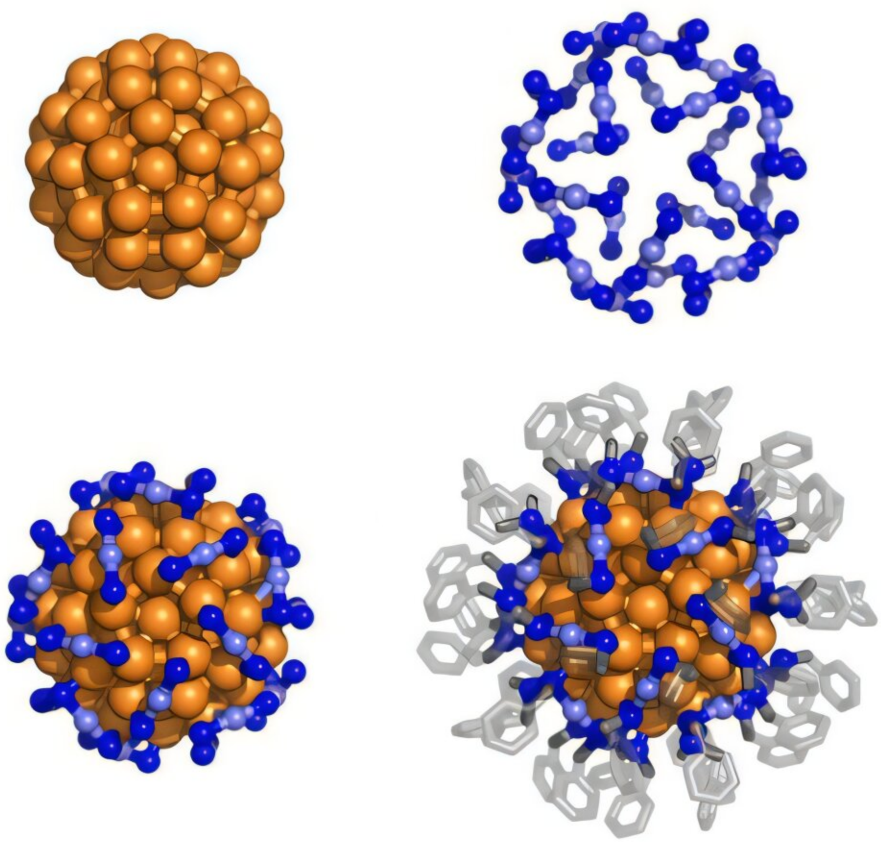
Gold clusters mimic atomic spin properties for scalable quantum computing applications

July 22 2025, by Gail McCormick



New research shows how gold clusters mimic the key properties of the most accurate systems currently used in quantum applications, showing promise for a tunable, scalable option for quantum devices. The cluster contains a gold core, on top left, as well as ligands, on the bottom right. Credit: Knappenberger Lab / Penn State

The efficiency of quantum computers, sensors and other applications often relies on the properties of electrons, including how they are spinning. One of the most accurate systems for high-performance quantum applications relies on tapping into the spin properties of electrons of atoms trapped in a gas, but these systems are difficult to scale up for use in larger quantum devices like quantum computers.

Now, a team of researchers from Penn State and Colorado State has demonstrated how a gold cluster can mimic these gaseous, trapped atoms, allowing scientists to take advantage of these spin properties in a system that can be easily scaled up.

"For the first time, we show that gold nanoclusters have the same key spin properties as the current state-of-the-art methods for quantum information systems," said Ken Knappenberger, department head and professor of chemistry in the Penn State Eberly College of Science and leader of the research team.

"Excitingly, we can also manipulate an important property called spin polarization in these clusters, which is usually fixed in a material. These clusters can be easily synthesized in relatively large quantities, making this work a promising proof-of-concept that gold clusters could be used to support a variety of quantum applications."

Two papers describing the gold clusters and confirming their spin properties appear in *ACS Central Science* and *The Journal of Physical Chemistry Letters*.

