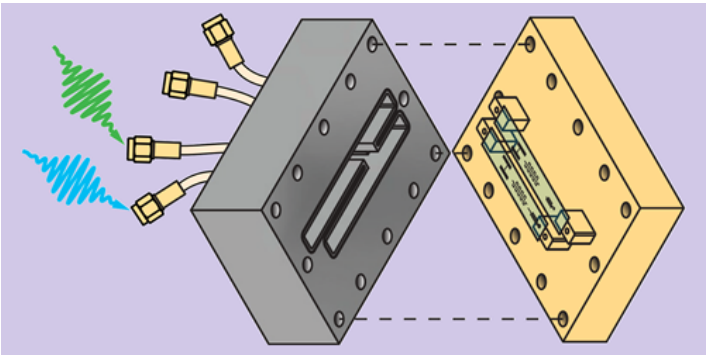
Quantum Circuit Simulates Chemistry

A tunable quantum device can model the energy profiles of chemical reactions and improve physicists' understanding of reaction dynamics.

By **Ryan Wilkinson**

Quantum physics allows particles to pass through energy barriers that they otherwise would not be able to cross. In chemistry, this "tunneling" can help explain how fast reactions occur as a system of particles moves through a barrier between two stable configurations. Now Max Schäfer at Yale University and his colleagues have demonstrated a quantum device that can precisely model such two-well systems [**1**]. This simulator could shed light on the dynamics of many chemical processes, ranging from catalysis to the mechanism by which genes are turned on and off.

The team's device was first introduced in 2024 (see **Focus: New Quantum Effect in Textbook Chemistry Law**). It comprises a superconducting quantum circuit known as a Kerr parametric oscillator. When driven by two microwave signals, this circuit's energy profile possesses two barrier-separated wells akin to those of chemical reactions. Carefully tuning the microwave signals allows the depths of each energy well and the height of the barrier between them to be independently varied in real time.



Credit: A. C. C. de Albornoz *et al.* [**1**]

Leveraging these capabilities, Schäfer and his colleagues observed two unexpected quantum effects. First, transitions from a shallow well to a deep well can occur more slowly than ones between wells of equal depth. This finding is surprising because systems normally transition more readily to lower-energy states than to equal-energy ones. Second, the transition rates show resonances that alternately sharpen and broaden as the well depths are varied. On the basis of numerical simulations, the researchers predict that both of these effects should manifest in the double-well systems associated with chemical reactions.

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REFERENCES

1. A. C. C. de Albornoz *et al.*, "Asymmetry control in a parametric oscillator for the quantum simulation of chemical activation," **PRX Quantum 7, 020309 (2026).**