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A magnetic nanographene butterfly poised to advance quantum technologies

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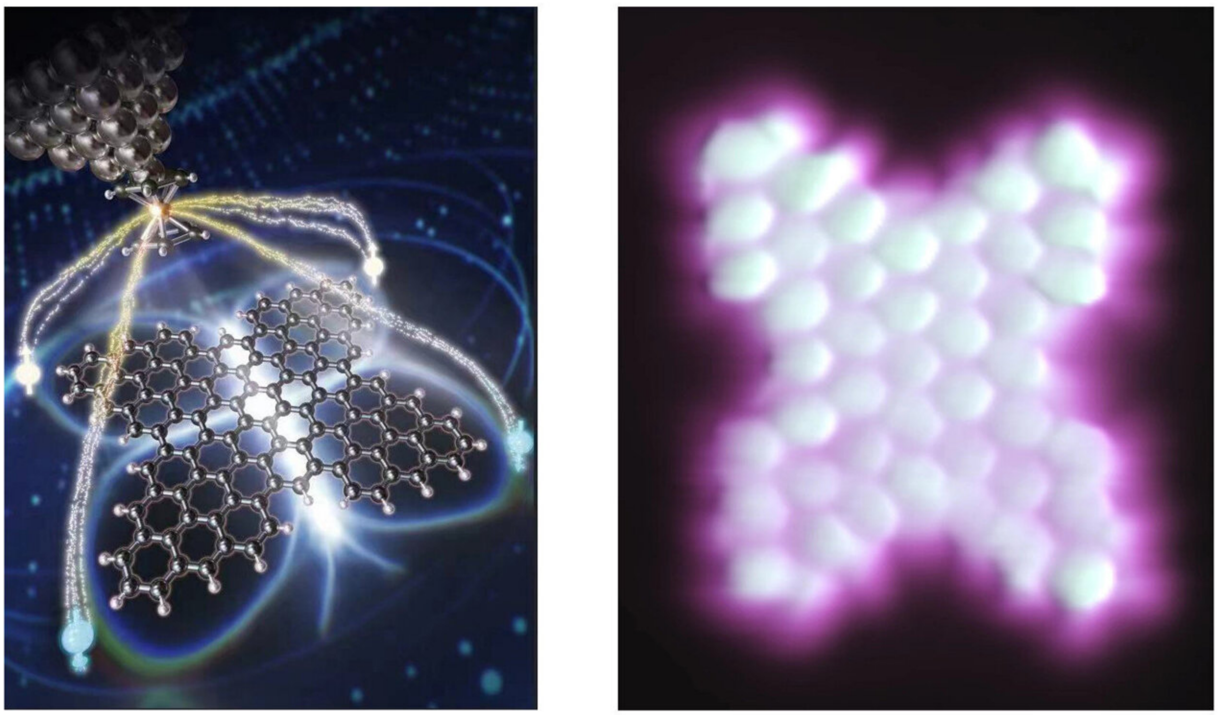

A visual impression of the magnetic “butterfly” hosting four entangled spins on “wings” (left) and its corresponding atomic-scale image obtained using scanning probe microscopy (right). Credit: National University of Singapore

Researchers from the National University of Singapore (NUS) have developed a new design concept for creating next-generation carbon-based quantum materials, in the form of a tiny magnetic nanographene with a unique butterfly-shape hosting highly correlated spins. This new design has the potential to accelerate the advancement of quantum materials which are pivotal for the development of sophisticated quantum computing technologies poised to revolutionize information processing and high density storage capabilities.

The team was led by Associate Professor Lu Jiong from the NUS Department of Chemistry and Institute for Functional Intelligent Materials, together with Professor Wu Jishan who is also from the NUS Department of Chemistry, and international collaborators. The research was published in*Nature Chemistry*.

Magnetic nanographene, a tiny structure made of graphene molecules, exhibits remarkable magnetic properties due to the behavior of specific electrons in the carbon atoms' π-orbitals. By precisely designing the arrangement of these carbon atoms at the nanoscale, control over the behavior of these unique electrons can be achieved. This renders nanographene highly promising for creating extremely small magnets and for fabricating fundamental building blocks needed for quantum computers, called quantum bits or qubits.

The unique structure of the butterfly-shaped magnetic graphene developed by the researchers has four rounded triangles resembling butterfly wings, with each of these wings holding an unpaired π-electron responsible for the observed magnetic properties. The structure was achieved through an atomic-precise design of the π-electron network in the nanostructured graphene.

Assoc Prof Lu said, "Magnetic nanographene, a tiny molecule composed of fused benzene rings, holds significant promise as a next-generation quantum material for hosting fascinating quantum spins due to its chemical versatility and long spin coherence time. However, creating multiple highly entangled spins in such systems is a daunting yet essential task for building scalable and complex quantum networks."

The achievement is a result of close collaboration among synthetic chemists, materials scientists, and physicists, including key contributors Professor Pavel Jelinek and Dr. Libor Vei, from the Czech Academy of Sciences in Prague.

A next-generation magnetic nanographene with highly entangled spins

The magnetic properties of nanographene are usually derived from the arrangement of its special electrons, known as π-electrons, or the strength of their interactions. However, it is difficult to make these properties work together to create multiple correlated spins. Nanographene also predominately exhibits a singular magnetic order, where spins align either in the same direction (ferromagnetic) or in opposite directions (antiferromagnetic).

The researchers developed a method to overcome these challenges. Their butterfly-shaped nanographene, with both ferromagnetic and antiferromagnetic properties, is formed by combining four smaller triangles into a rhombus at the center. The nanographene measures approximately 3 nanometers in size.

To produce the "butterfly" nanographene, the researchers initially designed a special molecule precursor via conventional in-solution chemistry. This precursor was then used for the subsequent on-surface synthesis, a new type of solid-phase chemical reaction performed in a vacuum environment. This approach allowed the researchers to precisely control the shape and structure of the nanographene at the atomic level.

An intriguing aspect of the "butterfly" nanographene its four unpaired π-electrons, with spins mainly delocalized in the "wing" regions and entangled together. Using an ultra-cold scanning probe microscope with a nickelocene tip as an atomic-scale spin sensor, the researchers measured the magnetism of the butterfly nanographenes. Additionally, this new technique helps scientists direct probe entangled spins to understand how nanographene's magnetism works at the atomic scale.

The breakthrough not only tackles existing challenges but opens up new possibilities for precisely controlling the magnetic properties at the smallest scale, leading to exciting advancements in quantum materials research.

"The insights gained from this study pave the way for creating new-generation organic quantum materials with designer quantum spin architectures. Looking ahead, our goal is to measure the spin dynamics and coherence time at the single-molecule level and manipulate these entangled spins coherently. This represents a significant stride towards achieving more powerful information processing and storage capabilities," said Assoc Prof Lu.

More information: Shaotang Song et al, Highly entangled polyradical nanographene with coexisting strong correlation and topological frustration, *Nature Chemistry* (2024). DOI: 10.1038/s41557-024-01453-9

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