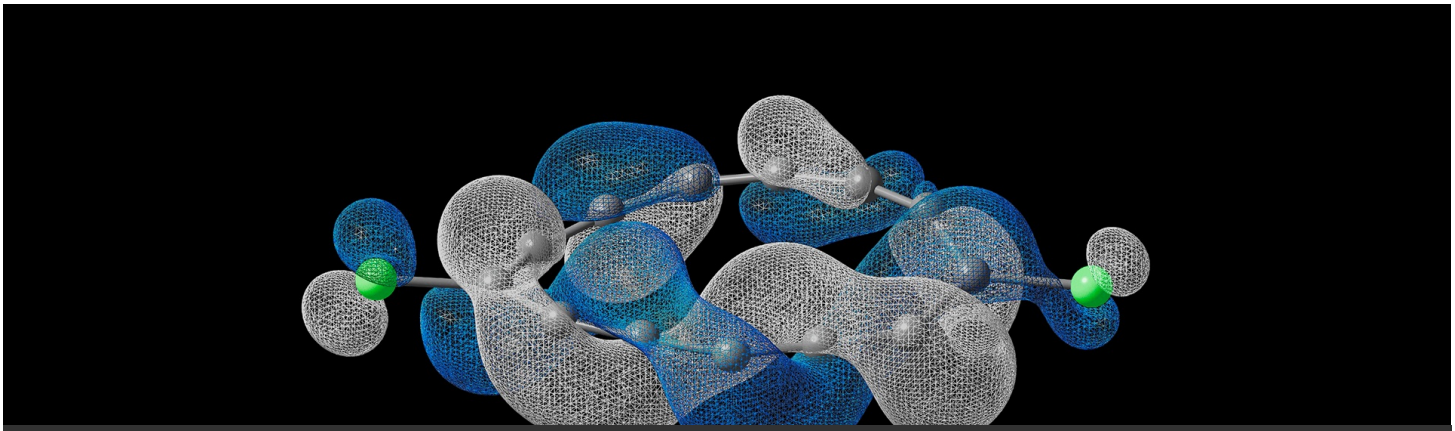
IBM Newsroom

IBM and University Researchers Create a Never-Before-Seen Molecule and Prove its Exotic Nature with Quantum Computing

- Published today in Science, the discovery marks the creation and observation of the first molecule with a half-Möbius electronic topology.

- It shows how quantum computers can directly contribute to understanding complex molecular behavior.



Dyson orbital for electron attachment, calculated using quantum hardware. Credit: IBM and the University of Manchester

YORKTOWN HEIGHTS, New York – March 5, 2026 – An international team of scientists from IBM (NYSE:IBM), The University of Manchester, Oxford University, ETH Zurich, EPFL and the University of Regensburg have created and characterized a molecule unlike any previously known — one whose electrons travel through its structure in a corkscrew-like pattern that fundamentally alters its chemical behavior. Published today in *Science*, it is the first experimental observation of a half-Möbius electronic topology in a single molecule.

To the scientists' knowledge, a molecule with such topology has never before been synthesized, observed, or even formally predicted. Understanding this molecule's behavior at the electronic structure level required something equally fundamental: a high fidelity quantum computing simulation.

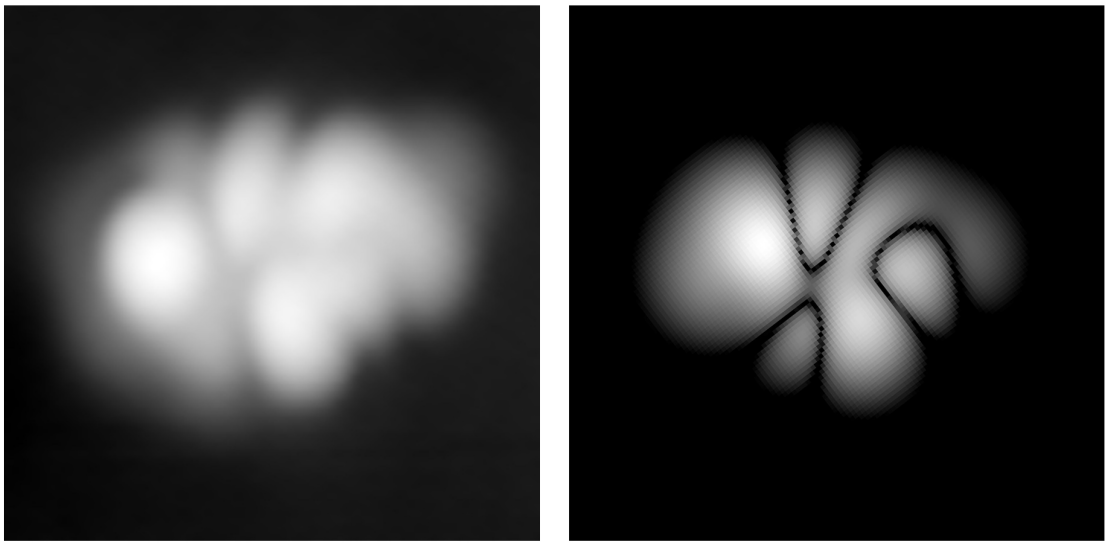
The discovery advances science on two fronts. For chemistry, it demonstrates that electronic topology — the property governing how electrons move through a molecule — can be deliberately engineered, not merely found in nature. For quantum computing, it is a concrete demonstration of a quantum simulation doing what it was designed to do: representing quantum mechanical behavior directly, at the molecular scale, to produce scientific insight that would otherwise have remained out of reach.

