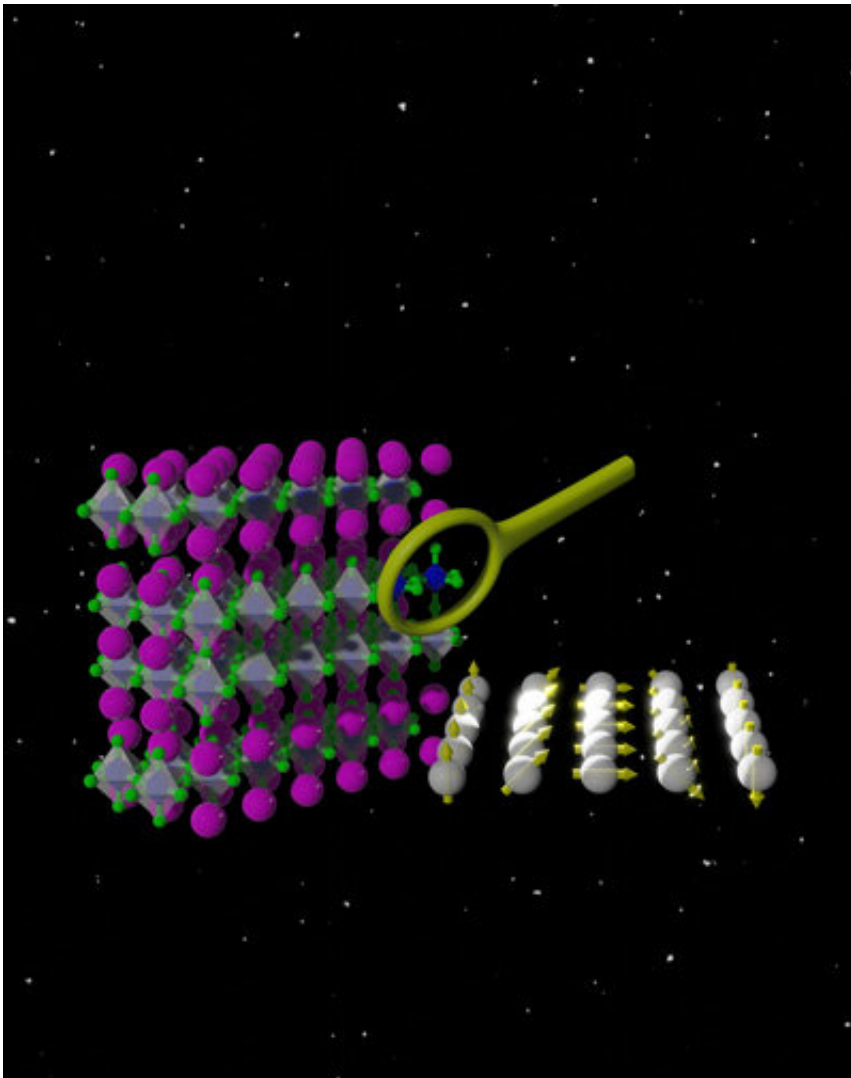


New design principles for spin-based quantum materials

September 18 2020, by Alex Gerage



A crystal structure (left) and a visual model of the spin helix (right). Credit: Northwestern University

As our lives become increasingly intertwined with technology—whether supporting communication while working remotely or streaming our favorite show—so too does our reliance on the data these devices create. Data centers supporting these technology ecosystems produce a significant carbon footprint—and consume 200 terawatt hours of energy each year, greater than the annual energy consumption of Iran. To balance ecological concerns yet meet growing demand, advances in microelectronic processors—the backbone of many Internet of Things (IoT) devices and data hubs—must be efficient and environmentally friendly.

Northwestern University materials scientists have developed new design principles that could help spur development of future quantum materials used to advance (IoT) devices and other resource-intensive technologies while limiting ecological damage.

"New path-breaking materials and computing paradigms are required to make [data centers](#) more energy-lean in the future," said James Rondinelli, professor of materials science and engineering and the Morris E. Fine Professor in Materials and Manufacturing at the McCormick School of Engineering, who led the research.

The study marks an important step in Rondinelli's efforts to create new materials that are non-volatile, energy efficient, and generate less heat—important aspects of future ultrafast, low-power electronics and quantum computers that can help meet the world's growing demand for data.

Rather than certain classes of semiconductors using the electron's charge in transistors to power computing, solid-state spin-based materials utilize the electron's spin and have the potential to support low-energy memory devices. In particular, materials with a high-quality persistent spin texture (PST) can exhibit a long-lived persistent spin helix (PSH), which

can be used to track or control the spin-based information in a transistor.

Although many spin-based materials already encode information using spins, that information can be corrupted as the spins propagate in the active portion of the transistor. The researchers' novel PST protects that spin information in helix form, making it a potential platform where ultralow energy and ultrafast spin-based logic and memory devices operate.

The research team used quantum-mechanical models and computational methods to develop a framework to identify and assess the spin textures in a group of non-centrosymmetric crystalline materials. The ability to control and optimize the spin lifetimes and transport properties in these materials is vital to realizing the future of quantum microelectronic devices that operate with low energy consumption.

"The limiting characteristic of spin-based computing is the difficulty in attaining both long-lived and fully controllable spins from conventional semiconductor and magnetic materials," Rondinelli said. "Our study will help future theoretical and experimental efforts aimed at controlling spins in otherwise non-[magnetic materials](#) to meet future scaling and economic demands."

Rondinelli's framework used microscopic effective models and group theory to identify three materials design criteria that would produce useful spin textures: carrier density, the number of electrons propagating through an effective magnetic field, Rashba anisotropy, the ratio between intrinsic spin-orbit coupling parameters of the materials, and momentum space occupation, the PST region active in the electronic band structure. These features were then assessed using quantum-mechanical simulations to discover high-performing PSHs in a range of oxide-based materials.

The researchers used these principles and numerical solutions to a series of differential spin-diffusion equations to assess the spin texture of each material and predict the spin lifetimes for the helix in the strong spin-orbit coupling limit. They also found they could adjust and improve the PST performance using atomic distortions at the picoscale. The group determined an optimal PST material, Sr₃Hf₂O₇, which showed a substantially longer spin lifetime for the helix than in any previously reported material.

"Our approach provides a unique chemistry-agnostic strategy to discover, identify, and assess symmetry-protected persistent spin textures in quantum materials using intrinsic and extrinsic criteria," Rondinelli said. "We proposed a way to expand the number of space groups hosting a PST, which may serve as a reservoir from which to design future PST materials, and found yet another use for ferroelectric oxides—compounds with a spontaneous electrical polarization. Our work also will help guide experimental efforts aimed at implementing the materials in real device structures."

A paper describing the work, titled "Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes," was published online on September 18 in the journal *Matter*.

More information: Xue-Zeng Lu et al, Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes, *Matter* (2020). [DOI: 10.1016/j.matt.2020.08.028](https://doi.org/10.1016/j.matt.2020.08.028)

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