"An electron's spin not only influences important chemical reactions, but also quantum applications like computation and sensing," said Nate Smith, graduate student in chemistry in the Penn State Eberly College of Science and first author of one of the papers. "The direction an electron spins and its alignment with respect to other electrons in the system can directly impact the accuracy and longevity of quantum information systems."

Much like the Earth spins around its axis, which is tilted with respect to the sun, an electron can spin around its axis, which can be tilted with respect to its nucleus. But unlike Earth, an electron can spin clockwise or counterclockwise. When many electrons in a material are spinning in the same direction and their tilts are aligned, the electrons are considered correlated, and the material is said to have a high degree of spin polarization.

"Materials with electrons that are highly correlated, with a high degree of spin polarization, can maintain this correlation for a much longer time, and thus remain accurate for much longer," Smith said.

The current state-of-the-art system for high accuracy and low error in quantum information systems involves trapped atomic ions—atoms with an electric charge—in a gaseous state. This system allows electrons to be excited to different energy levels, called Rydberg states, which have very specific spin polarizations that can last for a long period of time. It also allows for the superposition of electrons, with electrons existing in multiple states simultaneously until they are measured, which is a key property for quantum systems.

"These trapped gaseous ions are by nature dilute, which makes them very difficult to scale up," Knappenberger said. "The condensed phase required for a solid material, by definition, packs atoms together, losing that dilute nature. So, scaling up provides all the right electronic ingredients, but these systems become very sensitive to interference from the environment.

"The environment basically scrambles all the information that you encoded into the system, so the rate of error becomes very high. In this study, we found that gold clusters can mimic all the best properties of the trapped gaseous ions with the benefit of scalability."

Scientists have heavily studied gold nanostructures for their potential use in optical technology, sensing, therapeutics and to speed up chemical reactions, but less is known about their magnetic and spin-dependent properties. In the current studies, the researchers specifically explored monolayer-protected clusters, which have a core of gold and are surrounded by other molecules called ligands. The researchers can precisely control the construction of these clusters and can synthesize relatively large amounts at one time.

"These clusters are referred to as super atoms, because their electronic character is like that of an atom, and now we know their spin properties are also similar," Smith said. "We identified 19 distinguishable and unique Rydberg-like spin-polarized states that mimic the super-positions that we could do in the trapped, gas-phase dilute ions. This means the clusters have the key properties needed to carry out spin-based operations."

The researchers determined the spin polarization of the gold clusters using a similar method used with traditional atoms. While one type of gold cluster had 7% spin polarization, a cluster with a different ligand approached 40% spin polarization, which Knappenberger said is competitive with some of the leading two-dimensional quantum materials.

"This tells us that the spin properties of the electron are intimately related to the vibrations of the ligands," Knappenberger said. "Traditionally, quantum materials have a fixed value of spin polarization that cannot be significantly changed, but our results suggest we can modify the ligand of these gold clusters to tune this property widely."

The research team plans to explore how different structures within the ligands impact spin polarization and how they could be manipulated to fine tune spin properties.

"The quantum field is generally dominated by researchers in physics and materials science, and here we see the opportunity for chemists to use our synthesis skills to design materials with tunable results," Knappenberger said. "This is a new frontier in quantum information science."

In addition to Smith and Knappenberger, the research team includes Juniper Foxley, graduate student in chemistry at Penn State; Patrick Herbert, who earned a doctoral degree in chemistry at Penn State in 2019; Jane Knappenberger, researcher in the Penn State Eberly College of Science; and Marcus Tofanelli and Christopher Ackerson at Colorado State.

More information: Juniper Foxley et al, Diverse Superatomic Magnetic and Spin Properties of Au144(SC8H9)60 Clusters, *ACS Central Science* (2025). DOI: 10.1021/acscentsci.5c00139

Nathanael L. Smith et al, The Influence of Passivating Ligand Identity on Au25(SR)18 Spin-Polarized Emission, *The Journal of Physical Chemistry Letters* (2025). DOI: 10.1021/acs.jpclett.5c00723

Provided by Pennsylvania State University