Answering the mystery of what atoms do when liquids and gases meet

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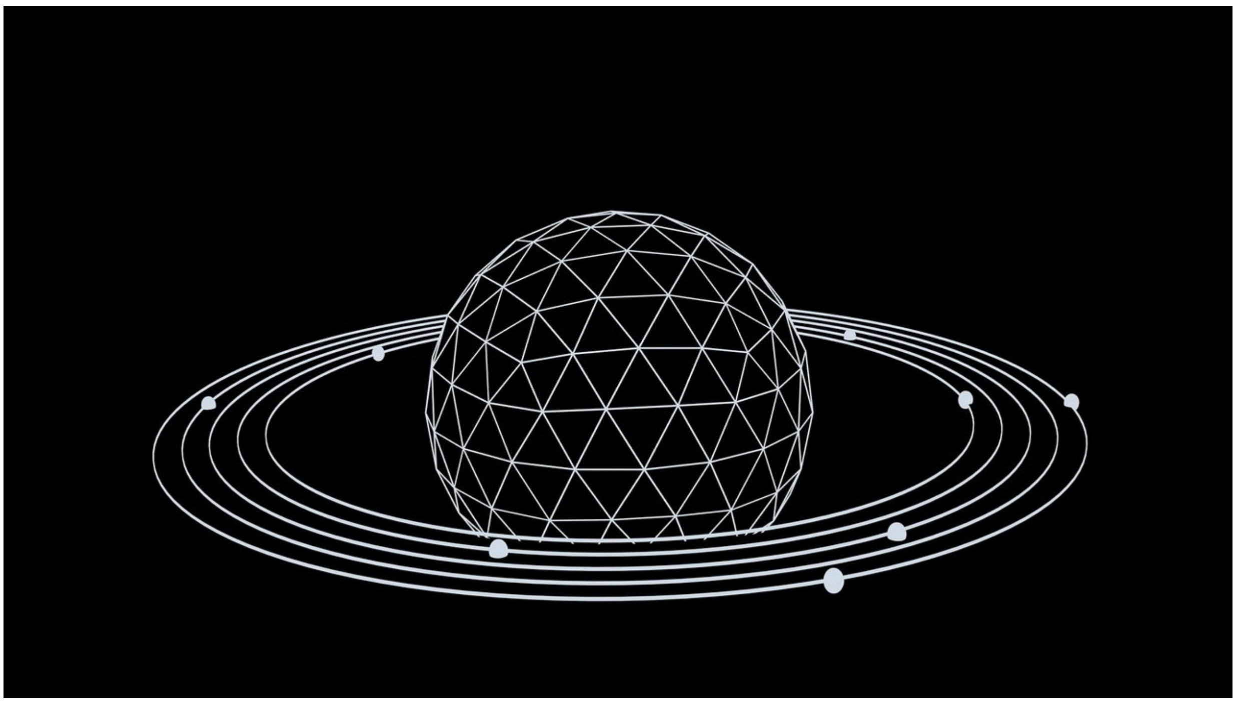

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How atoms arrange themselves at the smallest scale was thought to follow a 'drum-skin' rule, but mathematicians have now found a simpler solution.

Atomic arrangements in different materials can provide a lot of information about the properties of materials, and what the potential is for altering what they can be used for.

However, where two materials touch – at their interface – complex interactions arise that make predicting the arrangement of atoms difficult.

Now, in a paper published today in *Nature Physics*, researchers from Imperial College London and Universidad Carlos III de Madrid have come up with a new model that better predicts how atoms are arranged in relation to each other.

Co-author Professor Andrew Parry, from the Department of Mathematics at Imperial, said: "It's a completely new way of viewing the liquid-gas interface. It can also be applied to other kinds of interfaces: whenever two different materials come together and we want to know how the atoms relate to each other, these ideas can be used."

Where gases and liquids meet: a complex situation

When materials are in a solid state, their atoms are arranged in very uniform patterns – like grids, sheets and lattices. This means that knowing the position of one atom can reveal the positions of all its neighbouring atoms.

However, in liquids and gases, the arrangements of atoms can be very different across the volume of the material. Atoms may be 'locally' packed closer together, leading to denser areas, and can change quickly.

One of the most complex of these situations is when liquids and gases meet. Professor Parry said: "If you imagine a glass of water, the upper surface layer of water in contact with air acts differently to the water below; it has surface tension. When you disturb the surface, for example by tapping the glass, the ripples change the patterns of water atoms at the surface."

Across a glass of water, the arrangement of atoms created by ripples is thought of as arising from 'drum-skin'-like behaviour – the surface tension means the water is drawn taut like a drum and acts accordingly when disturbed.

Piercing the drum-skin analogy

It was previously believed that this kind of behaviour also worked on the atomic scale: that at the level of individual atoms, the same kind of drum-skin behaviour was taking place, ordering the atoms in a certain way.

However, large simulations and calculations of how the atoms behave in this situation do not show a scaled-down version of the drum-skin behaviour, as would be expected.

Now, Professor Parry and Dr. Carlos Rascón from the Universidad Carlos III de Madrid have found a series of new solutions to this problem that do not rely on the drum-skin analogy.

By combining information about the ripples created when the surface is disturbed and how atoms cluster locally, the duo were able to uncover how atoms arrange themselves in relation to one another.

Getting to the underlying simplicity of the system

Professor Parry said: "Whenever we see phenomena at the larger scale – such as temperature, pressure and surface tension – they usually arise out of concepts we observe in the microscopic world. Hence, in this case the drum-skin behaviour arises from something completely different at the microscopic level.

"We can now get to the underlying simplicity of the system without having to overstretch the drum-skin analogy."

The new theory and set of solutions matched the results of the largest-ever simulation of liquid-gas interface behaviour ever conducted much better than the drum-skin model.

"The Goldstone Mode and Resonances in the Fluid Interfacial Region' by A.O. Parry and C. Rascón is published in *Nature Physics*.

More information: A. O. Parry et al. The Goldstone mode and resonances in the fluid interfacial region, *Nature Physics* (2018). DOI: 10.1038/s41567-018-0361-z

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