"First, we designed a molecule we thought could be created, then we built it, and then we validated it and its exotic properties with a quantum computer," said Alessandro Curioni, IBM Fellow, Vice President, Europe and Africa, and Director of IBM Research Zurich. "This is a leap towards the dream laid out by renowned physicist Richard Feynman decades ago to build a computer that can best simulate quantum physics and a demonstration where, as he said, 'There's plenty of room at the bottom.' The success of this research signals a step towards this vision, opening the door for new ways to explore our world and the matter within it."

A Never-Before-Seen Molecule

The molecule, with the formula $C_{13}Cl_2$, was assembled atom-by-atom at IBM from a custom precursor synthesized at Oxford University, with individual atoms removed one at a time using precisely calibrated voltage pulses under ultra-high vacuum at near-absolute-zero temperatures.

Experiments with scanning tunneling and atomic force microscopy, both techniques pioneered at IBM, combined with quantum computing to reveal an electronic configuration with no counterpart in chemistry's existing record: an electronic structure that undergoes a 90-degree twist with each circuit, requiring four complete loops to return to the starting phase.



Left, a scanning tunneling microscopy image of the new half-Möbius molecule's electron orbital density; right, a simulated STM image of the molecule's orbital density, which was made using an IBM quantum computer.

This half-Möbius topology is qualitatively distinct from any previously known molecule and can be reversibly switched between clockwise-twisted, counterclockwise-twisted and untwisted states — demonstrating that electronic topology is not a property to be discovered, but one that can now be deliberately engineered under specific conditions.

A Disruptive Scientific Tool: Quantum-Centric Supercomputing

The scientists in this experiment created a molecule that had never existed. Now they had to figure out why it worked, a task which challenged conventional computers. The electrons within $C_{13}Cl_2$ interact in deeply entangled ways — each influencing all the others simultaneously. Modeling that behavior requires tracking every possible configuration of those interactions at once, requiring computational demands that grow exponentially and can quickly overwhelm classical machines.

Quantum computers are different by nature because they operate according to the same quantum mechanical laws that govern electrons in molecules, and they can represent these systems directly rather than approximate them. They “speak” the same fundamental language as the matter they are built to study and that distinction, once largely theoretical, can now contribute to concrete scientific results.

This capability offers tremendous potential for quantum computers to support real-world experimentation with quantum-centric supercomputing workflows. By integrating quantum processing units (QPUs), CPUs, and GPUs, quantum-centric supercomputing allows complex problems to be broken into parts that are orchestrated and solved according to each system's strengths — achieving what no single compute paradigm can deliver alone.

Utilizing an IBM quantum computer within such a workflow, the team found helical molecular orbitals for electron attachment, a fingerprint of the half-Möbius topology. Moreover, simulation via quantum computing helped reveal the mechanism behind the formation of the unusual topology: a helical pseudo-Jahn-Teller effect.

This achievement builds on IBM's long legacy in nanoscale science. The scanning tunneling microscope (STM) was invented at IBM in 1981, for which IBM scientists Gerd Binnig and Heinrich Rohrer were awarded the Nobel Prize in 1986. Its creation enabled researchers to image surfaces atom by atom. In 1989, IBM scientists developed the first reliable method for manipulating individual atoms. Over the past decades, the IBM team has extended these techniques to build and control increasingly exotic molecular structures.

RESEARCHER QUOTES

Dr. Igor Rončević, paper co-author, Lecturer in Computational and Theoretical Chemistry at Manchester University:

"Chemistry and solid-state physics advance by finding new ways to control matter. In the second half of the 20th century, substituent effects were very popular. For example, researchers explored how the potency of a drug or the elasticity of a material changes if, for example, a methyl is replaced with chlorine. The turn of the century brought us spintronics, introducing electron spin as a new degree of freedom to play with, and transforming data storage. Today, our work shows that topology can also serve as a switchable degree of freedom, opening a new powerful route for controlling material properties.

"The non-trivial topology of this molecule, and the exotic behavior of many other systems, arises from interactions between their electrons. Simulating electrons with classical computers is very hard – a decade ago we could exactly model 16 electrons, and today we can go up to 18. Quantum computers are naturally well-suited for this problem because their building blocks – qubits – are quantum objects, which mirror electrons. Using IBM's quantum computer, we were able to explore 32 electrons. However, the most exciting part is this is just the start. Quantum hardware is advancing rapidly, and the future is quantum."

Dr. Harry Anderson, paper co-author, Professor of Chemistry at Oxford University:

"It is remarkable that the Lewis structure of $C_{13}Cl_2$ already indicates it is chiral, as confirmed by the experiment and quantum chemical calculations. It is also amazing that the enantiomers can be interconverted by applying voltage pulses from the probe tip."

Dr. Jascha Repp, paper co-author, Professor of Physics at the University of Regensburg:

"I'm really excited to be part of a project where quantum hardware does real science, not just demos. It's fascinating that a tiny molecule can have such a complex electronic structure that is challenging to simulate classically, and is so twisted and strange that it almost twists your mind."

For more about this research, please read the blog:Quantum simulates properties of the first-ever half-Möbius molecule, designed by IBM and researchers.

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