New method predicts spin dynamics of materials for quantum computing

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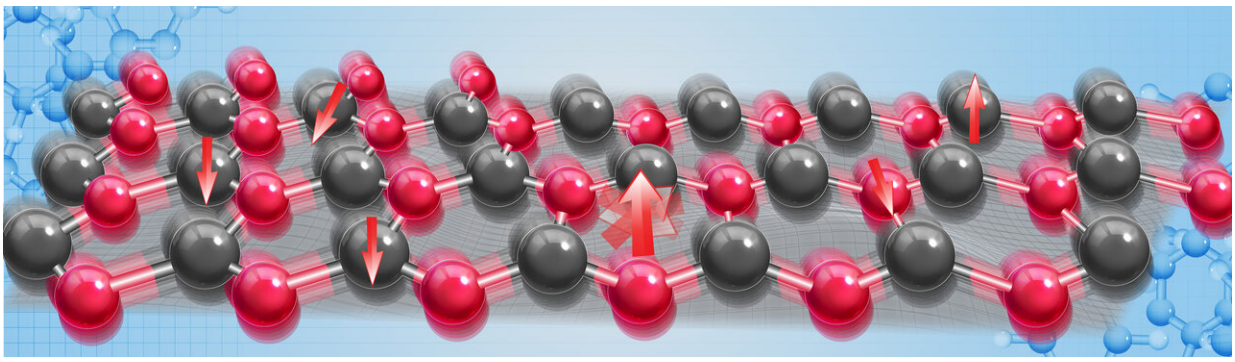

This illustration represents spin relaxation due to the coupling with lattice vibrations, as predicted from fully quantum-mechanical calculations. Credit: Xinran Dongfang

Researchers at UC Santa Cruz have developed a theoretical foundation and new computational tools for predicting a material's spin dynamics, a key property for building solid-state quantum computing platforms and other applications of spintronics.

Spin is a fundamental property of electrons and other particles, and the rapidly growing field of spintronics uses spin states in a manner analogous to the use of electrical charge in electronics. Spin can be used as the basis for qubits (quantum bits) and single-photon emitters in applications of quantum information science, including quantum

computation, communication, and sensing.

Qubits can be made from any quantum system that has two states, but the challenge is to maintain quantum coherence (a relationship between quantum states) long enough to allow manipulation of the qubits. Decoherence means a loss of information from the system, and spin qubits can lose coherence by interacting with their environment through, for example, lattice vibrations within the material.

"The key property for quantum information science is the lifetime of the spin states, known as the spin relaxation and decoherence time," said Yuan Ping, assistant professor of chemistry at UC Santa Cruz. "For quantum information applications, we need materials with long spin relaxation times."

In a paper published June 3 in *Nature Communications*, Ping and her coauthors at UCSC and Rensselaer Polytechnic Institute present a new theoretical framework and computational tools for accurately predicting the spin relaxation time of any material, which was not previously possible.

"These days, people just make a material and try it to see whether it works. Now we have the predictive capability from quantum mechanics that will allow us to design materials with the properties we want for applications in quantum information science," she said. "And if you have a promising material, this can tell you how to change it to make it better."

The researchers established methods for determining spin dynamics from first principles, meaning that no empirical parameters from experimental measurements are needed to do the calculations. They also showed that their approach is generalizable to different types of materials with vastly different crystal symmetries and electronic

structures.

For example, they predicted accurately the spin relaxation time of centrosymmetric materials such as silicon, ferromagnetic iron, and graphene, as well as non-centrosymmetric materials such as molybdenum disulfide and gallium nitride, highlighting the predictive power of their method for a broad range of quantum materials.

By enabling the rational design of materials, instead of searching blindly and testing a wide range of materials experimentally, these new methods could enable rapid advances in the field of quantum information technologies.

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