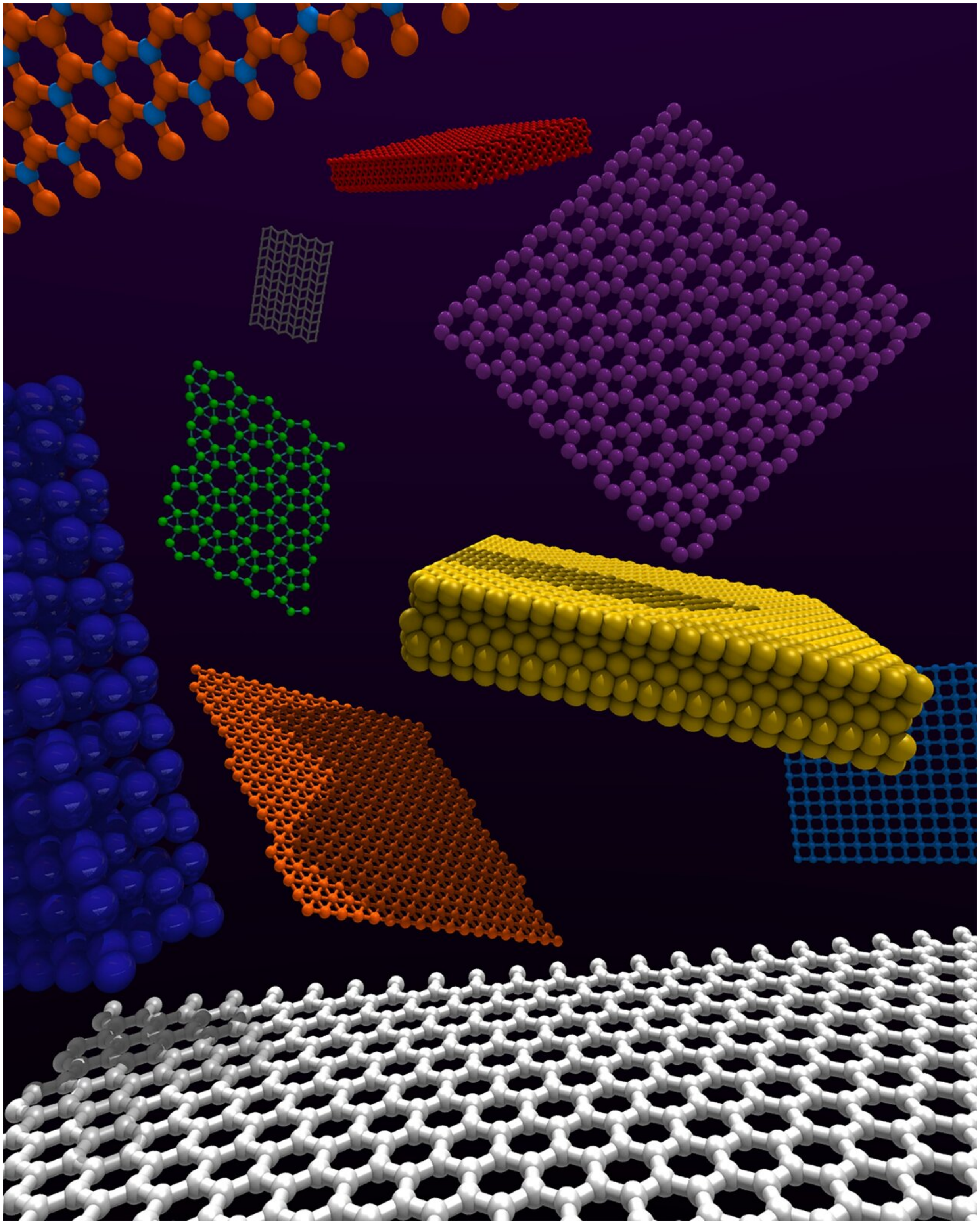
'IcePic' algorithm outperforms humans in predicting ice crystal formation

July 25 2022



A representation of the variety of materials under investigation for their potential to control ice formation. Credit: Michael B. Davies

Cambridge scientists have developed an artificially intelligent algorithm capable of beating scientists at predicting how and when different materials form ice crystals.

