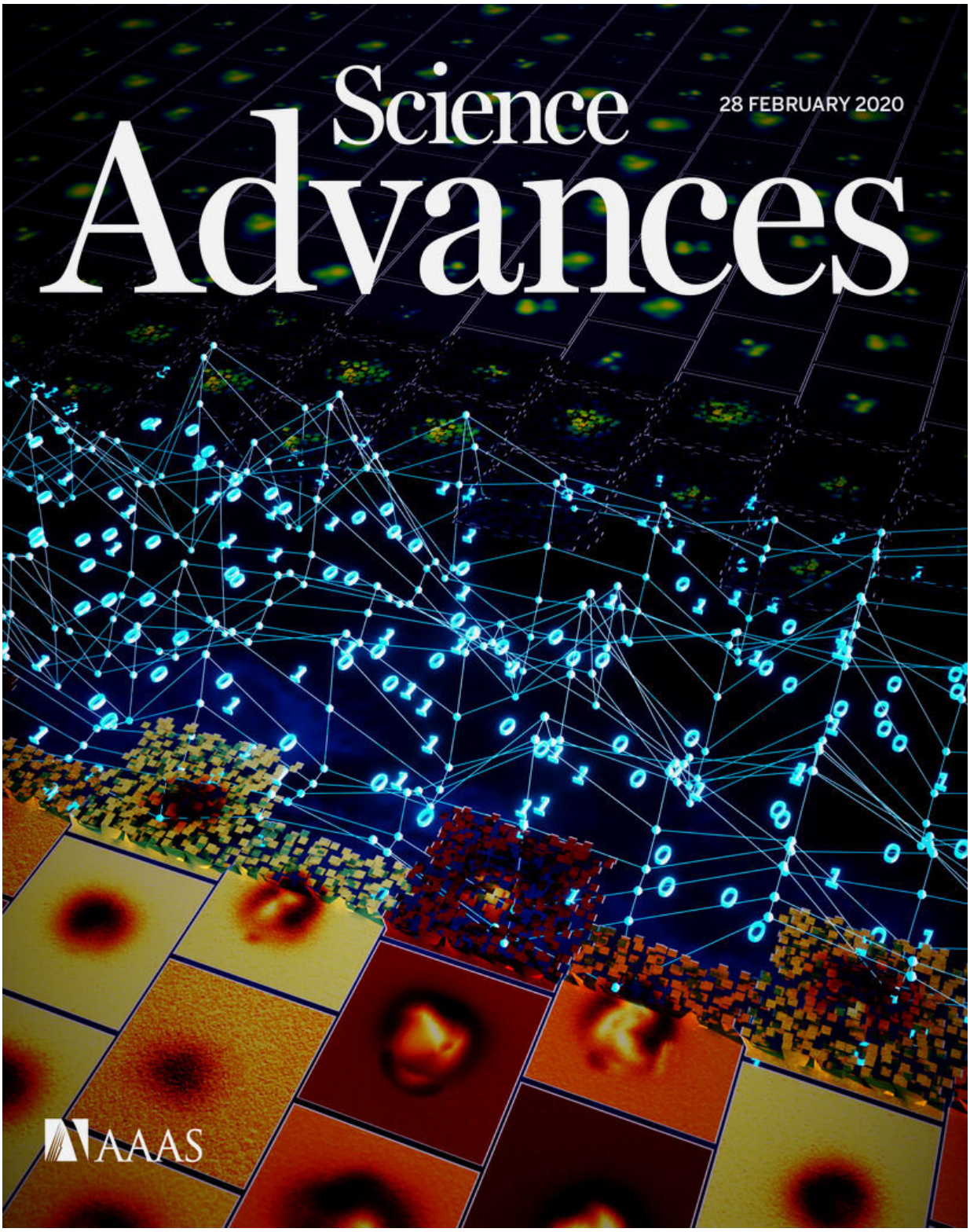


Credit: *Science Advances*

Scientists around the world are interested in developing new materials to help people live more sustainable and healthy lives, but the quest to produce these materials requires detailed knowledge of the mysterious structures of the molecules they are made from. Designers want to replace wasteful plastic with sustainable plant derived compounds, but this can be a challenge without knowledge of plant compound's molecular structure. A new technique developed at Aalto University should allow researchers to get this essential information.

To achieve this, the researchers combined a common materials analysis technique with artificial intelligence. Atomic Force Microscopy (AFM) uses an incredibly fine needle to measure the size and shape of nanometer sized objects, and can already be used to measure the structure of flat, pancake-like planar molecules. By training an artificial intelligence algorithm on lots of AFM data, scientists can now identify more complex molecules with exciting real-world applications.

The team are now able to take images of a single, 3-dimensional molecules, with enough detail that it is possible to understand the different chemical properties of different parts of the molecule. The work was carried out by researchers at Aalto University, led by Academy Professor Peter Liljeroth, and Professors Adam S. Foster and Juho Kannala; and was recently published in the journal *Science Advances*.

"The method researchers currently use guesses the structure, simulates AFM images and see if the guess was correct. When there are many possibilities, this is slow and difficult, and in the end one cannot be certain that all possible structures were thought of," explains Peter Liljeroth.

The researchers used a well understood biomolecule called 1S-camphor, that has a well-known atomic structure and, as a bioproduct of the wood industry, is similar to many of the molecules that other Aalto researchers

are interested in for producing sustainable products. Using a combination of machine learning and AFM simulations, Professor Foster's team developed a deep learning system that matches a set of AFM images with their molecular structure. First, the machine learning system was tested on simulated AFM data, analysing various molecules with planar and non-planar geometries. To test that it worked, experimental data was used with exciting results: The AI was able to reliably and rapidly interpret AFM images of complex 3-D molecules and say what their chemical properties would be.

Benjamin Alldritt, the first author of the paper explains "This research is exciting because it gives us new ways of understanding materials using current experiments. By combining machine learning with AFM, we can understand images of 3-D structures that were unable to before. Additionally, this new method is faster than already existing methods at working out how molecule sits on the surface, and it's quicker and more reliable than human experts for this task."

**More information:** Benjamin Alldritt et al. Automated structure discovery in atomic force microscopy, *Science Advances* (2020). DOI: 10.1126/sciadv.aay6913

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