

Q-NEWSLETTER

HIGHLIGHT

[Training AI on Quantum Chemistry](#)

In an IEEE Spectrum article, Chi Chen and Matthias Troyer explain that the real problem in computational chemistry is not just speed, but accuracy in describing how electrons interact inside molecules and materials. Many standard methods, such as Hartree–Fock and density functional theory, simplify these interactions by treating each electron as if moving in an average field created by the others. That works well in many cases, but it becomes unreliable for strongly correlated systems, where electron behaviour is tightly linked and must be treated collectively.

The article argues that quantum computers could generate much more faithful data for these difficult cases, and that AI models trained on this “quantum-accurate” data could then predict properties such as reactivity, conductivity, or stability far more quickly across huge numbers of candidate materials. Today’s most accurate chemistry calculations are extremely slow and expensive. If this hybrid approach works at scale, it could accelerate the discovery of new drugs, better batteries, cleaner catalysts, and advanced materials.

RESEARCH

[First Half-Möbius Molecule Simulated](#)

An international team from IBM, Oxford, the University of Manchester, ETH Zurich, EPFL, and the University of Regensburg has created

and analysed the first “half-Möbius” molecule, built atom by atom at IBM Research Europe in Zurich. Unlike a normal molecular ring, where electron orbitals connect smoothly around the loop, this structure contains a twist, similar to a Möbius strip formed by giving a band a half-turn before joining it. That twist changes the way electrons are distributed and move through the molecule, giving rise to unusual chemical properties.

Because this new molecule is too complex for standard chemistry methods alone, the researchers used quantum-centric computing, combining classical and quantum tools, to simulate its properties and explain the experimental results. Aside from the exciting new molecule, this shows quantum computers are starting to act as real scientific instruments for discovering and understanding new forms of matter.

MARKET

[Building Quantum Hardware in the UK](#)

Quantcore has raised £2.5 million in seed funding to expand quantum manufacturing in the UK. The company, a spin-out from the University of Glasgow, is based at the James Watt Nanofabrication Centre in Scotland and produces niobium superconducting components including processors, resonators, and sensors. This is notable not just as a funding story, but as a sign that the UK is investing in the physical infrastructure behind quantum technologies. Without firms that can fabricate specialised hardware, progress in quantum computing remains difficult to scale.