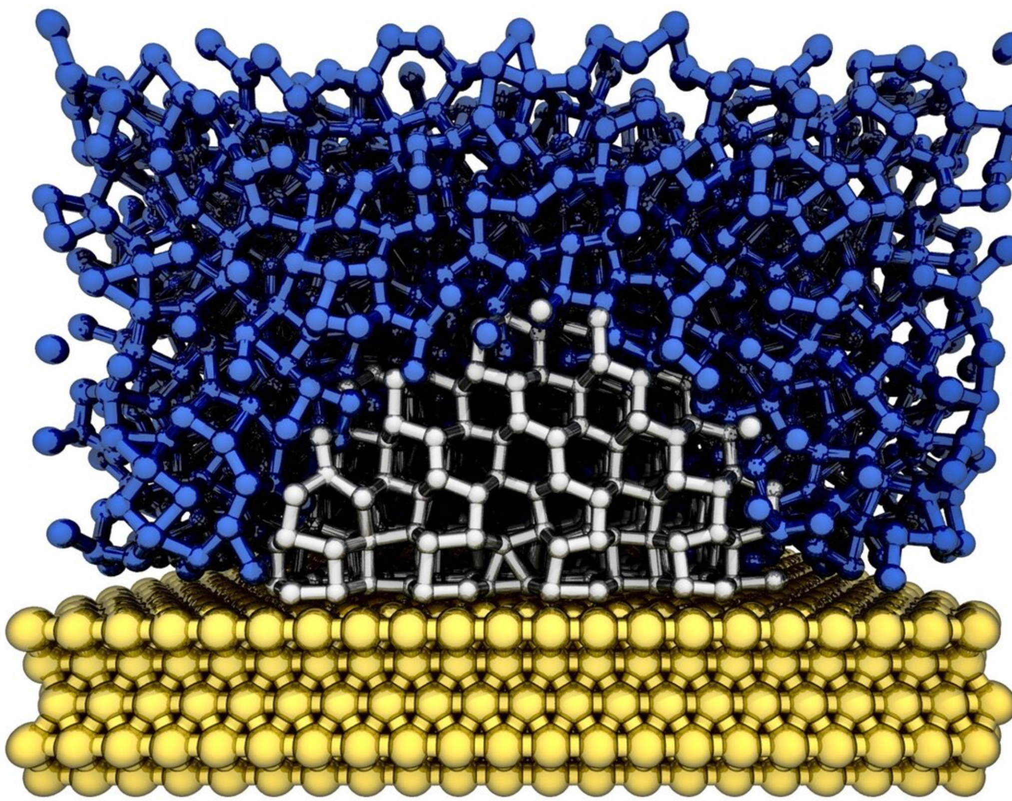
The program—IcePic—could help atmospheric scientists improve climate change models in the future. Details are published today in the journal *PNAS*.

Water has some unusual properties, such as expanding when it turns into ice. Understanding water and how it freezes around different molecules has wide-reaching implications in a broad range of areas, from weather systems that can affect whole continents to storing biological tissue samples in a hospital.

The Celsius temperature scale was designed based on the premise that it is the transition temperature between water and ice; however, whilst ice always melts at 0°C, water doesn't necessarily freeze at 0°C. Water can still be in liquid form at -40°C, and it is impurities in wate that enable ice to freeze at higher temperatures. One of the biggest aims of the field has been to predict the ability of different materials to promote the formation of ice—known as a material's "ice nucleation ability".

Researchers at the University of Cambridge, have developed a 'deep learning' tool able to predict the ice nucleation ability of different materials—and which was able to beat scientists in an online 'quiz' in which they were asked to predict when ice crystals would form.

Deep learning is how artificial intelligence (AI) learns to draw insights from raw data. It finds its own patterns in the data, freeing it of the need for human input so that it can process results faster and more precisely. In the case of IcePic, it can infer different ice crystal formation properties around different materials. IcePic has been trained on thousands of images so that it can look at completely new systems and infer accurate predictions from them.



A foreign material promotes the growth of ice in a film of water. Credit: Michael B. Davies

The team set up a quiz in which scientists were asked to predict when ice crystals would form in different conditions shown by 15 different images. These results were then measured against IcePic's performance. When put to the test, IcePic was far more accurate in determining a material's ice nucleation ability than over 50 researchers from across the globe. Moreover, it helped identify where humans were going wrong.

Michael Davies, a Ph.D. student in the ICE lab at the Yusuf Hamied Department of Chemistry, Cambridge, and University College London, London, first author of the study, said: "It was fascinating to learn that the images of water we showed IcePic contain enough information to actually predict ice nucleation.

"Despite us—that is, human scientists—having a 75 year head start in terms of the science, IcePic was still able to do something we couldn't."

Determining the formation of ice has become especially relevant in climate change research.

Water continuously moves within the Earth and its atmosphere, condensing to form clouds, and precipitating in the form of rain and snow. Different foreign particles affect how ice forms in these clouds, for example, smoke particles from pollution compared to smoke particles from a volcano. Understanding how different conditions affect our cloud systems is essential for more accurate weather predictions.

"The nucleation of ice is really important for the atmospheric science community and climate modeling," said Davies. "At the moment there is no viable way to predict ice nucleation other than direct experiments or expensive simulations. IcePic should open up a lot more applications for discovery."

More information: Accurate prediction of ice nucleation from room temperature water, *Proceedings of the National Academy of Sciences* (2022). DOI: 10.1073/pnas.2205347119.

Provided by University of Cambridge